
Gravitational waves from dark sector
phase transitions

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**“If we knew what it was we were
doing, it would not be called
research, would it?”**

– Albert Einstein

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List of publications

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2. T. Bringmann, T. Konstandin, J. Matuszak, K. Schmidt-Hoberg and C. Tasillo, *Tuning the violins: dark sector phase transition models for the PTA signal* [[2602.09092](#)]
3. J. Matuszak, C. Tasillo, *TransitionListener v2.0 – Robust Gravitational Wave Predictions for Cosmological Phase Transitions*, [[2605.15259](#)],

The work on the following publication started before the doctorate and will therefore not be discussed in detail:

- T. Bringmann, T. E. Gonzalo, F. Kahlhoefer, J. Matuszak, and C. Tasillo, *Hunting WIMPs with LISA: correlating dark matter and gravitational wave signals* *JCAP* **05** (2024) 065, [[2311.06346](#)].

Abstract

The observation of gravitational waves (GWs) promises a new avenue to study fundamental physics through processes that occurred in the early universe shortly after inflation. Such observations might provide insights into open questions in our description of the universe, including the nature of dark matter. In this thesis, we study the phenomenon of cosmological first-order phase transitions in dark sectors in light of the observation of a stochastic gravitational wave signal at nanohertz frequencies by the pulsar timing array (PTA) collaborations.

First, we present the numerical code **TransitionListener**, which allows the computation of first-order phase transitions and the resulting gravitational wave spectra for general models that exhibit spontaneous symmetry breaking. It implements the necessary computational steps from the construction of the effective potential to the evaluation of the GW signals and their detectability with current and future experiments.

Using this tool, we study the generic requirements for first-order phase transitions in dark sectors to explain the observed PTA signal. We investigate three representative model classes: an Abelian dark Higgs model, a two-step phase transition with two scalar singlets and a loop-induced symmetry breaking of a near conformal scalar field. We investigate their general prediction and discuss the tuning of model parameters needed to achieve a strong enough phase transition to explain the PTA data. While all considered models can describe the PTA signal, we find that only the conformal model can do so generically without significant tuning of the model parameters.

Finally, we explore whether such a dark sector phase transition can simultaneously generate the mass of a dark matter candidate. We extend the near conformal model, consisting of a dark Higgs and dark photon, by including a stable fermion as a dark matter candidate. Since the PTA data requires a phase transition at MeV temperatures, the spontaneous symmetry breaking gives rise to sub-GeV masses. The dark sector couples to the Standard Model (SM) through kinetic mixing of the dark and SM photon, enabling the dark matter candidate to obtain its relic abundance via thermal freeze-out, which proceeds through annihilations into dark Higgs bosons and electrons. This scenario is subject to strong constraints from dark photon searches at collider experiments and cosmological bounds on the decays of the dark Higgs bosons. We perform global fits and identify viable parameter space, where the model can explain the PTA signal, produce the observed DM relic abundance and satisfies all relevant cosmological, astrophysical and laboratory constraints.

Zusammenfassung

Die Beobachtung von Gravitationswellen (GWs) eröffnet einen neuen Zugang zur Untersuchung fundamentaler Physik durch Prozesse, die im frühen Universum kurz nach der Inflation stattgefunden haben könnten. Solche Beobachtungen können Einblicke in offene Fragen unseres Verständnisses des Universums liefern, darunter die Eigenschaften der Dunklen Materie. In dieser Dissertation untersuchen wir das Phänomen kosmologischer Phasenübergänge erster Ordnung in dunklen Sektoren im Kontext der Beobachtung eines stochastischen Gravitationswellensignals bei nanohertz Frequenzen durch Pulsar Timing Array (PTA) Kollaborationen.

Zunächst stellen wir den numerischen Code **TransitionListener** vor, der die Berechnung von Phasenübergängen erster Ordnung, sowie der daraus resultierenden Gravitationswellenspektren für allgemeine Modelle mit spontaner Symmetriebrechung ermöglicht. Er implementiert die notwendigen Rechenschritte von der Konstruktion des effektiven Potentials bis

zur Bestimmung der resultierenden Gravitationswellensignale und deren Nachweisbarkeit mit aktuellen und zukünftigen Experimenten.

Mithilfe dieses Werkzeugs untersuchen wir die allgemeinen Anforderungen an Phasenübergänge erster Ordnung in dunklen Sektoren, um das beobachtete PTA Signal zu erklären. Dazu untersuchen wir drei repräsentative Modellklassen: ein abelsches Dunkles Higgs Modell, einen zweistufigen Phasenübergang mit zwei skalaren Singulets sowie eine schleifeninduzierte Symmetriebrechung eines nahezu konformen skalaren Feldes. Wir analysieren deren Vorhersagen und untersuchen die Feinabstimmung der Modellparameter, die erforderlich ist, um einen ausreichend starken Phasenübergang zur Erklärung der PTA Daten zu erhalten. Obwohl alle betrachteten Modelle das PTA Signal beschreiben können, zeigen wir, dass nur das konforme Modell dies auf generische Weise ohne signifikante Feinabstimmung der Modellparameter ermöglicht.

Abschließend untersuchen wir, ob ein solcher Phasenübergang im dunklen Sektor gleichzeitig die Masse eines Dunkle Materie Kandidaten erzeugen kann. Wir erweitern das nahezu konforme Modell, bestehend aus einem Dunklen Higgs und einem Dunklen Photon, um ein stabiles Fermion als Dunkle Materie Kandidaten. Da die PTA Daten auf einen Phasenübergang bei MeV Temperaturen hindeuten, entstehen durch die spontane Symmetriebrechung Massen im Sub-GeV Bereich. Der dunkle Sektor koppelt über kinetische Mischung zwischen dem dunklen und dem Standardmodell (SM) Photon an das Standardmodell. Dadurch erhält der Dunkle Materie Kandidat seine Reliktdichte über thermisches Ausfrieren, das durch Annihilationen in Dunkle Higgs Bosonen und Elektronen erfolgt. Dieses Szenario unterliegt starken Einschränkungen durch Suchen nach Dunklen Photonen an Kollidern sowie durch kosmologische Grenzen für die Zerfälle der Dunklen Higgs Bosonen. Wir führen globale Fits durch und identifizieren einen zulässigen Parameterbereich, in dem das Modell gleichzeitig das PTA Signal erklären, die beobachtete Reliktdichte der Dunklen Materie erzeugen und alle relevanten kosmologischen, astrophysikalischen und experimentellen Einschränkungen erfüllen kann.

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List of Abbreviations

BBN	big-bang nucleosynthesis
BHB	black hole binaries
CMB	cosmic microwave background
DM	dark matter
DS	dark sector
EM	energy-momentum
ET	Einstein Telescope
EW	electroweak
FLRW	Friedmann-Lemaître-Robertson-Walker
FOPT	first-order phase transition
GW	gravitational wave
IPTA	International Pulsar Timing Array
LIGO	Laser Interferometer Gravitational-Wave Observatory
LISA	Laser Interferometer Space Antenna
LTE	local thermal equilibrium
MHD	magnetohydrodynamic
NLO	next-to-leading-order
PLI	power-law-integrated
PTA	pulsar timing array
QCD	quantum chromodynamics
QFT	quantum field theory
SM	Standard Model
SNR	signal-to-noise ratio
SSB	spontaneous symmetry breaking

TOA time-of-arrival

VEV vacuum expectation value

CHAPTER 1

Introduction

More than a century ago, in 1916, Albert Einstein predicted the existence of gravitational waves [1]: tiny ripples in the fabric of space time. While, at the time, it was believed that these could never be detected, about a hundred years later the Laser Interferometer Gravitational-Wave Observatory (LIGO) observed the gravitational wave signal of merging black holes [2]. Since then, not only individual astrophysical events have been detected through their gravitational wave (GW) signal, but also evidence for a stochastic GW background has been found by the pulsar timing array (PTA) collaborations [3–5]. This background humming, consisting of a huge multitude of GW signals reaching us from every region in the sky, could originate not only from astrophysics but also include a component from the earliest times of the universe. Together with the planned next generation of GW observatories, such as the Laser Interferometer Space Antenna (LISA) [6] or Einstein Telescope (ET) [7], this marks the beginning of an era of GW cosmology.

The observation of our early cosmos relies on the electromagnetic radiation – photons with different frequencies – that travels to our eyes and telescopes. However, large parts of the early universe’s thermal history remain hidden from direct observation. Up until roughly 380,000 years after the end of inflation, the primordial plasma that filled the universe was opaque to electromagnetic radiation. Only when the electrons and nuclei of the plasma formed neutral elements, did the plasma become transparent and the photons could travel unperturbed, which we see today as the cosmic microwave background (CMB) [8]. In contrast, GWs travelled freely through the dense plasma and therefore provide a unique way to probe the earliest moments of the universe. At the extreme temperatures and energies of these earliest times, processes of elementary particle physics could have released enough energy to generate a GW signal that would reach us today. There exist a number of possible mechanisms that could create such a GW signal in the primordial universe. These include GWs from quantum fluctuations that are amplified by inflation [9, 10], topological defects, such as cosmic strings [11, 12] or domain walls [13, 14], as well as cosmological phase transitions [15, 16].

Here, we focus on cosmological phase transitions. The Standard Model (SM) predicts two such transitions, the electroweak symmetry breaking through the Higgs mechanism, and the quantum chromodynamics (QCD) phase transition, where the quarks confined into baryons and mesons [17–20]. With the known content of the SM, these two proceed as smooth

crossover transitions, where no observable GWs are produced [21, 22]. However, the SM falls short of describing the full universe we observe today. Fundamental questions that remain unanswered are, for example, the origin of the asymmetry of matter over anti-matter [23], the nature of dark matter [24, 25] and the hierarchy problem [26, 27]. Often, the proposed solutions to these open questions, such as additional scalar fields [28], new gauge groups [29], grand unified theories [30] or hidden sectors [31] rely on extending the known content of the SM. These extensions often come with a richer vacuum structure, where transitions in the early universe from one vacuum to another can be first-order. These disruptive events can release significant amounts of energy and proceed through the nucleation and expansion of bubbles, which eventually collide and radiate parts of the released energy as GWs.

These first-order transitions are intriguing in several aspects. In the case of a modified electroweak phase transition, they can provide the departure from thermal equilibrium required to create the matter-antimatter asymmetry in the universe [32–35]. In the case of dark matter, they can offer a mechanism to produce the observed relic abundance [36–39], while simultaneously sourcing a stochastic signal that could be detected today. In this work, we will study the possibility of a dark sector phase transition in the light of the GW background recently observed by the PTA collaborations. In the observed range of nanohertz frequencies, a signal of astrophysical origin is expected. A plausible candidate is given by supermassive black hole binaries (BHBs) which form after galaxies merge. In the final phase of their inspiralling, the supermassive BHBs radiate a strong GW signal that falls into the frequency range of 1-100 nanohertz [40, 41]. However, the recent findings of the NANOGrav collaboration [42] and simulations of supermassive BHBs [43] indicate tensions of the expected signal with the large amplitude and spectral shape found in the data. Additionally, the mechanism that dissipates sufficient energy to bring the supermassive BHBs close enough together to drive their merging through GW emission is not fully understood yet [44, 45]. This leaves the exciting possibility that (part of) the PTA signal is of cosmological origin.

While it is already widely recognised that first-order phase transitions in dark sectors can fit the PTA data [46–51], it is often not clear how realistic or “natural” the underlying models are. We therefore study the question of what the general requirements on the microscopic particle physics models are, and how generic the prediction of a strong first-order phase transition, that can explain the PTA data is. In our analysis, we study three different representative model classes that realise a first-order phase transition in different ways. We will find that, only in a model with an additional, classically conformal symmetry, the prediction of a strong enough phase transition to fit the PTA data is generic. The other mechanisms, a two-step phase transition and a simple thermally induced potential barrier, require significant tuning of the underlying model parameters and typically predict too weak phase transitions to fit the PTA data.

To match the nanohertz frequencies of the PTA data, we will see that a dark sector phase transition has to occur around temperatures of $\mathcal{O}(10\text{ MeV})$, which is connected to a sub-GeV mass scale of the dark sector particles. The next question we study is therefore the possibility that a first-order phase transition can not only explain GW signal at the nanohertz frequencies, but also at the same time gives mass to a sub-GeV dark matter candidate that can reproduce the observed relic density of dark matter today. Here, we will consider a model with a classical conformal symmetry that consists of a dark Higgs, a dark photon and a fermionic dark matter candidate, charged under a $U(1)'$ gauge symmetry. We will study the phenomenology of this model in detail and consider the current constraints on sub-GeV dark sectors from cosmology and astrophysics, as well as from laboratory experiments. By performing a global fit using the tool **GAMBIT** [52], we will find viable parameter space for this rather minimal model where all constraints can be satisfied.

This thesis is structured as follows. In part I, we lay the groundwork to understand the GW signal of cosmological phase transitions. We start to review the Standard Model of cosmology and the necessity and evidence for dark matter in chapter 2. Additionally, we introduce the formalism necessary to understand the production and propagation of a stochastic GW background through an expanding universe. Lastly, we describe the recent measurement of a GW background by the PTA collaborations. In chapter 3, we introduce the formalism of finite-temperature field theory that we need to understand the thermodynamics of spontaneous symmetry breaking. Furthermore, we review the dynamics of first-order phase transitions and the hydrodynamics of expanding bubbles in the primordial plasma that lead to the radiation of GWs. Then, we discuss the resulting GW spectrum.

In part II we present the studies performed in this work. Chapter 4 discusses the tool `TransitionListener`, which we developed to perform the numerical steps of the computation of first-order phase transitions and the evaluation of the GW signals from the underlying particle physics model. Using this tool, we study the general requirements on dark sector phase transitions to fit the PTA data by analysing three dark sector models in chapter 5. These represent different ways in which the spontaneous symmetry breaking of scalar fields can lead to a first-order phase transition. Next, we connect phase transitions to the open question of the nature of dark matter. In chapter 6, we explore the possibility that a nearly conformal dark sector could produce both dark matter and simultaneously explain the PTA data. Finally, we conclude with a summary of this thesis in chapter 7.

Part I.

Background

Cosmology, dark matter and gravitational waves

In this chapter, we will review the relevant background on cosmology, the puzzle of dark matter, and gravitational waves. We start by reviewing the ingredients of our universe described by the cosmological standard model Λ CDM in sec. 2.1. Then we turn to the necessity and evidence of dark matter in sec. 2.2 and the description of particles in the expanding universe (sec. 2.3). Finally, we turn to GWs and their production in sec. 2.4 and the recent measurement of a stochastic GW background with pulsar timing arrays in sec. 2.5.

2.1. The expanding universe

In 1915, Albert Einstein published his groundbreaking theory of general relativity [53]. This classical field theory describes the interplay between curvature of space and the distribution of matter and can be summarised in the Einstein equations

$$G_{\mu\nu} + g_{\mu\nu}\Lambda = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + g_{\mu\nu}\Lambda = 8\pi GT_{\mu\nu}. \quad (2.1)$$

The left hand side describes the geometry of spacetime through the Einstein tensor $G_{\mu\nu}$, while the right hand side relates this geometry to the distribution of energy and matter through the energy-momentum tensor $T_{\mu\nu}$. These equations come with a vast array of implications and predictions that have been tested in the past 100 years with great success. They describe the dynamics of our universe from the perihelion shift of Mercury on its motion around the Sun, to the geometry of black holes, gravitational lensing, and the expansion of the universe from inflation up to today.

The Einstein tensor on the left hand side is composed of the Ricci tensor $R_{\mu\nu} \equiv R^\alpha_{\mu\alpha\nu}$ and the Ricci scalar $R \equiv R^\mu_{\mu}$, which are calculated from contractions of the Riemann curvature tensor

$$R^\mu_{\nu\alpha\beta} = \Gamma^\mu_{\nu\alpha,\beta} - \Gamma^\mu_{\nu\beta,\alpha} + \Gamma^\mu_{\alpha\rho}\Gamma^\rho_{\nu\beta} - \Gamma^\mu_{\beta\rho}\Gamma^\rho_{\nu\alpha}, \quad (2.2)$$

where we used the notation $A_{\nu,\mu} \equiv \partial_\mu A_\nu$. This object contains the information about the curvature of a manifold, or more illustratively, describes the change of a vector after parallel transporting it around the manifold. The Riemann tensor itself is computed from the Christoffel symbols

$$\Gamma^\mu_{\alpha\beta} = \frac{1}{2}g^{\mu\nu} (g_{\nu\alpha,\beta} + g_{\nu\beta,\alpha} - g_{\alpha\beta,\nu}), \quad (2.3)$$

which are derived from the measure of distance, the metric $g_{\mu\nu}$. The interplay between the geometry and the energy and matter distribution was summarised perfectly by Wheeler [54]: “*Space-time tells matter how to move; matter tells space-time how to curve.*”. As we will see, on very large scales, these equations describe a universe that is either in a state of expansion or collapsing. This lead Einstein to introduce a term containing the cosmological constant Λ to find a solution describing a static and non-changing universe, as it was believed to be. After debates and revoking this term again, observations have shown that the universe is indeed in a state of accelerated expansion. This acceleration is due to exactly this non-vanishing cosmological constant that can be interpreted as a contribution to the energy density $T_{\mu\nu}^\Lambda = g_{\mu\nu}\Lambda/(8\pi G)$ that does not dilute in an expanding space.

In total, the Einstein field equations form a system of 16 coupled differential equations, which are reduced to ten by the symmetry $g_{\mu\nu} = g_{\nu\mu}$, and further to 6 through the Bianchi identities $G^{\mu\nu}_{;\mu} = 0$. Here we use the notation $G^{\mu\nu}_{;\mu} \equiv \nabla_\mu G^{\mu\nu}$ for the covariant derivative. In general, they are very difficult to solve, but in the cosmological case, more simplifications can be made. On large scales, observations have shown that the universe is very well approximated as homogeneous and isotropic, which is called the *cosmological principle*. The most general solution to the Einstein equations for such a system is the metric that gives the infinitesimal distance [55, 56]

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = dt^2 - a^2(t) \left(\frac{1}{1-kr^2} dr^2 + r^2 (d\theta^2 + \sin^2\theta d\phi^2) \right). \quad (2.4)$$

The assumption of homogeneity rules out prefactors with a spatial dependence, while non-diagonal terms disappear due to isotropy. Still allowed is a global curvature, which can describe a closed universe $k > 0$ (sphere), an open universe $k < 0$ (hyperboloid) or a flat universe $k = 0$. This is known as the Friedmann-Lemaître-Robertson-Walker (FLRW) metric. On large scales, we can model the content of our universe as a perfect fluid, which in the homogeneous and isotropic case has the energy-momentum tensor in the cosmic rest frame

$$T^\mu_\nu = \text{diag}(\rho, -P, -P, -P). \quad (2.5)$$

Here ρ is the energy density and P the pressure of the fluid. Under these assumptions we only obtain two non-trivial components of the Einstein tensor

$$G_{00} = 3\frac{\dot{a}^2 + k}{a^2}, \quad G_{ij} = \left(2\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2} + \frac{k}{a^2} \right) \delta_{ij}, \quad (2.6)$$

and therefore two independent equations, which can be written as

$$H^2 \equiv \left(\frac{\dot{a}}{a} \right)^2 = \frac{8\pi G}{3} \rho - \frac{k}{a^2}, \quad (2.7)$$

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3P). \quad (2.8)$$

The first *Friedmann equation* describes how the energy density ρ in the universe leads to an expansion, the rate of which is captured by the Hubble parameter H , while the second Friedmann equation describes the change in this expansion. In order to see how in turn the energy density changes with this expansion, we can use the first Bianchi identity $G^\mu_{0;\mu} = 0$ to obtain [55, 56]

$$\dot{\rho} = -3\frac{\dot{a}}{a}(\rho + P). \quad (2.9)$$

Using the equations of state, that relate pressure and energy density for relativistic particles, non-relativistic particles and the cosmological constant, we can derive the expansion properties of the universe:

Relativistic matter

In the case of pure radiation, the pressure is given by the equation of state $P = \rho/3$, as we will see in sec. 2.3. Using the conservation equation (2.9), we obtain the following scaling of the energy density:

$$\dot{\rho} = -4\frac{\dot{a}}{a}\rho \quad \Rightarrow \quad \rho \propto a^{-4}. \quad (2.10)$$

By inserting this into the Friedmann eq. (2.7), we obtain the time-dependence of the scale factor for radiation domination

$$\frac{\dot{a}^2}{a^2} \propto a^{-4} \quad \Rightarrow \quad a(t) \propto t^{1/2}. \quad (2.11)$$

Hence, for an energy density dominated by radiation, the universe will be in a state of accelerated expansion.

Non-relativistic matter

In the case of purely non-relativistic matter, the pressure is negligible compared to the energy density ($P \simeq 0$), as we will see in sec. 2.3. Here, we obtain

$$\dot{\rho} = -3\frac{\dot{a}}{a}\rho \quad \Rightarrow \quad \rho \propto a^{-3}. \quad (2.12)$$

Therefore, a matter dominated universe will also be in a state of expansion, but this expansion decelerates less than in the case of radiation:

$$\frac{\dot{a}^2}{a^2} \propto a^{-3} \quad \Rightarrow \quad a(t) \propto t^{2/3}. \quad (2.13)$$

Curvature

In case the curvature term dominates and is negative $k < 0$, the expansion of the universe becomes linear

$$\frac{\dot{a}^2}{a^2} \propto a^{-2} \quad \Rightarrow \quad a(t) \propto t. \quad (2.14)$$

If the curvature term is instead positive $k > 0$, the right hand side of eq. (2.7) will become negative as the energy density dilutes, and the universe recollapses, unless a non-vanishing cosmological constant is present.

Cosmological constant

Since the energy density of the cosmological constant Λ does not dilute

$$\dot{\rho} = 0 \quad \Rightarrow \quad \rho = \text{const}, \quad (2.15)$$

it leads to an exponentially accelerated expansion:

$$\frac{\dot{a}^2}{a^2} \propto \text{const.} \quad \Rightarrow \quad a(t) \propto e^{Ht}. \quad (2.16)$$

2.1.1. The Standard Model of cosmology: Λ CDM

We now have the ingredients to sketch a picture of the expansion history of the universe using the results of the Planck collaboration, which has measured the energy composition of the universe by observing the cosmic microwave background (CMB) [8]. These observations have revealed that our universe is mostly composed of ingredients that we do not understand yet. As common in the literature, we express them here in terms of the fraction of the

total energy density today $\Omega_i = \rho_i/\rho_{c,0}$. The energy in radiation from photons contributes a tiny fraction to the energy density today $\Omega_\gamma \simeq 2.47 \cdot 10^{-5}$. A bigger portion is made out of energy density that behaves as non-relativistic matter $\Omega_m \simeq 0.31$. However, only a fifth of this consists of the ordinary matter described by the SM of particle physics in form of baryonic matter $\Omega_b \simeq 0.05$. The far bigger part is found to be made up of non-interacting matter that is invisible to us and hence called dark matter (DM) $\Omega_{DM} \simeq 0.26$. The biggest portion comes from the cosmological constant $\Omega_\Lambda \simeq 0.69$, also called dark energy, which no microphysical model can convincingly explain yet. Additionally, the measurements of the curvature $\Omega_k \simeq 0.001 \pm 0.002$ have shown that our universe is flat.

Using the scaling relations of the different energy components and the measured values today, we can trace back the composition of the energy density at earlier times. This is depicted in fig. 2.1 in terms of the scale factor a , where its value today is conventionally set to $a_0 = 1$. In the earliest times, the universe was in a state of radiation domination, but since the energy density of radiation dilutes quicker than that of non-relativistic particles, at some point the matter content started to dominate the energy density. After this period of matter domination, the universe entered into a state of accelerated expansion, driven by the non-diluting energy density from the cosmological constant. The earliest times that we can probe directly come from observations of the last scattering surface of photons, when electrons and nuclei formed neutral elements. This is known as the CMB. Still there are a number of events that must have taken place in the very early universe before these times.

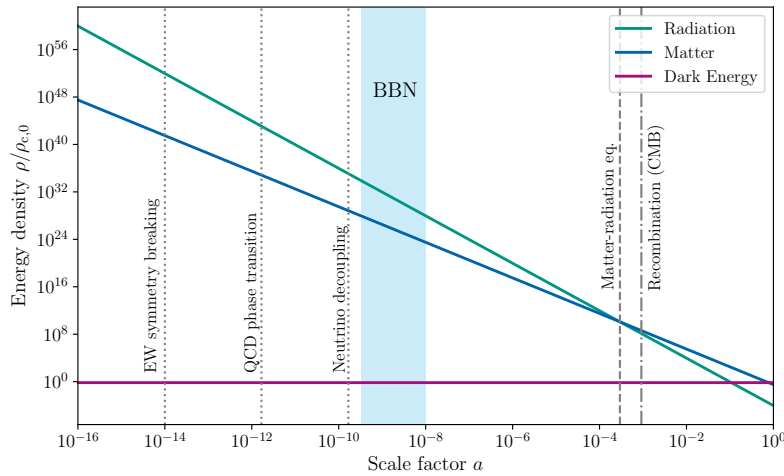


Figure 2.1.: Evolution of the different contributions to the energy density of the universe in terms of the scale factor a . Observations by the Planck collaboration indicate a stage of radiation domination (green line) at early times, followed by matter domination (blue line) and finally a stage of accelerated expansion due to positive cosmological constant (purple line).

The puzzle of a vanishing curvature can be solved by assuming that in the earliest times the universe was dominated by a vacuum energy density that led to an accelerated expansion known as inflation. This flattens out any existing curvature and also amplifies quantum fluctuations to macroscopic density fluctuations that are needed as the initial seeds for the structure formation in the late universe. Inflation is assumed to be sourced by the potential energy of a scalar field that subsequently decays into SM particles (and DM), which form a thermal bath and an era of radiation domination begins, where all the known elementary particles are unconfined. As the universe expanded and the temperature decreased below the electroweak and then the QCD scale, the electroweak phase transition gave mass to the

quarks and leptons and the QCD phase transition led the free quarks to confine into baryons and mesons. At temperatures around the MeV scale, the interactions between the neutrinos and the SM particles became inefficient and they decoupled from the thermal bath. When the temperature dropped below the electron mass, pairs of electrons and positrons annihilated into photons, after which protons and neutrons began to form the nuclei of the lightest elements. This process is known as big-bang nucleosynthesis (BBN). The measurement of the relative abundances of the helium isotopes is one of the probes that lets us draw conclusions about the earliest measurable times. Finally, due to the faster dilution of radiation than non-relativistic matter, around $T = 750 \text{ meV}$ the universe reached matter-radiation equality. At 250 meV electrons and protons combined into neutral elements and photons no longer constantly scattered off charged particles. They decoupled and now almost freely propagate to us today, giving us the picture of the CMB, observable with radio telescopes. Today, the energy density is dominated by a cosmological constant that gives us again an accelerated expansion.

2.2. Dark Matter

In the previous section, we saw that the standard model of cosmology describes a universe with a matter content that is mostly unknown to us. It requires the existence of particles that are invisible to us but provide gravitational interaction to explain our observations. In this section, we will discuss the necessity and evidence for dark matter in more detail. Extensive reviews can be found in refs. [57, 58].

2.2.1. Evidence for dark matter

The hints towards the existence of matter beyond what we can observe using light date back more than a century. In the 19th century, Kelvin estimated the necessary mass of our galaxy to produce the observed velocity dispersion of stars orbiting around the galactic centre. He found his estimate to be larger than the mass observed in the visible stars, which led him to the conclusion that most of the mass in the galaxy must come from “dark bodies”. The Swiss astronomer Fritz Zwicky arrived at the same conclusion in 1933, when he studied the motion of galaxy clusters by observing their Doppler-shifted light [24]. Also here, the visible mass in stars and gas was not enough to account for the gravitational attraction inferred from the movement of the galaxies. In the 1970s, the astronomer Vera Rubin analysed the rotation of spiral galaxies using an new type of spectograph that allowed to measure the velocity curves of individual galaxies [25]. These observed rotation curves again did not match the predictions if one only accounts for all the visible matter. The stars and matter in galaxy arms rotate too fast to be trapped by only the gravitational attraction of the visible matter according to our current understanding of gravity.

This leaves two possible conclusions: either the laws of gravity that perfectly describe the observations on the scale of the Solar System do not describe the dynamics on the large scales of galaxies and galaxy clusters, or there exists a form of matter that does not (or only very weakly) interact with the SM particles. The first possibility led to the development of theories of modified Newtonian dynamics (MOND) that change the gravitational laws on large scales, but even though they manage to explain individual observations, they yet fail to coherently describe the universe on all scales. Introducing new particles that predominantly interact gravitationally, however can describe the observations of the universe accurately on various scales.

More evidence towards the particle nature of DM is, for example, found in the gravitational lensing effects around two colliding galaxy clusters, with the most well-known example being

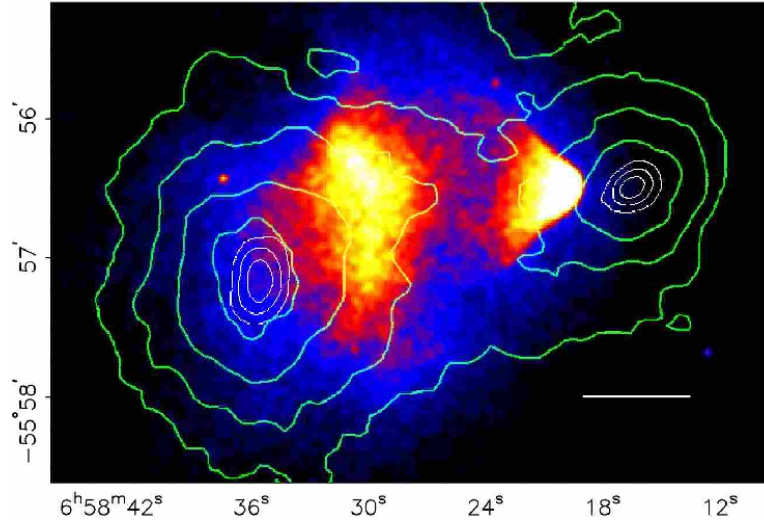


Figure 2.2.: Image of the Bullet Cluster showing two colliding galaxy clusters. The X-ray spectrum of the gas in the galaxies is shown by the coloured regions, while the mass distribution inferred from gravitational lensing is shown by the green contours. Image taken from [59].

the Bullet Cluster, shown in fig. 2.2. The observed SM matter lags behind the mass distribution reconstructed from the gravitational lensing around the cluster [59]. This can be explained if the majority of mass in the clusters is made up of non-interacting (dark) particles that pass almost freely through each other, while the visible SM particle in the interacting gases got slowed down during the collision. Additional strong hints come from the earliest observations of the earliest times of the universe, the CMB. The observed statistical properties of the temperature fluctuations of the CMB require the presence of non-interacting (dark) matter, which influenced the velocity and density of the SM matter. Due to the collision-less nature of the DM, it lacks the pressure that counteracts the formation of overdensities from primordial fluctuations and created gravitational wells. The pressure of the photon-electron fluid, however, counteracted the gravitational attraction and formed oscillations around regions of dark matter overdensities. The typical length scales of these oscillations are still visible in the spectrum of the temperature anisotropies of the CMB. Furthermore, these overdensities also acted as seeds for the structure formation in our universe, which we can observe today in the large-scale distribution of galaxies.

2.2.2. Dark matter detection

If dark matter is indeed of elementary particle nature, it must surround us in our galaxy and constantly pass through us. If we suppose that the DM mass were to be around $m_{\text{DM}} = 1 \text{ GeV}$, the estimates of the local DM density of $\rho_{\text{DM}} \approx 0.3 \text{ GeV cm}^{-3}$ and the local DM velocity $v_{\text{DM}} \approx 220 \text{ km s}^{-1}$ [60] suggest that around one million DM particles would pass through every cubic centimetre per second on Earth.

This motivates the direct detection approach to search for DM. Even if DM only interacts very weakly with the SM, eventually a DM particle will scatter off SM matter. Observing large quantities of SM matter yields the possibility that such a scattering event deposits recoil energy that can be measured. Since the DM particles can at most only very weakly interact with the SM particles, one has to observe very large quantities of SM matter to increase the number of observable interactions. This is done for example in the XENONnT experi-

ment [61], that consists of currently 5.9 tons of liquid xenon surrounded by photomultipliers in the expectation to measure the scintillation light from such interactions.

Another approach to search for DM is to observe regions of strong gravitation, such as stars or galactic centres. In these regions, we can expect an increased DM density, that could lead to DM annihilations into SM particles and anti-particles. Since particles are abundant in our region of the universe, while anti-particles are rare, the detection of an excess of anti-particles propagating from those regions of strong gravitational attraction could point towards DM. An example of such an experiment is hosted on the international space station (ISS). The Alpha Magnetic Spectrometer (AMS-02) is used to search for an excess in anti-protons and anti-helium that could originate from DM annihilations [62].

Existing collider experiments that probe the properties of SM through high-energy collisions can also be used to search for DM. In rare events, DM could be produced alongside the SM particles. If these DM particles are short-lived, they could decay back into SM particles within the detector. In the reconstruction of the particle tracks, this would show up as a displaced vertex from the collision point. Long-lived DM particles would instead decay outside the detector. In this case, the total energy measured by the detector does not match the collision energy, since the DM particles do not leave any trace in the detector [63]. An example for such a missing-energy experiment is the NA64 experiment [64]. Here, a high-intensity beam of electrons with energies of about 100 GeV is directed at a fixed target. A DM particle produced in the collisions of the electrons with the target nuclei would escape the experiment without interacting and show up in missing energy in the detector.

So far, these detection experiments have not yet succeeded in their efforts to find particle DM. These null-results encourage to think of different ways to shed light on its nature. One such possibility opens up if we consider the early universe, where the dark matter could have left unique imprints that give hints towards its characteristics. For this, we will first need to study the dynamics of particles in a thermal path in the next section.

2.3. Particles in an expanding universe

The early universe comprised a dense and hot thermal bath of a mix of relativistic and non-relativistic particles. The adequate tool to describe particles in such environments is the formalism of statistical mechanics and the Boltzmann equation. In this section, we review this topic by following along refs. [65–67]

For very large numbers of particles, we can best describe their behaviour through a distribution in phase-space instead of tracking the individual particles in space: the phase-space distribution $f_a(t, \mathbf{x}, \mathbf{p})$ of a particle species a describes what fraction of particles at time t and point $\mathbf{x}$ have the momentum $\mathbf{p}$. The evolution of the phase-space distribution in time and space is governed by the relativistic Boltzmann equation [68]:

$$\hat{\mathcal{L}}[f_a(t, \mathbf{x}, \mathbf{p})] = \left(p^\mu \frac{\partial}{\partial x^\mu} - \Gamma^i_{\mu\nu} p^\mu p^\nu \frac{\partial}{\partial p^i} \right) f_a(t, \mathbf{x}, \mathbf{p}) = \hat{\mathcal{C}}[f_a(t, \mathbf{x}, \mathbf{p}), \dots]. \quad (2.17)$$

On the left-hand side, the Liouville operator $\hat{\mathcal{L}}$ accounts for the effects of gravity, whereas the collision operator $\hat{\mathcal{C}}$ on the right-hand side describes the interaction of the particle species a with itself and other particles species indicated by [...]. As we will see below, the collision operator renders this an integro-differential equation, which is, in general, highly non-linear and complicated to solve. In the case of an isotropic and homogeneous universe, we can make some simplifications: homogeneity implies that the phase-space distribution cannot depend on the position $\mathbf{x}$, while isotropy implies that there is no dependence on the momentum $\mathbf{p}$

direction, but only on the modulus p or equivalently on the energy E_a . Using the Christoffel symbols obtained from the FLRW metric, the left-hand side of eq. (2.17) simplifies to

$$\hat{\mathcal{L}}[f_a(t, p)] = \left(E_a(p) \frac{\partial}{\partial t} - H(t) E_a(p) p \frac{\partial}{\partial p} \right) f_a(t, p) = \hat{\mathcal{C}}[f_a(t, p), \dots]. \quad (2.18)$$

Instead of describing the particles on the phase-space level, it is often simpler to track the number density of particles. It is obtained by integrating the phase-space distribution over the momenta and multiplying by the degrees of freedom g_a of the particle species

$$n_a(t) = \int \frac{d^3 p}{(2\pi)^3} g_a f_a(t, p). \quad (2.19)$$

We can obtain the evolution of the number density by dividing eq. (2.18) by the energy and integrating the momenta

$$\dot{n}_a(t) + 3Hn_a(t) = \int d^3 p \frac{g_a}{(2\pi)^3} \frac{\hat{\mathcal{C}}[f_a(t, p), \dots]}{E_a(p)}. \quad (2.20)$$

We can interpret this equation as follows: the number density can change due to two mechanisms. On the left hand side, the Hubble rate H describes the dilution of the number density through the expansion of the universe and on the right hand side, the creation, annihilation, or decay of particles is described by the collision operator. This operator is defined as the sum over all the processes $r \in \mathcal{R}_r$ involving the particle a in the initial state and processes $\bar{r} \in \mathcal{R}_{\bar{r}}$ involving a in the final state:

$$\begin{aligned} \hat{\mathcal{C}}[f_a(p, t), \dots] = & \frac{1}{2g_a} \sum_{\bar{r} \in \mathcal{R}_{\bar{r}}} \int \prod_{i, f \neq a} \frac{d^3 p_{i/f}}{(2\pi)^3 2E_{i/f}} (1 \pm f_a)(1 \pm f_{\bar{f}}) f_i |M_{\bar{r}}|^2 (2\pi)^4 \delta(\Sigma p) \\ & - \frac{1}{2g_a} \sum_{r \in \mathcal{R}_r} \int \prod_{i, f \neq a} \frac{d^3 p_{i/f}}{(2\pi)^3 2E_{i/f}} (1 \pm f_{\bar{f}}) f_i f_a |M_r|^2 (2\pi)^4 \delta(\Sigma p). \end{aligned} \quad (2.21)$$

Here, the squared matrix element $|M_r|^2$ encodes the probability of a given process. For the interaction to take place, particles must be present in the initial states, for which the factors f_i give the probability. The Bose enhancement or Pauli exclusion in the final states is accounted for by the factors $(1 \pm f_{\bar{f}})$, where the sign is positive (negative) for bosonic (fermionic) particles. Lastly, the conservation of energy in a process is ensured by the delta distribution $\delta(\Sigma p) \equiv \delta^4(\sum_f p_f - \sum_i p_i)$.

In the case that interactions are very frequent, the particles will thermalise, i.e. the momentum distribution will eventually be described by a Bose-Einstein or Fermi-Dirac distribution with a common temperature $T(t)$ and read

$$f_a(t, p) = \frac{1}{\exp\left(\frac{E_a(p) - \mu_a(t)}{T(t)}\right) \mp 1}, \quad (2.22)$$

where the sign is positive for fermions and negative for bosons. In the following scenarios, the chemical potential $\mu_a(t)$ will not play a role, which is why we neglect it from here on.

If all particle species are in thermal equilibrium, the collision operator vanishes for a process r invariant under time reversal, i.e. $|M_r|^2 = |M_{\bar{r}}|^2$, with $\bar{r}$ denoting the inverse process. In this case, the collision operator is proportional to

$$\hat{\mathcal{C}}_r[f_a, \dots] \propto \left(\prod_{i, f} (1 \pm f_{\bar{f}}) f_i - \prod_{\bar{i}, \bar{f}} (1 \pm f_{\bar{f}}) f_{\bar{i}} \right) \delta(\Sigma p), \quad (2.23)$$

where the indices i, f stand for the final states of the interaction, while $\bar{i}, \bar{f}$ stand for the states of the reverse interaction. Using the expression for equilibrium phase-space distributions (2.22) with equal temperatures, it can be shown that this expression vanishes. This is known as the *principle of detailed balance*.

2.3.1. Non-relativistic collision operator for $2 \rightarrow 2$ processes

Often, the evolution of a particle species is dominated by $2 \rightarrow 2$ processes. Thus, we will take a closer look at the collision operator for this case here. For the general process $a + b \rightarrow c + d$ the collision operator is given by

$$\hat{C} = -\frac{1}{2g_a} \int \frac{d^3p_b}{(2\pi)^3 2E_b} \frac{d^3p_c}{(2\pi)^3 2E_c} \frac{d^3p_d}{(2\pi)^3 2E_d} |M|_{ab \rightarrow cd}^2 (2\pi)^4 \delta(\Sigma p) (1 \pm f_c)(1 \pm f_d) f_a f_b. \quad (2.24)$$

In the regime of non-relativistic particles, i.e. $T \ll m$, we can approximate the statistical factors $(1 \pm f) \simeq 1$ and introduce the cross section as

$$\sigma_{ab \rightarrow cd} = \frac{1}{(2E_a)(2E_b)|\mathbf{v}_a - \mathbf{v}_b|} \int \frac{d^3p_c}{(2\pi)^3 2E_c} \frac{d^3p_d}{(2\pi)^3 2E_d} |M|_{ab \rightarrow cd}^2 (2\pi)^4 \delta(\Sigma p). \quad (2.25)$$

This lets us express the collision operator in terms of $\sigma_{ab \rightarrow cd}$ and the number densities of the initial state particles

$$\begin{aligned} \int \frac{d^3p_a}{(2\pi)^3 2E_a} g_a \hat{C} &= -\frac{1}{2} \int \frac{d^3p_a}{(2\pi)^3} \frac{d^3p_b}{(2\pi)^3} f_a f_b |\mathbf{v}_a - \mathbf{v}_b| \sigma_{ab \rightarrow cd} \\ &= -\frac{1}{2} n_a(t) n_b(t) \langle \sigma_{ab \rightarrow cd} v \rangle. \end{aligned} \quad (2.26)$$

In the second line, we introduced the thermally averaged cross section

$$\langle \sigma v \rangle \equiv \frac{\int d^3p_a d^3p_b f_a(p_a, T) f_b(p_b, T) \sigma v_{\text{rel}}}{\int d^3p_a d^3p_b f_a(p_a, T) f_b(p_b, T)}, \quad (2.27)$$

where $v_{\text{rel}} = |\mathbf{v}_a - \mathbf{v}_b|$ is the relative velocity between the initial-state particles.

The evolution of the number density for a non-relativistic particle species a can then be expressed in terms of the thermally averaged cross sections for the annihilation and production processes

$$\dot{n}_a(t) + 3H(t)n_a = -\frac{1}{2} \sum_{i,j \in \mathcal{I}} n_i(t) n_j(t) \langle \sigma_{\text{ann},ij} v \rangle + \frac{1}{2} \sum_{l,k \in \mathcal{F}} n_l(t) n_k(t) \langle \sigma_{\text{prod},kl} v \rangle. \quad (2.28)$$

Here, the first sum runs over the initial states of the (annihilation) processes $\mathcal{I}$ that contain a in the initial state. The second sum runs over the (production) processes $\mathcal{F}$ that have a in a final state. Note that the factor $1/2$ is needed because we double-count processes that have a twice in the initial or final state, i.e the processes $a_1 + a_2 \rightarrow c + d$ and $a_2 + a_1 \rightarrow c + d$ are counted separately.

2.3.2. Thermodynamic quantities

Now that we have studied the evolution of the number density, we also briefly review the other thermodynamic quantities. The energy density ρ and pressure P of a particle species can be obtained by computing the following moments of the phase-space distribution

$$\rho_a(t) = \int \frac{d^3p}{(2\pi)^3} g_a E_a(p) f_a(p, t), \quad (2.29)$$

$$P_a(t) = \int \frac{d^3p}{(2\pi)^3} g_a \frac{p^2}{3E_a(p)} f_a(p, t). \quad (2.30)$$

A useful approximation for these quantities can be found in the relativistic regime, where $T \gg m$. Here they become

$$n_a(T) \simeq \frac{\zeta(3)}{\pi^2} g_a T^3 \quad (\times \frac{3}{4} \text{ for fermions}), \quad (2.31a)$$

$$\rho_a(T) \simeq \frac{\pi^2}{30} g_a T^4 \quad (\times \frac{7}{8} \text{ for fermions}), \quad (2.31b)$$

$$P_a(T) \simeq \frac{\rho_a(T)}{3}, \quad (2.31c)$$

where $\zeta(x)$ denotes the Riemann zeta function. Note that, due to their difference in the phase-space distribution, fermions receive additional factors in these expressions. In the opposite limit, the non-relativistic regime with $T \ll m$, we obtain instead

$$n_a(T) \simeq \left(\frac{m_a T}{2\pi} \right)^{3/2} n_a e^{-m_a/T}, \quad (2.32a)$$

$$\rho_a(T) \simeq \left(m_a + \frac{3T}{2} \right) n_a(T), \quad (2.32b)$$

$$P_a(T) \simeq T n_a(T). \quad (2.32c)$$

An additional expression for the entropy density of the thermal bath can be obtained using the first law of thermodynamics

$$s_a(T) = \frac{\rho_a(T) + P_a(T)}{T} \simeq \begin{cases} 2\pi^2 g_a T^3 / 45 & \text{relativistic } (T \gg m), \\ m_a n_a(T) / T & \text{non-relativistic } (T \ll m). \end{cases} \quad (2.33)$$

Using this expression for the entropy density and the conservation eq. (2.9), it follows that the entropy of a thermal bath is conserved in a co-moving volume

$$\sum_a s_a(T) a^3(T) = \text{const.}, \quad (2.34)$$

where the sum runs over the different particle species that are in thermal equilibrium. Note that the injection of energy from e.g. other species that are initially not in thermal contact leads to an increase of entropy. To see this, we can reformulate the Boltzmann equation (2.18) in terms of the entropy evolution

$$\dot{s}_a(t) + 3H(t)s_a(t) = - \int \frac{d^3p}{(2\pi)^3} g_a \frac{\hat{C}[f_a, \dots]}{E_a(p)} \ln \left(\frac{f_a}{1 \pm f_a} \right). \quad (2.35)$$

In the case of thermal equilibrium, the principle of detailed balance causes the collision operator to vanish, however, if a species is not in thermal equilibrium, it can inject heat into the thermal bath and cause an increase in the entropy.

2.3.3. Effective degrees of freedom

To describe a thermal bath composed of both relativistic and non-relativistic particles, it is convenient to count their respective contribution to the energy density using *effective degrees of freedom*. We can rewrite the energy density (2.29) for particles in thermal equilibrium as

$$\rho_a(T) = \int \frac{d^3p}{(2\pi)^3} g_a E_a(p) \left(e^{E_a(p)/T} \mp 1 \right)^{-1} \quad (2.36)$$

$$= \frac{\pi^2}{30} T^4 \underbrace{\left(g_a \frac{15}{\pi^4} \int_{m/T}^{\infty} du u^2 \frac{\sqrt{u^2 - m^2/T^2}}{e^u \mp 1} \right)}_{\equiv g_{\text{eff},a}} = \frac{\pi^2}{30} g_{\text{eff},a} T^4, \quad (2.37)$$

where we defined the effective energy degrees of freedom $g_{\text{eff},a}$, that take values between g_a (for $m_a/T \rightarrow 0$) and 0 (for $m_a/T \rightarrow \infty$). Similarly, the pressure and entropy can also be mapped to their relativistic expressions

$$P_a(T) = \frac{\pi}{90} k_{\text{eff},a} T^4, \quad (2.38)$$

$$s_a(T) = \frac{2\pi^2}{45} \left(\frac{3g_{\text{eff},a} + k_{\text{eff},a}}{4} \right) T^3 = \frac{2\pi^2}{45} h_{\text{eff},a} T^3. \quad (2.39)$$

Here, we defined the effective entropy degrees of freedom as $h_{\text{eff},a} = (3g_{\text{eff},a} + k_{\text{eff},a})/4$ and used the effective pressure degrees of freedom $k_{\text{eff},i}$ obtained from

$$k_{\text{eff},a} = g_a \frac{15}{\pi^4} \int_{m/T}^{\infty} du \frac{(u^2 - m^2/T^2)^{3/2}}{e^u \mp 1}. \quad (2.40)$$

The total energy density, pressure, and entropy density of a thermal bath that can include relativistic and non-relativistic particles are then simply given in terms of the total effective degrees of freedom

$$\rho_{\text{tot}}(T) = \frac{\pi^2}{30} g_{\text{eff}} T^4 \quad \text{with} \quad g_{\text{eff}} \equiv \sum_a g_{\text{eff},a}, \quad (2.41)$$

$$P_{\text{tot}}(T) = \frac{\pi^2}{90} k_{\text{eff}} T^4 \quad \text{with} \quad k_{\text{eff}} \equiv \sum_a k_{\text{eff},a}, \quad (2.42)$$

$$s_{\text{tot}}(T) = \frac{2\pi^2}{45} h_{\text{eff}} T^3 \quad \text{with} \quad h_{\text{eff}} \equiv \sum_a h_{\text{eff},a}. \quad (2.43)$$

2.3.4. Freeze-out mechanism

If we assume that DM and SM particles interact weakly, the large number densities in the hot and dense early universe could have made the interactions frequent enough to bring them into thermal equilibrium. In such a scenario, the Boltzmann eq. (2.28) can be employed to calculate the amount of DM we observe today. As the universe expands and cools down, we can describe the evolution of the number density of DM as

$$\begin{aligned} \dot{n}_{\text{DM}} + 3Hn_{\text{DM}} &= -\langle\sigma_{\text{ann}}v\rangle n_{\text{DM}}^2 + \langle\sigma_{\text{prod}}v\rangle n_{\text{SM}}^2 \\ &= -\langle\sigma_{\text{ann}}v\rangle \left[n_{\text{DM}}^2 - (n_{\text{DM}}^{\text{eq}})^2 \right]. \end{aligned} \quad (2.44)$$

In the second line, we assumed that the SM follows an equilibrium distribution and used the principle of detailed balance $\langle\sigma_{\text{ann}}v\rangle (n_{\text{DM}}^{\text{eq}})^2 = \langle\sigma_{\text{prod}}v\rangle (n_{\text{SM}}^{\text{eq}})^2$. This evolution can be further rewritten in terms of the ratio of the number density and the total entropy $s = s_{\text{SM}} + s_{\text{DM}}$, that defines the yield $Y_{\text{DM}} = n_{\text{DM}}/s$ and the dimensionless measure of time $x = m_{\text{DM}}/T$,

$$\frac{dY_{\text{DM}}}{dx} = -\frac{Y_{\text{DM}}^{\text{eq}}}{x} \frac{\Gamma_{\text{ann}}^{\text{eq}}}{H} \left[\left(\frac{Y_{\text{DM}}}{Y_{\text{DM}}^{\text{eq}}} \right)^2 - 1 \right] \quad \text{with} \quad \Gamma_{\text{ann}}^{\text{eq}} = n_{\text{DM}}^{\text{eq}} \langle\sigma_{\text{ann}}v\rangle. \quad (2.45)$$

We can see that as long as the particles are interacting efficiently ($\Gamma_{\text{ann}}^{\text{eq}} \gg H$) the DM species follows the equilibrium distribution. Once the particles become non-relativistic, i.e. $x \gg 1$, their number density becomes exponentially suppressed, cf. eq. (2.32a), and thus also the yield goes to zero. However, as the DM number density becomes suppressed, also its annihilation rate into the SM particles decreases. Eventually, the annihilations become so infrequent

($\Gamma_{\text{ann}}^{\text{eq}} \ll H$), that the DM leaves the thermal equilibrium with the SM. From here on, the DM particles evolve separately and Y_{DM} stays to good approximation constant:

$$\lim_{x \rightarrow \infty} Y_{\text{DM}}(x) \approx Y_{\text{DM}}^{\text{eq}}(x_f). \quad (2.46)$$

Here, the freeze-out condition $\Gamma_{\text{ann}}(T_f) = H(T_f)$ determines the point $x_f = m_{\text{DM}}/T_f$ from which on the interactions become too inefficient to change the yield. Fig. 2.3 shows this freeze-out of the yield for increasing values of the cross sections. One can see that larger cross sections keep the particles in thermal equilibrium for longer and thus they freeze out later with a lower yield.

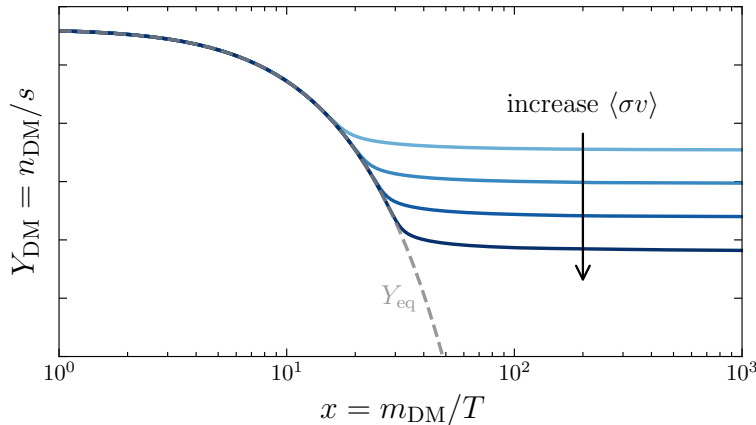


Figure 2.3.: The evolution of the DM yield for different values of the annihilation cross sections. The larger the cross section, the longer the DM stays in equilibrium (grey dashed line) and the smaller the relic abundance becomes (light to dark blue).

With the number density at the freeze-out temperature, an estimate of the DM relic abundance today can be obtained by

$$h^2 \Omega_{\text{DM}} \simeq h^2 \frac{\rho_{\text{DM},0}}{\rho_{c,0}} = h^2 \frac{m_{\text{DM}} Y_{\text{DM}}(x_f) s_0}{3H_0^2/(8\pi G)} \quad (2.47)$$

The abundance depends here on the DM mass and the yield at freeze-out. Here, the critical energy density $\rho_{c,0}$ is the total energy density today and the reduced Hubble parameter h is defined in terms of today's Hubble parameter as $H_0 = 100 h \text{ km s}^{-1} \text{ Mpc}^{-1}$. Lastly, the entropy density today s_0 can be computed from the photon temperature $T_{\gamma,0} \simeq 2.725 \text{ K}$ and the effective entropy degrees of freedom $h_{\text{eff},0} \simeq 3.93$.

2.4. Gravitational waves

In the last section, we have seen that DM could have been in thermal contact with the SM and abundant in the early universe. This motivates to consider to search for hints at the nature of dark matter in cosmological observations. Especially promising messengers that could reach us from the earliest times are gravitational waves. Gravitational waves, predicted by Einstein [1] over 100 years ago, were first detected in 2015 by the LIGO/Virgo collaboration [2]. At a distance of roughly one billion light years two black holes of masses 29 and 39 times the mass of our Sun merged into one of 62 solar masses. Part of the missing mass was radiated away in form of ripples in spacetime – gravitational waves (GWs). This has not only detected and confirmed the existence of astrophysical objects like black hole binaries,

but also opened up a new window into our universe and marked the beginning of gravitational wave cosmology. Unlike photons, gravitational waves did not thermalise in the early universe, but travelled freely and unperturbed. That means that GWs produced in the early universe still retain information about their production. Their spectrum, frequency, and intensity, which can contain a wealth of information about the early universe, are not washed out into a thermal distribution by interactions. Therefore, they can deliver information about the earliest times where energy scales beyond any experimental reach determined the dynamics.

Planned new GW observatories like LISA [69] or the Einstein Telescope [70] will use these messengers to not only probe astrophysics, but also cosmology. Already in the summer of 2023, the PTA collaborations NANOGrav [3], EPTA & InPTA [4] and PPTA [5] have found evidence for a stochastic gravitational wave signal at nanohertz (nHz) frequencies. As we will discuss further in sec. 2.5.2, an astrophysical signal is expected from the supermassive black hole binary that formed after the collision of galaxies. However, as of now, the theoretical modelling of the expected signal predicts a smaller amplitude and a lower spectral index than found in data. This leaves the exciting possibility that new physics, such as DM, could have left an imprint in this signal from processes in the early universe [71].

Understanding the processes behind the creation of such GWs and the properties of the signal could thus enable us to gather new hints on the nature of DM from these observations. In this section we will therefore review GW and their production. For a more detailed introduction, see e.g. [72–74] that we will follow along here.

2.4.1. Gravitational waves in vacuum

We start the study of GWs by considering the metric for a weak gravitational field. If we neglect cosmic expansion for the moment, we can choose a coordinate system that separates the metric into a flat background part and perturbations around it

$$g_{\mu\nu}(x) = \eta_{\mu\nu} + h_{\mu\nu}(x). \quad (2.48)$$

Such a decomposition is possible when the perturbations are small $|h_{\mu\nu}| \ll 1$ compared to the Minkowski metric that describes the flat space $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$. This scenario allows to use perturbation theory and leaves us in the regime of linearised gravity if we neglect higher-order terms in the Einstein equations. The dynamics of the spacetime are then all contained in the perturbations $h_{\mu\nu}$ around the static background $\eta_{\mu\nu}$. We note here that in contrast to the full metric, $h_{\mu\nu}$ is not a tensor as it does not maintain the decomposition eq. (2.48) for general coordinate transformations. Still, it is useful to restrict ourselves to transformations that leave this decomposition intact, which are given by the constant Lorentz transformations from special relativity

$$x^{\bar{\mu}} = \Lambda^{\bar{\mu}}_{\alpha} x^{\alpha}. \quad (2.49)$$

Under this restriction, we can treat the perturbations as if they were tensors in flat Minkowski space by defining the transformed perturbations as

$$h_{\bar{\mu}\bar{\nu}} \equiv \Lambda^{\alpha}_{\bar{\mu}} \Lambda^{\beta}_{\bar{\nu}} h_{\alpha\beta} \quad \text{and} \quad h^{\alpha\beta} \equiv \eta^{\alpha\mu} \eta^{\beta\nu} h_{\mu\nu}. \quad (2.50)$$

Another type of transformations that keep the decomposition eq. (2.48) unchanged are small changes in the coordinates of the form $x^{\mu} \rightarrow x^{\mu} + \xi^{\mu}(x)$ with the property $|\xi^{\mu}_{,\alpha}| \ll 1$. To first order in $\xi^{\mu}_{,a}$, the transformed metric is

$$g_{\bar{\mu}\bar{\nu}} = \eta_{\mu\nu} + h_{\mu\nu} - \xi_{\mu,\nu} - \xi_{\nu,\mu}. \quad (2.51)$$

The effect of the coordinate transformation on the perturbations is therefore

$$h_{\bar{\mu}\bar{\nu}} = h_{\mu\nu} - \xi_{\mu,\nu} - \xi_{\nu,\mu} . \quad (2.52)$$

Since we are free to choose the coordinate system, we can use this gauge transformation to eliminate four degrees of freedom in $h_{\mu\nu}$. One convenient choice is here the so-called Lorenz gauge, which sets $h^{\mu\nu}_{,\nu} = 0$.

We continue by computing the Riemann tensor, which is now given purely in terms of the perturbations $h_{\mu\nu}$:

$$R^\mu{}_{\nu\alpha\beta} = \frac{1}{2} \left(h^\mu{}_{\beta,\nu\alpha} + h_{\nu\alpha,}{}^\mu{}_\beta - h^\mu{}_{\alpha,\nu\beta} - h_{\nu\beta,}{}^\mu{}_\alpha \right) . \quad (2.53)$$

If we additionally introduce the trace reverse of $h_{\mu\nu}$ as

$$\bar{h}_{\mu\nu} \equiv h_{\mu\nu} - \frac{1}{2} \eta_{\mu\nu} h^\alpha{}_\alpha , \quad (2.54)$$

the Einstein tensor computed from eq. (2.53) becomes

$$G_{\mu\nu} = -\frac{1}{2} \left(\bar{h}_{\mu\nu,\alpha}{}^\alpha + \eta_{\mu\nu} \bar{h}^{\alpha\beta}{}_{,\alpha\beta} - \bar{h}_{\mu\alpha,\nu}{}^\alpha - \bar{h}_{\nu\alpha,\mu}{}^\alpha + \mathcal{O}(h^2) \right) . \quad (2.55)$$

Here, we can now employ the gauge freedom eq. (2.52) and choose the Lorenz gauge, where the Einstein tensor significantly simplifies and the linearised Einstein equations become

$$\square \bar{h}_{\mu\nu} = -16\pi G T_{\mu\nu} . \quad (2.56)$$

The d'Alembert operator $\square$ is here defined as $\square = \partial_\mu \partial^\mu = \partial_t^2 - \Delta$ and the Laplace operator Δ denotes the second derivative in all spatial directions $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$.

2.4.2. Propagation of gravitational waves

Before we study the full linearised Einstein equations, let us first turn to the homogeneous case, which describes the propagation of the metric perturbations, i.e. gravitational waves in vacuum. Far away from any source ($T_{\mu\nu} = 0$), eq. (2.56) reduces to the homogeneous wave equation

$$(\partial_t^2 - \Delta) \bar{h}_{\mu\nu} = 0 . \quad (2.57)$$

It is easy to see that it has the solution

$$\bar{h}_{\mu\nu} = A_{\mu\nu} \text{Re}(e^{ik_\alpha x^\alpha}) , \quad (2.58)$$

with amplitude $A_{\mu\nu}$ and wave vector k_α , known as the plane-wave solution. The dispersion relation obtained from $\square \bar{h}_{\mu\nu} = -k^2 \bar{h}_{\mu\nu} = 0$ is $k^2 = E^2 - p^2 = 0$ and immediately shows that GWs behave as radiation, i.e. they are massless and travel at the speed of light.

To study this solution further, we take again advantage of the gauge freedom that resulted from the transformation eq. (2.52) and use it to impose restrictions on the amplitude:

$$A^{\alpha\beta} k_\beta = 0 , \quad A^\alpha{}_\alpha = 0 , \quad \text{and} \quad A^{\alpha\beta} U_\beta = 0 , \quad (2.59)$$

where U_β is any constant four-velocity vector. These restrictions compose the *transverse-traceless* (TT) gauge. For concreteness, we choose $U_\beta = \delta_\beta^0$ and the wave propagation

direction $k = (\omega, 0, 0, \omega)$ along the z -axis, such that the perturbation can be written in matrix form as

$$\bar{h}_{\mu\nu}^{\text{TT}}(t, z) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & A_+ & A_\times & 0 \\ 0 & A_\times & -A_+ & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \cos(\omega(t - z)) . \quad (2.60)$$

We see that there are only two independent components A_+ and $A_\times$, that can be interpreted as the two polarisation states of the gravitational wave. The generalisation of a plane wave propagating in the direction of an arbitrary unit vector $\hat{n}$ follows simply by constructing the orthonormal basis tensors

$$e_{ij}^+(\hat{n}) = \hat{l}_i \hat{l}_j - \hat{m}_i \hat{m}_j \quad \text{and} \quad e_{ij}^\times(\hat{n}) = \hat{l}_i \hat{m}_j + \hat{m}_i \hat{l}_j , \quad (2.61)$$

from the orthonormal basis vectors $\hat{n}$, $\hat{l}$, and $\hat{m}$. With this, we can express a general GW coming from a source in the direction $\hat{n}$ as

$$h_{ij}(t, \vec{x}) = \sum_{a=+, \times} \int_{-\infty}^{\infty} df A_a(f) e^{2\pi i f(t + \hat{n} \cdot \vec{x})} e_{ij}^a(\hat{n}) , \quad (2.62)$$

with $A_a(f)$ being the Fourier amplitudes.

The effect of a GW can be demonstrated by considering two close particles separated in the $x - y$ plane. In the absence of external forces, they move along their geodesic U^μ and the separation S^μ between them is described by the geodesic deviation equation [75]

$$\nabla_U \nabla_U S^\alpha = R^\alpha_{\mu\nu\beta} U^\mu U^\nu S^\beta . \quad (2.63)$$

Here ∇_U denotes the derivative along the geodesic U^μ . In the weak field limit, this equation simplifies to

$$\frac{d^2}{dt^2} S^\alpha = \frac{1}{2} S^\beta (\bar{h}^\alpha_{\beta,00})^{\text{TT}} . \quad (2.64)$$

If we now assume a GW with only a A_+ component ($A_\times = 0$), it is easy to see that the solutions for the separation in the x - and y -direction are

$$\begin{aligned} S^x(t) &= S^x(0) + \frac{1}{2} A_+ \cos(\omega(t - z)) S^x(0) , \\ S^y(t) &= S^y(0) - \frac{1}{2} A_+ \cos(\omega(t - z)) S^y(0) . \end{aligned} \quad (2.65)$$

As sketched in the top row of fig. 2.4, the effect of a $+$ -polarised GW is to let the test particles that are initially separated in the x (y) direction oscillate in the x (y) direction. For a $\times$ -polarised GW ($A_+ = 0$), the solutions are instead

$$\begin{aligned} S^x(t) &= S^x(0) + \frac{1}{2} A_\times \cos(\omega(t - z)) S^y(0) , \\ S^y(t) &= S^y(0) + \frac{1}{2} A_\times \cos(\omega(t - z)) S^x(0) . \end{aligned} \quad (2.66)$$

As illustrated in the bottom row of fig. 2.4, the $\times$ -polarised GW lets the test particles oscillate in the x (y) direction proportional to their initial y (x) separation.

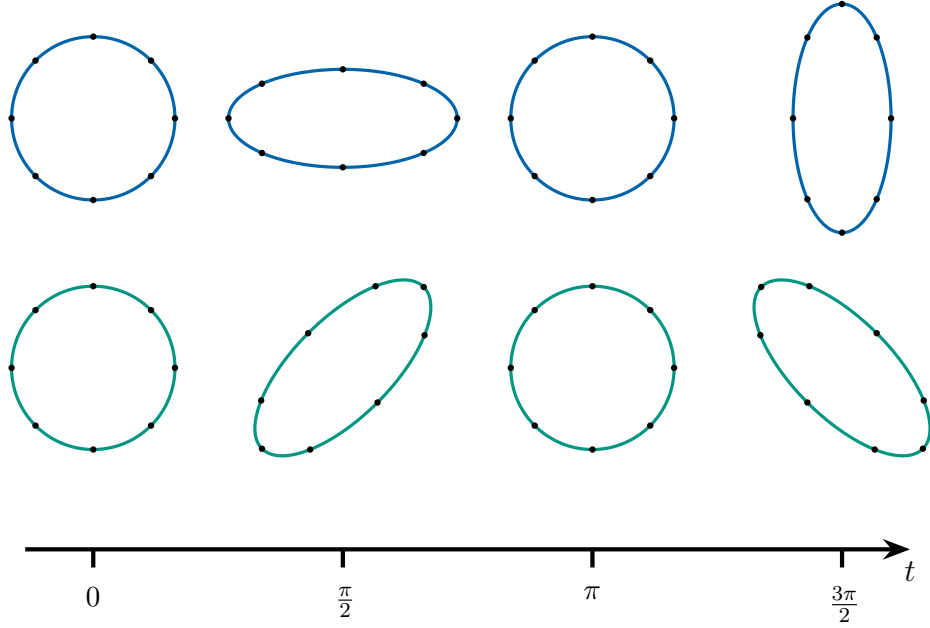


Figure 2.4.: Effect of a $+$ -polarised (top row) and $\times$ -polarised (bottom row) GW on test particles distributed on a ring. As suggested by the naming convention, the $+$ -polarisation causes the particles to oscillate in a plus shape, whereas the $\times$ -polarisation causes a cross-shaped pattern.

2.4.3. Sources of gravitational waves

Let us now turn to the sources of gravitational waves, described by the inhomogeneous eq. (2.56), which can be solved by the method of the Green's function for the d'Alembert operator

$$\square_x G(x^\mu - y^\mu) = \delta^4(x^\mu - y^\mu). \quad (2.67)$$

This equation has the well-known solution [56]

$$G(x^\mu - y^\mu) = -\frac{\delta(|\mathbf{x} - \mathbf{y}| - (x^0 - y^0))}{4\pi|\mathbf{x} - \mathbf{y}|} \theta(x^0 - y^0). \quad (2.68)$$

By inserting the Green's function back into the linearised Einstein eqs. (2.56) and integrating over the source, we get

$$\begin{aligned} \bar{h}_{\mu\nu}(t, \mathbf{x}) &= -16\pi G \int d^4y G(x^\mu - y^\nu) T_{\mu\nu}(y), \\ &\approx 4G \int d^3y \frac{T_{\mu\nu}(t - r, \mathbf{y})}{r}. \end{aligned} \quad (2.69)$$

In the second line we performed the integration over y^0 and approximated $|\mathbf{x} - \mathbf{y}| = r \approx x$ for an observer far away from the source. We can further use the conservation law $T^{\mu\nu}_{;\nu} = 0$, to rewrite the metric perturbations as [73]

$$\bar{h}_{ij}(t, \mathbf{x}) = \frac{2G}{r} \partial_t^2 \int d^3y y_i y_j T_{00}(t - r, \mathbf{y}). \quad (2.70)$$

To bring this into the familiar form of the transverse traceless gauge, we can use the projection operator $\Lambda_{ij,kl} = P_{ik}P_{jl} - 1/2 P_{ij}P_{kl}$ with $P_{ij} = \delta_{ij} - n_i n_j$, which projects out the metric perturbation into the TT gauge. Finally, we then obtain

$$\bar{h}_{ij}^{\text{TT}}(t, \mathbf{x}) = \frac{2G}{r} \Lambda_{ij,kl} \partial_t^2 Q_{kl}(t - r), \quad (2.71)$$

where we defined the reduced quadrupole moment in terms of the energy density of the source T_{00}

$$Q_{ij} \equiv \int d^3y (y_i y_j - \frac{1}{3} y^2 \delta_{ij}) T_{00}. \quad (2.72)$$

A source has therefore two properties to fulfil in order to radiate GWs. The first one is that change of the energy density T_{00} has to be time dependent ($\partial_t^2 T_{00} \neq 0$), the second one is that the energy density has to be non-spherical, as the quadrupole moment vanishes otherwise.

The energy density in the radiated GWs can be computed by evaluating the Einstein tensor up to second order in the metric perturbations. Explicit evaluation gives [56]

$$\langle G_{\mu\nu}^{(2)} \rangle = -\frac{1}{32\pi G} \langle \partial_\mu \bar{h}_{\alpha\beta} \partial_\nu \bar{h}^{\alpha\beta} \rangle, \quad (2.73)$$

where the brackets denote a spatial average over several wavelengths of the GW. With this, the energy density in GWs is given by

$$\rho_{\text{GW}} = \frac{1}{32\pi G} \langle \partial_t \bar{h}_{ij}^{\text{TT}} \partial_t \bar{h}^{ij\text{TT}} \rangle. \quad (2.74)$$

2.4.4. Stochastic gravitational wave backgrounds

If we now consider a process that produces GWs in the early universe, we will see that today we would receive a magnitude of overlapping signals from different regions of our sky rendering it into a stochastic background signal. This is a basic consequence of the expansion of the universe we discussed in sec. 2.1. Here we review the properties of such a stochastic GW background, following refs. [74, 76].

We start by assuming that the length scale of the source is smaller or comparable to the Hubble radius given by the inverse Hubble rate $L_* H_* \lesssim 1$, where the subscript $*$ denotes the values at emission. This length scale today receives a redshift factor a_0/a_* and compared to the size of the universe today becomes

$$L_0 H_0 = H_0 L_* \frac{a_0}{a_*} \lesssim \frac{H_0}{H_*} \frac{a_0}{a_*} \stackrel{\text{rad.dom.}}{\approx} \frac{1}{\sqrt{\Omega_{\text{rad}}(1+z_*)}}, \quad (2.75)$$

where in the last step we assumed the emission to occur during radiation domination, which let us write $H_* \approx H_0 \sqrt{\Omega_{\text{rad}}(1+z_*)^4}$. We can evaluate this for a process at e.g. the electroweak scale, where we have a redshift value of $z_{\text{ew}} \sim 10^{14}$. Together with the fraction of energy density in radiation today $\Omega_{\text{rad}} \simeq 9 \cdot 10^{-5}$ this gives

$$L_0 H_0 \lesssim 10^{-12}. \quad (2.76)$$

This means that the correlation scale of a GW signal today is tiny compared to the present size of the universe. We can further translate this into the number of causally disconnected patches in the sky by using the angular diameter distance

$$d_A(z_*) = \frac{1}{H_0(1+z_p)} \int_0^{z_*} dz \frac{1}{\sqrt{\Omega_{\text{m}}(z) + \Omega_{\text{rad}}(z) + \Omega_\Lambda}}, \quad (2.77)$$

that relates the length L and the angular size θ : $d_A = L/\theta$. A rough estimate of the number of independent patches from the electroweak (EW) scale is then obtained by θ^{-2} , which is, inserting again the EW redshift,

$$\theta_*^{-2} = \frac{d_A(z_*)^2}{L_*^2} \gtrsim \frac{d_A(z_*)^2}{H_*^2} \stackrel{z_*=10^{14}}{\approx} 10^{24}. \quad (2.78)$$

Hence, any GW signal emitted at temperatures around the electroweak scale, even if it was correlated across the whole Hubble radius, gives a signal today that is superposed of a huge number of uncorrelated components and therefore cannot carry any information beyond its statistical properties.

The metric perturbations $h_{\mu\nu}$ from early universe processes that reach us as GWs today can therefore be treated as random variables and inherit their properties from the cosmological principle. On large scales, we saw that the universe is homogeneous and isotropic, so different patches have the same properties and the same processes happened at the same time, which is inherited by the GW background. Additionally, in the absence of parity violating production mechanisms, we also expect the signal to be unpolarised, i.e. both polarisation states are produced with equal probability and hence the spatial and temporal average of the Fourier amplitudes of the two polarisations is uncorrelated

$$\langle A_+(\hat{n}, f) A_\times(\hat{n}, f) \rangle = 0, \quad (2.79)$$

where the Fourier amplitudes A_a now also have a direction dependence $\hat{n}$. In total, we can summarise these properties in the two point correlation function

$$\langle A_a(\hat{n}, f) A_b^*(\hat{n}', f') \rangle = \frac{1}{4\pi} \delta_{ab} \delta(f - f') \delta(\phi - \phi') \delta(\cos \theta - \cos \theta') \frac{1}{2} S(f). \quad (2.80)$$

Here, isotropy and homogeneity dictate that signals from different angles of the sky are uncorrelated ($\delta(\phi - \phi') \delta(\cos \theta - \cos \theta')$), while the absence of polarisation gives δ_{ab} . The only information about the source is then encoded in the spectral function $S(f)$, that propagates into the frequency dependence of the energy density

$$h^2 \Omega_{\text{GW}}(f) = \frac{h^2}{\rho_c} \frac{d\rho_{\text{GW}}}{d \ln f} = \frac{h^2}{32\pi G \rho_c} \frac{d}{d \ln f} \langle \partial_t \bar{h}_{ij}^{TT} \partial_t \bar{h}^{ijTT} \rangle. \quad (2.81)$$

We can evaluate this by decomposing the GW amplitudes again in their plane wave expansion, where each Fourier amplitude now receives contribution from all sky directions $\hat{n}$ [76]

$$h_{ij}(\vec{x}, t) = \sum_{a=+, \times} \int_{-\infty}^{\infty} df \int d^2 \Omega_{\hat{n}} A_a(\hat{n}, f) e^{2\pi i f(t + \hat{n} \cdot \vec{x})} e_{ij}^a(\hat{n}). \quad (2.82)$$

With this, the two point correlation function reduces to

$$\langle \partial_t \bar{h}_{ij}^{TT} \partial_t \bar{h}^{ijTT} \rangle = \sum_{a, a'} \int_{-\infty}^{\infty} df df' \int d^2 \Omega_{\hat{n}} d^2 \Omega_{\hat{n}'} \langle A_a(f, \hat{n}) A_{a'}^*(f', \hat{n}') \rangle \quad (2.83)$$

$$e_{ij}^a(\hat{n}) e^{ija'}(\hat{n}') 4\pi^2 f f' e^{2\pi i(f-f')t + 2\pi i(\hat{n} - \hat{n}') \cdot \vec{x}} \quad (2.84)$$

$$= 8\pi^2 \int_0^{\infty} df f^2 S(f) \quad (2.85)$$

where we used $\int d\Omega_{\hat{n}} = 4\pi$ and $e_{ij}^a e^{ija} = 4$. Therefore, we have the fractional energy density

$$h^2 \Omega_{\text{GW}}(f) = \frac{2\pi^2 h^2}{3H_0} f^3 S(f), \quad (2.86)$$

where the physics of the source is encoded only in the shape and amplitude of the spectral function.

2.4.5. Cosmological bounds on stochastic gravitational waves

Since the GWs are decoupled from the plasma below the Planck scale, they do not interfere directly with particle processes in the early universe. Nonetheless, if the GWs carry a significant fraction of the energy density, they contribute to the Hubble expansion and possibly modify the standard cosmological history. Here we will discuss the two relevant bounds for this thesis, which come from BBN and observations of the CMB, following along ref. [77].

Bounds from BBN

Stringent bounds on the composition of the universe below MeV temperature come from the observation of light element abundances through the process of big-bang nucleosynthesis (BBN). It predicts the abundances of deuterium, helium isotopes (^3He , ^4He) and Lithium (^7Li), that can be measured today [78, 79]. These abundances are very sensitive to the ratio between protons (p) and neutrons (n), as the latter end up almost exclusively in the nuclei of the light elements. In thermal equilibrium, we have the ratio between the number densities of the non-relativistic nucleons

$$\frac{n_n}{n_p} = e^{-\Delta m/T} \quad \text{with} \quad \Delta m = m_n - m_p \simeq 1.3 \text{ MeV}, \quad (2.87)$$

where the process $n\nu_e \leftrightarrow pe$ maintains the equilibrium. This ratio is exponentially sensitive to the freeze-out temperature below which the process stops to efficiently convert protons to neutrons and the ratio n_n/n_p remains frozen. This determines the number of neutrons available to form the light nuclei of BBN.

Analogous to the discussion of the dark matter freeze-out mechanism (sec. 2.3.4), the freeze-out temperature can be roughly determined by equating the nucleon conversion rate with the Hubble rate $\Gamma_{pe \rightarrow n\nu_e}(T_f) = H(T_f)$. At BBN the energy density of the universe resides almost exclusively in radiation and the Hubble rate can be written as

$$H^2 = \frac{8\pi G}{3} (\rho_\gamma + \rho_\nu + \rho_{\text{extra}}) = \frac{8\pi G}{3} \left(1 + N_{\text{eff}} \frac{7}{8} \left(\frac{4}{11} \right)^{4/3} \right) \rho_\gamma, \quad (2.88)$$

$$\text{with} \quad \rho_\nu + \rho_{\text{extra}} \equiv N_{\text{eff}} \frac{7}{8} \left(\frac{4}{11} \right)^{4/3} \rho_\gamma, \quad (2.89)$$

where we employed the standard parameterisation of the effective degrees of neutrinos N_{eff} . The standard three neutrino generations with corrections through finite temperature QED effects give $N_{\text{eff}}^\nu \simeq 3.044$ [80]. Adding additional energy density ρ_{extra} through e.g. new light particles or GWs, then increases the Hubble rate and the freeze-out condition $\Gamma/H = 1$ is reached at a higher temperature, which in turn leads to a larger number of neutrons. From this we would expect an overproduction of deuterium that propagates into an overproduction of ^4He . For a proper determination of the effect, the full coupled Boltzmann equations for the BBN reaction chains have to be solved and additional effects like the modification of the baryon-to-photon ratio have to be taken into account.

CMB bounds on extra radiation

An additional, more direct bound comes from the observation of the CMB. Small overdensities in the density of the primordial plasma gravitationally attracted the tightly coupled photon, electron and baryon fluid that counteracted with pressure resulting in acoustic oscillations in the fluid. These froze out as the photons decoupled at CMB, leaving behind a characteristic length scale in the CMB anisotropies. Adding additional radiation would have shifted the moment of this freeze-out and with it the peak in the power spectrum of these oscillations. These additionally constrain N_{eff} at this later time and, together with the BBN bound, give a tight constraint. The value determined by the Planck collaboration is $N_{\text{eff}} = 2.99 \pm 0.17$ [8].

Combining both bounds at BBN and CMB times gives a tighter result of $N_{\text{eff}} = 2.925 \pm 0.082$ [81]. We can define the non-neutrino contribution to N_{eff} as the difference between the observed value and the SM neutrino contribution $\Delta N_{\text{eff}} = N_{\text{eff}}^{\text{obs}} - N_{\text{eff}}^\nu$. Using now the upper limit on N_{eff} at the 95% confidence limit, we obtain $\Delta N_{\text{eff}} < 0.125$ [81]. The contribution of GWs to this is then simply given by

$$\Delta N_{\text{eff}}^{\text{GW}} = \frac{8}{7} \left(\frac{11}{4} \right)^{4/3} \frac{1}{\Omega_\gamma h^2} \int_{f_{\text{BBN}}}^{\infty} h^2 \Omega_{\text{GW}}(f) d \log f, \quad (2.90)$$

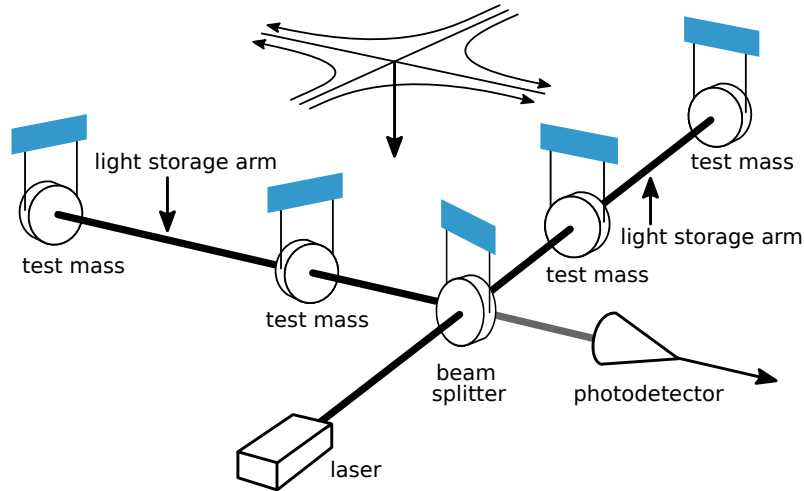


Figure 2.5.: Basic design of a laser interferometer to detect GWs. A beam splitter divides a laser beam into two arms, where the beam travels back and forth multiple times, before forming an interference pattern in a photodetector. Taken from [82].

such that we can set a bound on a GW background through $\Delta N_{\text{eff}}^{\text{GW}} < 0.125$. The lower bound of the frequency integral comes from the fact that only frequencies modes smaller than the Hubble horizon contributed to the signal. For BBN temperatures of $T \sim 0.1 \text{ MeV}$ this corresponds to $f_{\text{BBN}} \simeq 1.5 \cdot 10^{-11} \text{ Hz}$ [77].

2.4.6. Gravitational wave detection

The detection of GWs relies on the quadrupolar deformation of spacetime that we discussed in sec. 2.4.1. One way to measure this effect is to construct a Michelson-Morley interferometer, consisting of two perpendicular arms, as sketched in fig. 2.5. A beam splitter divides a laser into two beams that travel back and forth in each arm multiple times before forming an interference pattern in a photodetector. A GW with the polarisation axes aligned with the detector arms will cause one arm to contract, while the other expands. This causes the photons in the arms to travel different distances, inducing a phase shift and changing the interference pattern in the photodetector. The measurement of GWs from even the strongest sources, like binary mergers, still requires extreme precision. The LIGO interferometer [83], for example, is sensitive to changes in distances of 10^{-22} m by letting the photons travel around 280 times through its 4 km long arms.

Generally, the ability of an interferometer to detect a signal is determined by the *signal-to-noise ratio*

$$\text{SNR}^2 = C t_{\text{obs}} \int df \left[\frac{h^2 \Omega_{\text{GW}}(f)}{h^2 \Omega_{\text{noise}}(f)} \right]^2, \quad (2.91)$$

where the measurement is performed over the observation time t_{obs} and the details of the experiment enter through the detector-specific noise curve $\Omega_{\text{noise}}(f)$. The factor $C = 2$ accounts for cases where a cross-correlation can be performed through a multi-detector network. In a single detector scenario, $C = 1$ instead [84]. A signal is then considered detectable if the SNR exceeds a threshold SNR_{thr} after some observation time.

If the GW signal follows a power-law, a simplified criterion to determine whether it will be detectable can be constructed through the so-called power-law-integrated (PLI) sensitivity curves [85]. A signal given by $\Omega_q(f) = \Omega_q(f/\text{Hz})^q$ will be detectable if it satisfies

$$\text{SNR}_q \geq \text{SNR}_{\text{thr}}. \quad (2.92)$$

Observatory	Status	SNR _{thr}	t_{obs} [years]	References
SKA (5, 10, 20 yr)	Planned	4	5, 10, 20	[86, 87]
EPTA (18 yr)	Current	1.19	18	[88, 89]
NANOGrav (11, 15 yr)	Current	0.697	11, 15	[90]
μ Ares	Proposed	10	7	[91]
LISA	Planned	10	4	[6]
BBO	Proposed	10	4	[92]
ET	Proposed	5	5	[70]
HLV (O2)	Current	1	1	[93, 94]

Table 2.1.: Overview of running and proposed gravitational wave experiments.

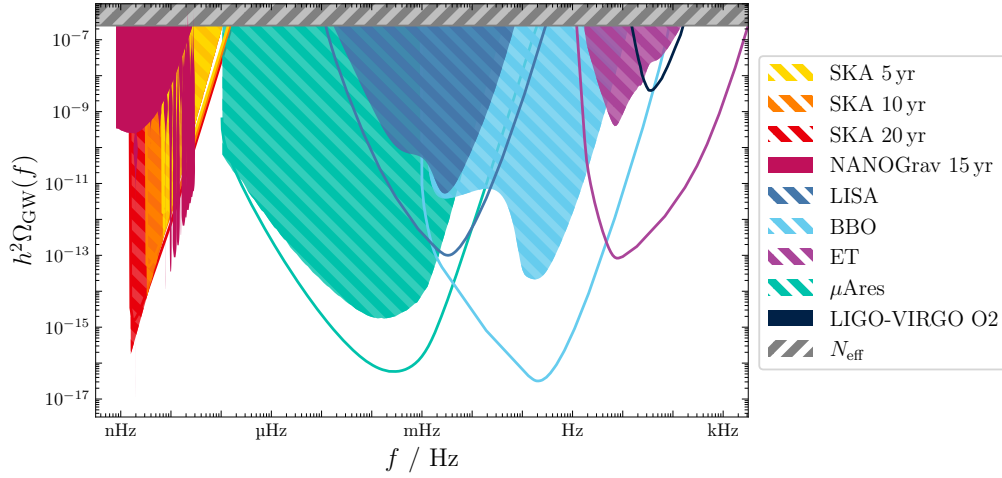


Figure 2.6.: Noise curves (shaded areas) and power law integrated sensitivity curves (solid lines) for the GW experiments listed in tab. 2.1. The grey hatched region shows the ΔN_{eff} bounds from BBN and CMB observations.

We can reformulate this condition into a threshold of the amplitude Ω_q , using the definition of the signal-to-noise ratio (SNR) eq. (2.91):

$$\Omega_q \geq \text{SNR}_{\text{thr}} \left[\sqrt{C t_{\text{obs}} \int_{-\infty}^{\infty} df \left(\frac{(f/\text{Hz})^q}{\Omega_{\text{noise}}(f)} \right)^2} \right]^{-1}. \quad (2.93)$$

From this criterion, we can construct the PLI sensitivity curve by taking the maximum of all possible power laws at each frequency

$$\Omega_{\text{PLI}}(f) = \max_q \left(\Omega_q^{\text{thr}} (f/\text{Hz})^q \right), \quad (2.94)$$

where Ω_q^{thr} is the amplitude for each q which fulfils the equality eq. (2.93).

A list of running experiments, as well as planned and proposed experiments, is listed in tab. 2.1, which is based on ref. [84]. In fig. 2.6 we show the PLI sensitivity curves (solid lines) constructed from the detector noise curves (hatched regions) for these experiments. Additionally, the bound from ΔN_{eff} on stochastic GW backgrounds is shown as the grey hatching.

2.5. Gravitational wave cosmology with pulsar timing arrays

In the previous section, we gave the example of a terrestrial interferometer with an arm length of a few kilometres, giving an optimal sensitivity in the frequency range associated with the wave length of the GWs, i.e. Hz to kHz (cf. fig 2.6). To observe lower frequencies, larger arm lengths of the interferometer are required. The idea to search for gravitational waves on astrophysical scales was proposed in the late 70s by Sazhin [95] and Detweiler [96]. It is based on the idea of using astrophysical objects as test masses to construct the interferometer arms. Ideal candidates for this are so-called pulsars – fast spinning neutrons stars that have a strong magnetic dipole misaligned from the axis of rotation. This precessing of the magnetic dipole creates an electric field and accelerates charged particles along the dipole axis [97], sweeping the universe like a lighthouse beam of a radio signal. These pulsars are sometimes referred to as “cosmic clocks”, as they have very stable orbital periods, with $P = 0.1 - 1$ s. The typical spin-down rate is $\dot{P} \sim 10^{-15}$ corresponding to a slow-down of only 1 nanosecond per month, which allows precise prediction of pulse timing with timing models. Using the quadrupole nature of GWs and correlating the timing residuals between pulsars makes it possible to distinguish between noise, pulsar modelling errors and GW signals.

To understand what response we can expect from a stochastic GW background from the early universe, we will review the calculation of the effect of GW on the observation of the pulse arrival times following along the review [76].

2.5.1. Pulsars and gravitational waves

The timing of the pulsar emission t_{em} can be modelled by the pulse time-of-arrival (TOA) t_{TOA} observed by radio telescopes and the effects that the pulse undergoes while travelling from the pulsar to Earth

$$t_{\text{em}} = t_{\text{TOA}} - \Delta_{\odot} - \Delta_{\text{ISM}} - \Delta_B. \quad (2.95)$$

This timing model includes the term $\Delta_{\odot}$ that accounts for timing corrections due to the reference frame of the detector (Earth) in the Solar System Barycenter (SSB), i.e. time dilation and redshift due to the gravitational potentials of the Sun and other bodies in the Solar System, delays through the propagation through the atmosphere and solar-wind and clock corrections. The second term Δ_{ISM} accounts for dispersion effects of the pulse travelling through the interstellar medium (ISM). The last term Δ_B is needed if the pulsar is part of a binary system, and encompasses the effect of time dilation and redshift as the pulse leaves the gravitational field of the system.

Differences between the predicted TOAs and the measured TOAs, called timing residuals, indicate the effects that are not accounted for by the deterministic timing model eq. (2.95). These include intrinsic pulsar noise due to irregularities in the rotational frequency from pulsar internal processes or detector noise, but also inaccuracies in the modelling of the Earths motion in the Solar System. These effects, however, can be distinguished from the effect of GWs that have a distinct quadrupole nature that shows up when correlating the timing residuals of pulsar pairs at different angles. In the following, we will derive this correlation for a stochastic background of GWs.

First, we will compute the effect of a single gravitational wave on the arrival time of the pulsar before turning to the case of a stochastic background. For this treatment, we follow along the derivation presented in refs.[76, 98]. Let us first look at the effect of a single GW on the arrival time of a pulse, by inspecting a pulse travelling from a pulsar to our detector in the presence of a GW. The line element for the pulse is

$$0 = ds^2 = -dt^2 + (\delta_{ij} + \bar{h}_{ij}^{TT} dx^i dx^j). \quad (2.96)$$

To simplify things, we can assume that the pulse is travelling along the x-axis, which gives

$$dx = \frac{dt}{\sqrt{1 + \bar{h}_{xx}^{TT}}} \approx \left(1 - \frac{1}{2}\bar{h}_{xx}^{TT}\right) dt, \quad (2.97)$$

where we used $|\bar{h}_{ij}^{TT}| \ll 1$. From this, we can express the distance to the pulsar L as

$$L = t_{\text{obs}} - t_{\text{em}} - \frac{1}{2} \int_{t_{\text{em}}}^{t_{\text{obs}}} dt' \bar{h}_{xx}^{TT}. \quad (2.98)$$

We can generalise this by rotating the result to an arbitrary pulsar location $\bar{h}_{xx}^{TT} \rightarrow n^i n^j \bar{h}_{ij}^{TT}$ and rearrange for the observation time

$$t_{\text{obs}} = t_{\text{em}} + L + \frac{n^i n^j}{2} \int_{t_{\text{em}}}^{t_{\text{em}}+L} dt' \bar{h}_{ij}^{TT}. \quad (2.99)$$

Here, we also approximated $t_{\text{obs}} \approx t_{\text{em}} + L$ in the integral boundary. The difference in the emission time of two subsequent pulses is simply the period $t'_{\text{em}} = t_{\text{em}} + P$ and we can write the observed difference

$$t'_{\text{obs}} - t_{\text{obs}} = P + \Delta P, \quad (2.100)$$

where the difference ΔP comes here from the effect of the gravitational wave

$$\Delta P = \frac{n^i n^j}{2} \int_{t_{\text{em}}}^{t_{\text{em}}+L} dt' [h_{ij}^{TT}(t' + P, x_0(t')) - h_{ij}^{TT}(t', x_0(t'))] \quad (2.101)$$

$$\approx \frac{n^i n^j}{2} \int_{t_{\text{em}}}^{t_{\text{em}}+L} dt' \left(\frac{\partial}{\partial t'} \bar{h}_{ij}^{TT}(t', x_0(t')) \right) P. \quad (2.102)$$

In the second step, we expanded the metric perturbation to first order since the orbital period is tiny compared to GW periods on these astrophysical length scales. For the case of a single plane-wave propagating in the direction $\hat{\Omega}$ with

$$\bar{h}_{ij}^{TT} = A_{ij}(\hat{\Omega}) \cos(\omega(t - \hat{\Omega} \cdot \vec{x})), \quad (2.103)$$

the shift in the arrival time of the pulse, also called the GW induced redshift $z(t, \hat{\Omega})$ becomes

$$z(t, \hat{\Omega}) \equiv \frac{\Delta P}{P} = \frac{n^i n^j A_{ij}}{2(1 + \hat{\Omega} \cdot \hat{n})} \left(\cos(\omega t_{\text{obs}}) - \cos(\omega(t_{\text{em}} - L \hat{\Omega} \cdot \hat{n})) \right). \quad (2.104)$$

Depending on the angle between the GW propagation and the pulsar-detector direction (encoded in $n^i n^j A_{ij}$), we recover the same quadrupole behaviour as the ring of test-particles discussed in sec. 2.4.3.

Next, we turn to the case of an isotropic signal coming from all sky directions. Using the general Fourier decomposition of the GW signal eq. (2.82), the redshift between two successive pulses through this isotropic GW is given by

$$z(t) = \sum_{a=+, \times} \int_{-\infty}^{\infty} df \int d^2 \hat{\Omega} A_a(f, \hat{\Omega}) F^a(\hat{\Omega}) e^{-2\pi i f t} \left(1 - e^{2\pi i f L(1 + \hat{\Omega} \cdot \hat{x})} \right), \quad (2.105)$$

$$\text{with} \quad F^a(\hat{\Omega}) = \frac{n^i n^j e_{ij}^a(\hat{\Omega})}{2(1 + \hat{\Omega} \cdot \hat{n})}. \quad (2.106)$$

To distinguish the effect of the GW from noise, mismodelling of effects in the timing model eq. (2.95) or other effects, we can correlate the redshifts between pulsar pairs. For a pulsar pair at the positions $\vec{x}_i$ and $\vec{x}_j$ and with distances L_i and L_j , the correlation is

$$\begin{aligned} \langle z_i(t) z_j(t) \rangle &= \int \int d\hat{\Omega} d\hat{\Omega}' \sum_{a,a'} \int_{-\infty}^{\infty} df df' F^a(\hat{\Omega}) e^{-2\pi i f t} \left(1 - e^{2\pi i f L_i (1 + \hat{\Omega} \vec{x}_i)} \right) \\ &\quad \times F^{a'}(\hat{\Omega}') e^{2\pi i f' t} \left(1 - e^{-2\pi i f' L_j (1 + \hat{\Omega}' \vec{x}_j)} \right) \left\langle A_a(f, \hat{\Omega}) A_b^*(f', \hat{\Omega}') \right\rangle. \end{aligned} \quad (2.107)$$

Using the assumptions of a homogeneous, isotropic and unpolarised signal i.e. eq. (2.80), the correlation between the redshift of pulsar pairs becomes

$$\langle z_i(t) z_j(t) \rangle = \frac{1}{4\pi} \int_0^\infty df S(f) \int d\hat{\Omega} \kappa_{ij}(\hat{\Omega}) \sum_{a=+, \times} F_i^a(\hat{\Omega}) F_j^a(\hat{\Omega}) \quad (2.108)$$

$$\text{with} \quad \kappa_{ij} = \left(1 - e^{-2\pi i f L_i (1 + \hat{\Omega} \vec{x}_i)} \right) \left(1 - e^{2\pi i f L_j (1 + \hat{\Omega} \vec{x}_j)} \right). \quad (2.109)$$

Here, the function κ_{ij} captures the spatial correlation between pulsar signals. For pulsars with typical distances larger than 400 light years and the probed frequencies of $f = 10^{-9}$ Hz we have $fL \gg 1$ and κ_{ij} becomes a rapidly oscillating function. Therefore, it does not contribute to the integral ($\kappa_{ij} \rightarrow 1$), except for identical pulsars, for which $\kappa_{ij} \rightarrow 2$ approaches the auto-correlation limit. In a good approximation we can therefore safely set $\kappa_{ij} \rightarrow 1 + \delta_{ij}$. We can define the overlap reduction function, which measures how much of the GW signal is shared between pulsar pairs, as

$$\Gamma_{ij} = \frac{3}{2} \int \frac{d^2 \hat{\Omega}}{4\pi} \kappa_{ij}(f, \hat{\Omega}) \sum_a F_i^a(\hat{\Omega}) F_j^a(\hat{\Omega}) = \frac{3}{2} x_{ij} \ln x_{ij} - \frac{1}{4} x_{ij} + \frac{1}{2} (1 + \delta_{ij}), \quad (2.110)$$

with $x_{ij} = 1/2(1 - \cos \theta_{ij})$ and θ_{ij} denoting the angle between pulsar pairs. This result, first presented by Hellings and Downs [99] and hence known as the Hellings and Downs correlation, is shown as the black dashed line in fig. 2.7. The correlation follows the expected quadrupole characteristics with positive correlation at 0 and 180° pulsar separation and anti-correlation for a 90° separation. The blue data points show the result of 15 years of pulsar observation by the NANOGrav (North American Nanohertz Observatory for Gravitational Waves) collaboration, which has found evidence for such a stochastic GW background.

2.5.2. The PTA data

In June 2023, the PTA collaborations announced that they found evidence for a stochastic GW background in the nanohertz frequency range with an amplitude of $h^2 \Omega_{\text{GW}} \sim 10^{-9} - 10^{-8}$. The significance for this was found to reach evidence level, with $3.5\sigma - 4\sigma$ reported by NANOGrav, which observed 68 pulsars over 15 years [3], 3σ by the EPTA-InPTA (European and Indian PTA) collaboration which observed 25 pulsars over 11 years [4], and 2σ by the PPTA (Parks PTA) collaboration, which observed 32 pulsars over 18 years [5]. The reported measurement of the Hellings and Downs correlation of the NANOGrav collaboration is shown as the blue data points in fig. 2.7. An observation of a GW background in this frequency range is not unexpected, as there are astrophysical processes that give such a signal: inspiralling supermassive black hole binaries (BHB) from galaxy merges.

The general consensus in astrophysics is that galaxies usually host a very massive black hole in their centres [101, 102]. As galaxies merge throughout the cosmic history, the massive black holes in their centres form binaries. If the BHB reach close separations (milliparsecs), their binding energy is radiated away in GWs, leading to an inspiralling and finally merging of the two black holes. In the case that the BHBs have a mass range of $\mathcal{O}(10^8 - 10^{10})$ solar

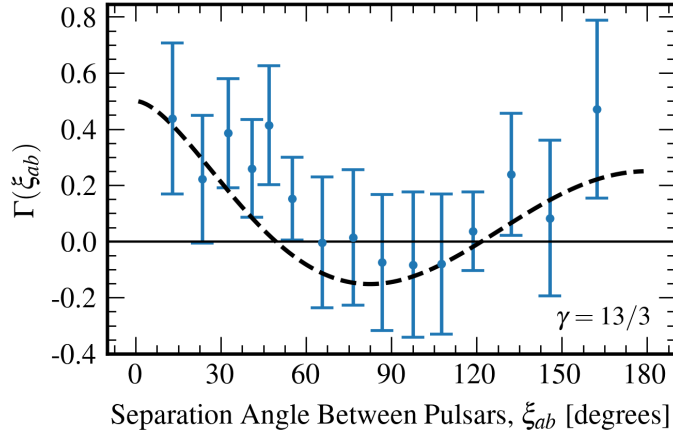


Figure 2.7.: Overlap reduction function as a function of the pulsar separation angle. The dashed black line shows the prediction for a homogeneous and isotropic GW signal, while the measurement by the NANOGrav collaboration with their 15 yr data set [100] is shown in blue. Image taken from [3].

masses (also called supermassive black holes), their GW emission falls into the nanohertz region probed by the PTA.

A very simple relation between the GW spectrum and the number density of sources was derived by Phinney [40]. The signal of the cosmological distribution of discrete sources can be written as

$$\frac{d\rho}{d \ln f} = \int_0^\infty dz \frac{dn}{dz} \frac{1}{1+z} \frac{dE}{d \ln f_r} \Big|_{f_r=f(1+z)}. \quad (2.111)$$

Here dn/dz is the number density of sources over redshift, $1/(1+z)$ accounts for the redshift of the energy of the signal emitted at the logarithmic frequency interval $dE/d \ln f_r$. For a population of binaries, we can use very simple scaling arguments to evaluate the frequency dependence of the energy emission. We start with the quadrupole formula for the power emitted by a compact binary [76]

$$P_{\text{GW}} = \frac{dE}{dt} = -\frac{G}{5} \left\langle \frac{d^3 Q_{ij}}{dt^3} \frac{d^3 Q_{ij}}{dt^3} \right\rangle \propto -GM^2 R^4 \omega^6, \quad (2.112)$$

where the proportionality holds for an equal mass binary. In the Newtonian approximation, we can use Kepler's third law to eliminate the R dependence

$$\omega = \left(\frac{GM}{4R^3} \right)^{1/2}, \quad (2.113)$$

such that

$$\frac{dE}{dt} = G^{7/3} M^{10/3} \omega^{10/3}. \quad (2.114)$$

To obtain the frequency scaling of the energy, we can approximate that the loss in the binding energy of the binary $E_{\text{bind}} \propto G^{2/3} M^{5/3} \omega^{2/3}$ is only due to the gravitational radiation, i.e. $\dot{E}_{\text{bind}} = P_{\text{GW}}$. With $\omega = 2\pi f$, we get the scaling $\dot{f} \propto f^{11/3}$. In total, these simple scaling relations give us a simple power law of the spectrum from the binaries [76]

$$\frac{dE}{d \ln f_r} = f_r \frac{dE}{dt_r} \frac{dt_r}{df_r} \propto f_r \times f_r^{10/3} \times f_r^{-11/3} = f_r^{2/3}. \quad (2.115)$$

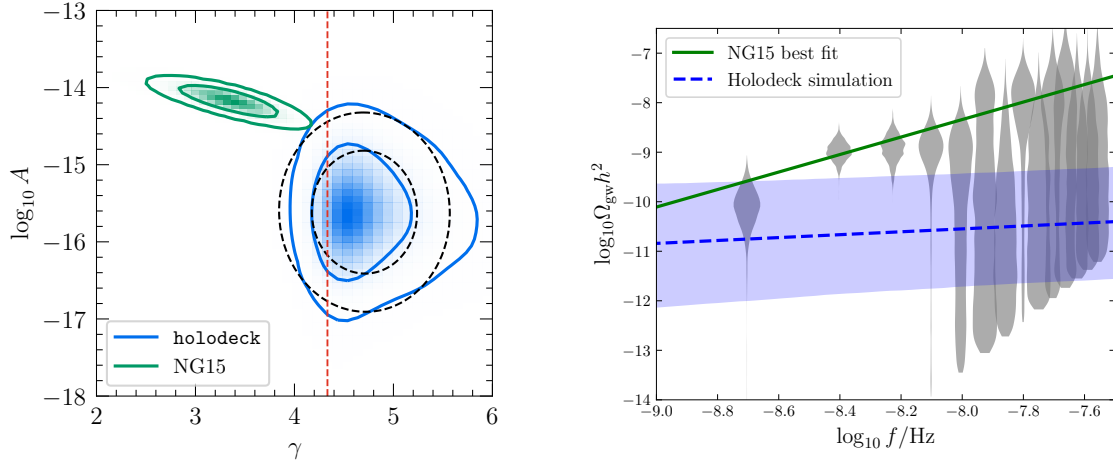


Figure 2.8.: *Left panel:* Predictions for the spectral index γ and the amplitude of the black hole binary signal at nHz (blue) and the best fit to the data taken by the PTA collaboration. The prediction $\gamma = 13/3$ from simple scaling arguments is shown as the red dashed line. Image taken from [71]. *Right panel:* NANOGrav 15 yr data represented as Fourier spectrograms (grey violins, extracted from the tool **PTArcade** [103]) and best fit of supermassive black hole binary signal (cf. eq. 2.116) (green). The GW spectrum from the Holodeck simulation [42] is shown as the blue dashed line with the 1σ band as the blue shading.

Conventionally, the signal from the supermassive BHB is then written as

$$h^2 \Omega_{\text{GW}}(f) = \frac{8\pi^4 h^2 f^5}{H_0} \frac{\Phi(f)}{T_{\text{obs}}} \quad \text{with} \quad \Phi_{\text{BHB}}(f) = \frac{A_{\text{BHB}}^2}{12\pi} T_{\text{obs}} \left(\frac{f}{\text{yr}^{-1}} \right)^{-\gamma_{\text{BHB}}}, \quad (2.116)$$

with the spectral index $\gamma_{\text{BHB}} = 13/3$ and the amplitude A_{BHB} depends on the source distribution $n(z)$. This power law scaling can only be valid in a finite frequency range, as otherwise the energy of the GWs would be unbounded.

The NANOGrav collaboration simulated the signal of a binary population based on realistic astrophysical distributions [42]. The prediction for the amplitude and spectral index of the simulation is shown in the left panel of fig. 2.8 as the blue contours, while the values inferred by the observations are shown in green. In the right panel of the figure, the NANOGrav data is shown by the grey violins that represent the posterior probability distribution of the amplitude of the GW background at each Fourier bin. For details on how the likelihood for a stochastic background is computed using this data, we refer to app. A.1. Clearly, there is a tension between the prediction and measurement. This leaves the possibility to improve the explanation of the signal by adding a cosmological source. Possible candidates are GWs from cosmic inflation, phase transitions and topological defects like domain walls and cosmic strings [71], that produce gravitational waves in the very early universe and each comes with a distinct gravitational wave spectrum. Therefore, there exists the exciting possibility that the stochastic gravitational wave background at nanohertz frequencies could shed light on processes that occurred in the very early universe.

In particular, in this thesis we will explore the possibility that DM could contribute to the measured signal through a cosmological first-order phase transition. The dynamics of this mechanism will be reviewed in the next chapter in detail.

Cosmological phase transitions

This chapter aims at providing the necessary background on the theory of cosmological phase transitions and the gravitational wave signatures one can expect from these events. First, the thermodynamics of quantum fields is discussed before reviewing phase transitions in the context of spontaneous symmetry breaking of scalar fields. We study the nucleation of bubbles and how the energy released in a first-order phase transition can be converted into gravitational waves and lastly review the spectra of the GW backgrounds produced.

3.1. Thermal field theory

This section will lay the groundwork to understand phase transitions in the early universe. We review the necessary thermodynamic concepts and introduce the mechanism of spontaneous symmetry breaking that will be responsible for phase transitions in the early universe. For the introduction to the thermodynamics of quantum fields, we follow the statistical field theoretical treatment as can be found in the textbooks [104, 105].

3.1.1. Basic thermodynamics of fields

The early universe was comprised of a hot and dense plasma where the elementary particles frequently interacted and maintained kinetic equilibrium. The most natural description for such a thermodynamic system is the *grand canonical* ensemble, which describes a system that can exchange particles as well as energy with a reservoir. The average energy of the particles is fixed by the temperature T and the average particle number by the chemical potential μ .

In the notation of quantum mechanics, such a thermal bath is denoted by a state $|\rho\rangle$ that can be expressed through the Hamiltonian $\hat{H}$ and the number operator $\hat{N}_i$ for each particle species of the system, together with the inverse temperature β and the chemical potentials μ_i . From this, the density matrix describing the state of the system is defined as

$$\hat{\rho} = |\rho\rangle \langle \rho| = e^{-\beta(\hat{H} - \mu_i \hat{N}_i)} \quad \text{with} \quad \beta = \frac{1}{T}, \quad (3.1)$$

where repeated indices are summed over. Using the density matrix, the ensemble average – or expectation value – of an operator $\mathcal{O}$ can be calculated as

$$\langle \mathcal{O} \rangle_{\text{T}} = \frac{\langle \rho | \mathcal{O} | \rho \rangle}{\langle \rho | \rho \rangle} = \frac{\text{tr } \mathcal{O} e^{-\beta(\hat{H} - \mu_i \hat{N}_i)}}{\text{tr } e^{-\beta(\hat{H} - \mu_i \hat{N}_i)}} = \frac{1}{Z} \text{tr } \mathcal{O} e^{-\beta(\hat{H} - \mu_i \hat{N}_i)}. \quad (3.2)$$

It turns out that the normalisation factor $Z = \text{tr} e^{-\beta(\hat{H} - \mu_i \hat{N}_i)}$ plays the role of one of the most important quantities in statistical mechanics. This object is called the grand canonical partition function

$$Z(T, \mu_1, \dots, \mu_n) = \text{Tr} \hat{\rho} = \text{Tr} e^{-\beta(\hat{H} - \mu_i \hat{N}_i)}. \quad (3.3)$$

Once computed, we can derive all the usual thermodynamic quantities from it. Pressure, particle number, entropy and energy are obtained as follows:

$$P = \frac{\partial(T \ln Z)}{\partial V} \quad (3.4)$$

$$N_i = \frac{\partial(T \ln Z)}{\partial \mu_i} \quad (3.5)$$

$$S = \frac{\partial(T \ln Z)}{\partial T} \quad (3.6)$$

$$E = -PV + TS + \mu_i N_i \quad (3.7)$$

In this thesis the chemical potential μ_i will play no role, and we therefore neglect it in the following discussion.

This temperature-dependent background state has some profound implications for the dynamics of quantum fields that represent the particle states. One of those is the Kubo-Martin-Schwinger relation [106]. The propagator (or thermal Green's function) for bosons is defined as

$$G_b(x, y, \tau_1, \tau_2) \equiv \langle T_\tau [\phi_x(\tau) \phi_y(0)] \rangle_T = Z^{-1} \text{tr} \left(T_\tau [\phi_x(\tau_1) \phi_y(\tau_2)] e^{-\beta \hat{H}} \right), \quad (3.8)$$

with the imaginary time ordering operator T_τ

$$T_\tau [\phi_x(\tau_1) \phi_y(\tau_2)] = \phi_x(\tau_1) \phi_y(\tau_2) \theta(\tau_1 - \tau_2) + \phi_y(\tau_2) \phi_x(\tau_1) \theta(\tau_2 - \tau_1). \quad (3.9)$$

Here, the only difference to zero temperature quantum field theory (QFT) is that we expressed the fields in terms of the imaginary time $\tau = it$. This allows to view the density matrix as the analog of the real-time Heisenberg evolution operator of the fields $\phi_x(\beta) = e^{\beta \hat{H}} \phi_x(0) e^{-\beta \hat{H}}$, where the inverse temperature takes the role of (imaginary) time. With this and the fact that T_τ commutes with $\hat{\rho}$, we can write the propagator as

$$G_b(x, y, \tau, 0) = Z^{-1} \text{tr} \left(T_\tau [\phi_x(\tau) \phi_y(0) e^{-\beta \hat{H}}] \right) \quad (3.10)$$

$$= Z^{-1} \text{tr} \left(T_\tau [e^{-\beta \hat{H}} e^{\beta \hat{H}} \phi_y(0) e^{-\beta \hat{H}} \phi_x(\tau)] \right) \quad (3.11)$$

$$= Z^{-1} \text{tr} \left(T_\tau [e^{-\beta \hat{H}} \phi_y(\beta) \phi_x(\tau)] \right) \quad (3.12)$$

$$= G_b(x, y, \tau, \beta). \quad (3.13)$$

Therefore, our fields satisfy $\phi_x(\tau) = \phi_x(\tau + \beta)$, i.e. they are periodic in time. The analogous relationship for fermions follows from the fermionic imaginary time-ordering operator

$$T_\tau [\psi_x(\tau_1) \psi_y(\tau_2)] = \psi_x(\tau_1) \psi_y(\tau_2) \theta(\tau_1 - \tau_2) - \psi_y(\tau_2) \psi_x(\tau_1) \theta(\tau_2 - \tau_1) \quad (3.14)$$

which gives an antiperiodic behaviour $\psi_x(\tau) = -\psi_x(\tau + \beta)$. This implies that we can decompose both bosonic and fermionic fields into a Fourier series

$$\chi(x, \tau)_T = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \tilde{\chi}(x) e^{i\omega_n \tau} \quad \text{with} \quad \omega_n = \begin{cases} 2n\pi/\beta & \text{bosons,} \\ (2n+1)\pi/\beta & \text{fermions.} \end{cases} \quad (3.15)$$

where ω_n denotes the so-called Matsubara frequencies. Note that the factor $1/\beta = \Delta\omega/(2\pi)$ is introduced such that we recover the usual continuum result in the limit of zero temperature

$$\frac{1}{\beta} \sum_n = \frac{1}{2\pi} \sum \Delta\omega \xrightarrow{\beta \rightarrow \infty} \int \frac{d\omega}{2\pi}. \quad (3.16)$$

We can understand this periodicity of the fields as follows: After the (imaginary) time β , the thermodynamic system returns to its original state.

3.1.2. Computing the partition function for quantum fields

In order to determine the thermodynamic properties of the early universe plasma, we have to compute the partition function. Previously, we wrote the partition function Z as a function of the Hamiltonian of the system. If we want to translate this to the language of quantum field theory employed in particle physics, it is more convenient to express it in terms of the Lagrange density $\mathcal{L}$ and the path integral formalism. Starting with the case of a simple scalar field, we can write out the trace operator using the eigenstates of the field operator $|\phi_a\rangle$

$$Z = \text{Tr} e^{-\beta \hat{H}} = \sum_a \int d\phi_a \langle \phi_a | e^{-\beta \hat{H}} | \phi_a \rangle. \quad (3.17)$$

Computing this will reveal some insights into the properties of the fields at finite temperature. First we recall the conjugate momentum operator $\hat{\pi}$, and the completeness condition and the overlap of quantum fields

$$\hat{\pi} |\pi\rangle = \pi(x) |\pi\rangle, \quad \int \frac{d\pi}{2\pi} |\pi\rangle \langle \pi| = 1, \quad \langle \phi | \pi \rangle = e^{i \int d^3x \pi(x) \phi(x)}. \quad (3.18)$$

Next, we can inspect the transition amplitude of the state $|\phi_a\rangle$ returning to itself $|\phi_a\rangle$ after some time t_f , similar to the expression appearing in the partition function. To evaluate it, we split it into N intervals between $[0, t_f]$ and approximate the Hamiltonian to be constant in these intervals

$$\begin{aligned} \langle \phi_a | e^{-iHt_f} | \phi_a \rangle &= \lim_{N \rightarrow \infty} \int d\phi_a \left(\prod_{i=1}^N \frac{d\pi_i}{2\pi} d\phi_i \right) \\ &\quad \times \langle \phi_a | \pi_N \rangle \langle \pi_N | e^{-iH_N \Delta t} | \phi_N \rangle \langle \phi_N | \pi_{N-1} \rangle \dots \\ &\quad \times \langle \phi_2 | \pi_1 \rangle \langle \pi_1 | e^{-iH_1 \Delta t} | \phi_1 \rangle \langle \phi_1 | \phi_a \rangle. \end{aligned} \quad (3.19)$$

Now we evaluate the Hamilton operator acting on the field states

$$\langle \pi_i | e^{-iH_i \Delta t} | \phi_i \rangle = \langle \pi_i | \phi_i \rangle e^{-iH(\pi_i, \phi_i) \Delta t}, \quad (3.20)$$

and obtain with the orthogonality relation $\langle \phi_i | \phi_j \rangle = \delta(\phi_i - \phi_j)$

$$\langle \phi_a | e^{-iHt_f} | \phi_a \rangle = \lim_{N \rightarrow \infty} \int \left(\prod_{i=1}^N \frac{d\pi_i}{2\pi} d\phi_i \right) \delta(\phi_a - \phi_1) \quad (3.21)$$

$$\times \exp \left(-i \Delta t \sum_{j=1}^{\infty} \int d^3x [\mathcal{H}(\pi_j, \phi_j) - \pi_j(\phi_{j+1} - \phi_j)/\Delta t] \right) \quad (3.22)$$

$$= \int D\pi_a \int_{\phi(x,0)}^{\phi(x,t_f)} D\phi_a \exp \left(i \int_0^t dt \int d^3x [\pi \partial_t \phi - \mathcal{H}(\pi, \phi)] \right) \quad (3.23)$$

The integration over the conjugate of the fields π gives the Legendre transformation of the Hamilton density, i.e. we end up with the Lagrange density $\mathcal{L}$

$$\langle \phi_a | e^{-i\hat{H}t_f} | \phi_a \rangle = \int_{\phi(x,0)}^{\phi(x,t_f)} D\phi_a \exp \left(i \int_0^t dt \int d^3x \mathcal{L}[\phi, \partial_\mu \phi] \right), \quad (3.24)$$

The last step is to connect this back to the partition function eq. (3.17). Here, we have to perform the trace (integral) over all the field eigenstates $D\phi = \prod_a D\phi_a$ and replace the time variable with an imaginary time $\tau = it$, also known as a *Wick rotation*:

$$Z = \int_{\text{periodic}} D\phi \exp \left(\int_0^\beta d\tau \int d^3x \mathcal{L}_E[\phi, \partial_\mu \phi] \right) \quad (3.25)$$

The periodicity restriction means that the fields obey $\phi(x, 0) = \phi(x, \beta)$ and the subscript denotes a Euclidean signature of the metric, which comes from the imaginary time. This reminds very closely of the path integral known from standard QFT. Indeed if we approach the zero temperature limit $\beta \rightarrow \infty$ and go back to real time, we recover exactly the *generating functional* without a source term.

Now let us turn to the task of computing this partition function at finite temperature for the simplest case of a non-interacting neutral scalar field with the Lagrangian

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{m^2}{2} \phi^2. \quad (3.26)$$

The Euclidean action expressed in imaginary time is then

$$S_E = \frac{1}{2} \int_0^\beta d\tau \int d^3x \left[\left(\frac{\partial \phi}{\partial \tau} \right)^2 + (\nabla \phi)^2 + m^2 \phi^2 \right], \quad (3.27)$$

and the partition function becomes after integrating by parts

$$Z = \int D\phi e^{-S_E} = \int D\phi \exp \left(-\frac{1}{2} \int_0^\beta d\tau \int d^3x \phi \left[-\frac{\partial^2}{\partial \tau^2} - \nabla^2 + m^2 \right] \phi \right). \quad (3.28)$$

Before performing the path integral, it is useful to go into the finite limit in the spatial coordinates for the moment and to write the fields as the Fourier series

$$\phi(x, \tau) = T \sum_{n=-\infty}^{\infty} \frac{1}{V} \sum_{\vec{p}} e^{i(\vec{p} \cdot \vec{x} + \omega_n \tau)} \phi_n(p). \quad (3.29)$$

where $1/V = 1/(L_x L_y L_z)$ is the volume that is understood to be taken to infinity $L_i \rightarrow \infty$. Substituting the Fourier series in eq. (3.28), and performing the spatial and time integrals we have

$$Z = \int D\phi_n(p) \left| \det \left(\frac{\delta \phi_x(\tau)}{\delta \phi_n(p)} \right) \right| \exp \left(-\frac{1}{2} T \sum_{n=-\infty}^{\infty} \frac{1}{V} \sum_{\vec{p}} (\omega_n^2 + p^2 + m^2) |\phi_n(p)|^2 \right). \quad (3.30)$$

Here, the switch of the integration measure to the Fourier amplitudes introduces the Jacobian determinant. This expression is now only quadratic in the field modes, and hence can be integrated using the standard Gaussian integral, giving the expression

$$Z = N \prod_n \prod_{\vec{p}} (\omega_n^2 + p^2 + m^2)^{-1/2}. \quad (3.31)$$

Here we absorbed all the prefactors, including the determinant, into a normalisation constant N . For a more detailed treatment, see e.g. [104]. After taking the logarithm of the previous expression, we obtain

$$\ln Z = -V \frac{1}{2} \sum_n \int \frac{d^3 p}{(2\pi)^3} \ln (\omega_n^2 + p^2 + m^2) . \quad (3.32)$$

In order to evaluate the sum over the Matsubara frequencies, we use the standard identities

$$\ln [(2\pi n)^2 + \beta^2 \omega^2] = \int_1^{\beta^2 \omega^2} \frac{d\theta^2}{\theta^2 + (2\pi n)^2} + \ln (1 + (2\pi n)^2) , \quad (3.33)$$

$$\sum_{n=-\infty}^{\infty} \frac{1}{n^2 + (\theta/2\pi)^2} = \frac{2\pi^2}{\theta} \left(1 + \frac{2}{e^\theta - 1} \right) , \quad (3.34)$$

and finally obtain

$$\ln Z = -V \int \frac{d^3 p}{(2\pi)^3} \left(\frac{1}{2} \beta \omega + \ln (1 - e^{-\beta \omega}) \right) , \quad (3.35)$$

with $\omega = \sqrt{p^2 + m^2}$. From this, we can now obtain the free energy density (or pressure) for our single bosonic degree of freedom

$$f = -\frac{T \ln Z}{V} = \int \frac{d^3 p}{(2\pi)^3} \left(\frac{1}{2} \omega + T \ln (1 - e^{-\beta \omega}) \right) . \quad (3.36)$$

The first term is the zero point energy, while the second describes the temperature dependent term. Now let us compute another familiar quantity, e.g. the energy density

$$e = f - T \frac{\partial f}{\partial T} = \int \frac{d^3 p}{(2\pi)^3} \left(\frac{\omega}{2} + \frac{\omega}{e^{\omega\beta} - 1} \right) = \int \frac{d^3 p}{(2\pi)^3} \frac{\omega}{e^{\omega\beta} - 1} + e_0 \quad (3.37)$$

the e_0 term is the zero point energy and can be subtracted since only energy differences are physical. Unsurprisingly, what we have recovered is our familiar expression for the energy density of a bosonic gas following the Bose-Einstein distribution function as encountered in sec. 2.3.

Fermions

The calculation for fermions follows analogously, however, we have to take into account the anti-commuting nature of these spin 1/2 particles. The Lagrangian for a Dirac fermion without interactions is

$$\mathcal{L} = \bar{\psi} (i\partial - m) \psi , \quad (3.38)$$

and the partition function becomes

$$Z_\psi = \int D\bar{\psi} D\psi \exp \left(\int_0^\beta d\tau \int d^3 x \bar{\psi} (i\partial - m) \psi \right) . \quad (3.39)$$

The anti-commuting nature of the fermions is here accounted for by the Grassmann numbers $\bar{\psi}$ and ψ . A single Grassmann variable η is defined by the algebra

$$\{\eta, \eta\} = 0 , \quad (3.40)$$

with $\{a, b\} = ab + ba$ and the integration rules

$$\int d\eta = 0, \int d\eta \eta = 1. \quad (3.41)$$

For a detailed treatment of the path integral using Grassmann numbers and their properties, see for example [105, 107]. Here, we only need the result for the Gaussian integral, which for a general operator becomes

$$\int D\bar{\psi} D\psi e^{\int_{\beta} \int_x \bar{\psi} D\psi} = \mathcal{N} \det(D)^{-1} \quad \text{with} \quad D = i\rlap{\not{D}} - m. \quad (3.42)$$

The evaluation of the functional determinant follows from the standard trick $\det[\exp D] = \exp[\text{tr} D]$. This expression is a generalisation of the previous result for the scalar and gives

$$\ln Z_{\psi} = 2 \sum_n \sum_p \ln(\omega_n^2 + p^2 + m^2), \quad (3.43)$$

where we neglected a constant term again. Using analogous identities to eqs. (3.33) and (3.34) for the fermionic Matsubara frequencies, we obtain the result

$$f_{\psi} = \frac{T \ln Z}{V} = -4 \int \frac{d^3 p}{(2\pi)^3} \left(\frac{1}{2} \omega + T \ln(1 + e^{-\omega\beta}) \right). \quad (3.44)$$

The difference compared to the scalar field is apparent. The integral was carried out over field and anti-field which gives, with the two spin states each, the factor 4 in front. Additionally, the opposite sign in the argument of the logarithm ensures the familiar Fermi-Dirac distribution.

Gauge bosons

For massless gauge theories, we have the Lagrangian

$$\mathcal{L} = -\frac{1}{4} A_{\mu\nu} A^{\mu\nu}, \quad (3.45)$$

with the field strength tensor $A_{\mu\nu} = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu}$. Before we simply insert this into the partition function we have to remember that a massless gauge field only has two degrees of freedom, which manifests e.g. in the invariance of eq. (3.45) under a gauge transformation $A_{\mu} \rightarrow A_{\mu} - \partial_{\mu} \alpha(x)$. In order to write the path integral over all components of A_{μ} , we can introduce a gauge fixing term and the gauge fixing condition F

$$\mathcal{L}_{\text{gauge-fix}} = -\frac{1}{2\xi} (\partial_{\mu} A^{\mu})^2 \quad \text{and} \quad F = \partial^{\mu} A_{\mu} - f(x, \tau) = 0, \quad (3.46)$$

which define the class of so-called R_{ξ} gauges. Here, f is an arbitrary function. Using the gauge fixing term, we can write the path integral as [105, 107]

$$Z_A = \int DA_{\mu} \det\left(\frac{\partial F}{\partial \alpha}\right) \exp\left(\int_0^{\beta} d\tau \int d^3 x (\mathcal{L} + \mathcal{L}_{\text{gauge-fix}})\right). \quad (3.47)$$

For our gauge fixing functional F the determinant becomes $\det(-\partial^2)$. Here, we can employ the standard trick to write the determinant of an operator as the integral

$$\det(-\partial^2) = \int D\bar{c} Dc \exp\left(\int_0^{\beta} d\tau \int d^3 x (\partial_{\mu} \bar{c})(\partial^{\mu} c)\right) \quad (3.48)$$

over fictitious complex Grassmann fields with spin 0, called ghost fields (cf. eq. (3.42)). Note that these are not physical fields as they do not appear in the Hamiltonian and also violate

the spin-statistics theorem. They are merely a convenient way to write the determinant. The result is easily obtained in Feynman gauge $\xi = 1$

$$\ln Z_A = \sum_n \sum_p [-2 \ln(\omega_n^2 + p^2) + 4 \ln(\omega_n^2 + p^2)] , \quad (3.49)$$

$$f_A = \frac{T \ln Z_A}{V} = -2 \int \frac{d^3 p}{(2\pi)^3} \left(\frac{1}{2} \beta \omega + \ln(1 - e^{-\beta \omega}) \right) , \quad (3.50)$$

which gives the expected result: the ghosts cancel the time-like and longitudinal degree of freedom of the vector boson, leaving us with the result for two bosonic degrees of freedom, which correspond to the two physical polarisation states of massless gauge bosons.

3.2. Spontaneous symmetry breaking

Next, we inspect the phenomenon of spontaneous symmetry breaking in relativistic field theory, also known as the Higgs mechanism [108–110]. For our purposes, it is enough to consider the simplest case as encountered in the standard textbooks [107, 111]. The theory under consideration is again a neutral scalar field, but this time we include a self-interaction term

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi + \underbrace{\frac{\mu^2}{2} \phi^2 - \frac{\lambda}{4!} \phi^4}_{-V(\Phi)} . \quad (3.51)$$

Evidently, the scalar field exhibits a $\mathbb{Z}_2$ symmetry through the invariance under the transformation $\phi \rightarrow -\phi$. In the case that $\mu^2 \leq 0$, the potential has its minimum at $\Phi = 0$, for $\mu^2 > 0$ the minimum shifts to non-vanishing field values. In the latter case, the minimum takes the value

$$\phi = \pm \sqrt{\frac{6\mu^2}{\lambda}} . \quad (3.52)$$

We can compute the classical limit of the expectation value of the field value ϕ , by taking the limit $\hbar \rightarrow 0$ in the zero temperature case and obtain

$$\langle \Omega | \phi | \Omega \rangle = \lim_{\hbar \rightarrow 0} \int D\phi e^{\frac{i}{\hbar} \int d^4 x \mathcal{L}[\phi]} \phi = \sqrt{\frac{6\mu^2}{\lambda}} \equiv v . \quad (3.53)$$

The limit $\hbar \rightarrow 0$ singles out the minimal value of the action, this is also called the saddle point or steepest descent evaluation. It recovers exactly the value minimising the action, i.e. $\partial_\phi \mathcal{L}[\phi] = 0$, which is called the vacuum expectation value (VEV) of the scalar field and is taken by the field all over space. The propagating excitations that form around this vacuum expectation value (VEV) are what we call particles. This motivates an expansion of the original field into a classical background value v and quantum excitations φ

$$\phi = v + \varphi . \quad (3.54)$$

Inserting this decomposition into the original Lagrangian (3.51), we see that the $\mathbb{Z}_2$ symmetry is no longer obeyed by the new quantum field φ :

$$\mathcal{L} = \frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi - \frac{1}{2} (-\mu^2 + 3\lambda v^2) \varphi^2 - \frac{\lambda v}{3!} \varphi^3 - \frac{\lambda}{4!} \varphi^4 , \quad (3.55)$$

where we dropped constant terms. The original symmetry is still present but realised in a different way. One can convince oneself that this Lagrangian is invariant under $\varphi \rightarrow -\varphi - 2v$. This mechanism is known as spontaneous symmetry breaking (SSB), since the VEV chooses randomly between $\langle \phi \rangle = \pm v$. In this new description, the fields obtained a mass term which depends on the value the VEV takes: $m_\varphi^2(v) = -\mu^2 + \lambda v^2$. This acquiring of a VEV-dependent mass term is a general feature of particles interacting with the symmetry-breaking scalar. For example, the electroweak symmetry-breaking of the Higgs field gives mass to the SM particles.

3.3. Thermodynamics of spontaneous symmetry breaking

Our description of the spontaneous symmetry breaking (SSB) took place in the usual zero temperature vacuum of QFT and in the classical limit. Things however get even more interesting when we combine it with the particle bath the fields create at finite temperature. We turn to the task of computing the partition function with the scalar field expanded around a VEV, so that we can derive the thermodynamic properties from it.

3.3.1. Partition function with spontaneous symmetry breaking

Here, it is illustrative to go beyond the simplest model and now consider an Abelian gauge theory with a spontaneously broken symmetry

$$\mathcal{L} = |D_\mu \Phi|^2 + \mu^2 |\Phi|^2 - \lambda |\Phi|^4 - \frac{1}{4} A_{\mu\nu} A^{\mu\nu}. \quad (3.56)$$

The covariant derivative $D_\mu = \partial_\mu + igA_\mu$ ensures gauge invariance and couples the scalar to the gauge boson. The scalar field now enjoys the invariance under the (local) transformation $\Phi \rightarrow \Phi e^{-ig\alpha(x)}$. We can decompose the complex scalar into the background field value, a real part ϕ and a complex part φ , i.e. a Goldstone boson

$$\Phi = \frac{\phi + \phi_b + i\varphi}{\sqrt{2}}. \quad (3.57)$$

The non-propagating background part is denoted by ϕ_b and has a minimum at $\phi_b = \sqrt{\mu^2/\lambda}$. We chose the minimum to be real and positive as any complex part can be rotated away by the gauge transformation $\Phi \rightarrow \Phi e^{-ig\alpha(x)}$. In order to write the partition function as a path integral over all components of the vector field A_μ we again have to fix the gauge choice to remove unphysical degrees of freedom. Here, a convenient choice is the following gauge fixing term, again in the R_ξ gauge

$$\mathcal{L}_{\text{gauge-fix}} = -\frac{1}{2\xi} (\partial^\mu A'_\mu - \xi g v \varphi)^2. \quad (3.58)$$

This gives the gauge fixing functional $F = \partial_\mu A^\mu - \xi g v \varphi - f(x, \tau) = 0$. In the expanded Lagrangian, we see the reason for this choice. Now the ξ independent term from eq. (3.58) cancels the mixing between the Goldstone φ and the gauge boson, so that $\mathcal{L}_{\text{eff}} = \mathcal{L} + \mathcal{L}_{\text{gauge-fix}}$ becomes

$$\begin{aligned} \mathcal{L}_{\text{eff}} = & \frac{1}{2} \partial_\mu \phi \partial^\mu \phi + \frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi - \frac{m_\phi^2}{2} \phi^2 - \frac{m_\varphi^2}{2} \varphi^2 - \frac{1}{4} F_{\mu\nu}^2 + \frac{m_A^2}{2} A_\mu^2 \\ & - \frac{\xi}{2} m_A^2 \varphi^2 - \frac{1}{2\xi} (\partial_\mu A^\mu)^2 - V_0(\phi_b) \end{aligned} \quad (3.59)$$

$$\text{with} \quad V_0(\phi_b) = \frac{-\mu^2}{2} \phi_b^2 + \frac{\lambda}{4} \phi_b^4. \quad (3.60)$$

Here, we collected quadratic terms in the propagating fields into background field dependent mass terms

$$m_\phi^2 = -\mu^2 + 3\lambda\phi_b^2, \quad m_\varphi^2 = -\mu^2 + \lambda\phi_b^2 \quad \text{and} \quad m_A^2 = g^2\phi_b^2. \quad (3.61)$$

Hence, we can write the partition function as a function of the background field value

$$Z[\phi_b] = \int D\phi D\varphi DA_\mu \det \left(\frac{\delta F}{\delta \alpha} \right) \exp \left(\int_0^\beta d\tau \int d^3x \mathcal{L}_\phi + \mathcal{L}_\varphi + \mathcal{L}_A - V_0(\phi_b) \right). \quad (3.62)$$

The scalar and Goldstone give the usual result, however, note that the Goldstone term is now gauge dependent

$$\ln Z_\phi = \sum_n \sum_p \ln (\omega_n^2 + p^2 + m_\phi^2) , \quad (3.63)$$

$$\ln Z_\varphi = \sum_n \sum_p \ln (\omega_n^2 + p^2 + m_\varphi^2 + \xi m_A^2) . \quad (3.64)$$

As we saw previously, the gauge fixing determinant $\det(-\partial^2 - \xi m_A^2)$ can be written as a contribution from ghost fields, which is now also gauge dependent

$$\ln Z_c = -2 \sum_n \sum_p \ln (\omega_n^2 + p^2 + \xi m_A^2) . \quad (3.65)$$

Lastly, the gauge field term in the partition function is given by

$$\int DA_\mu \exp \left(-\frac{1}{2} \int_0^\beta d\tau \int d^3x A_\mu \underbrace{(-\delta^{\mu\nu} \square - (1 - 1/\xi) \partial^\mu \partial^\nu + \delta^{\mu\nu} m_A^2)}_{O^{\mu\nu}} A_\nu \right) . \quad (3.66)$$

In Fourier-space we can split the operator $O^{\mu\nu}$ acting on the gauge field into two components

$$O_{\mu\nu} = (k^2 + m_A^2) \Pi_{\mu\nu}^T + \frac{1}{\xi} (k^2 + \xi m_A^2) \Pi_{\mu\nu}^L , \quad (3.67)$$

with the transverse and longitudinal projection operators

$$\Pi_{\mu\nu}^T = \delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \quad \text{and} \quad \Pi_{\mu\nu}^L = \frac{k_\mu k_\nu}{k^2} . \quad (3.68)$$

These have the properties $\text{tr} \Pi_{\mu\nu}^T = 3$ and $\text{tr} \Pi_{\mu\nu}^L = 1$ and therefore the contribution to the partition function is

$$\ln Z_A = \sum_n \sum_p [3 \ln (\omega_n^2 + p^2 + m_A^2) + \ln (\omega_n^2 + p^2 + \xi m_A^2)] . \quad (3.69)$$

Now we fix the gauge to the Landau gauge $\xi = 0$ and observe that the one ghost degree of freedom in eq. (3.65) cancels the longitudinal gauge boson contribution. The remaining one gives an additional massless contribution which cancels the gauge boson contribution in the symmetric phase and the (massless) Goldstone contribution in the broken phase. This is also known as the Goldstone boson theorem: the degree of freedom of the Goldstone boson is “eaten” by the gauge boson which now has an additional longitudinal degree of freedom.

The last term contributing to the partition function is the space- and time-independent potential of the background field

$$\ln Z_{\phi_b} = V \beta V_0(\phi_b) . \quad (3.70)$$

Zero energy shift

So far, we have studied the behaviour of the thermodynamic system by inspecting the thermal effects of the plasma on the minimum of the free energy, but we neglected zero-temperature effects, i.e. the shift in the zero point energy. However, if we want an accurate description of the dynamics of the system, we cannot neglect them. Therefore, we turn to the task to

determine the shift of the vacuum. The free energy receives a contribution from each particle species of the form

$$f_0(m) = \int \frac{d^3p}{(2\pi)^3} \frac{\omega}{2} = \int \frac{d^3p}{(2\pi)^3} \frac{\sqrt{p^2 + m^2}}{2}. \quad (3.71)$$

This integral is formally UV-divergent. In order to evaluate this, we use the technique of dimensional regularisation from QFT and make use of the result for general integrals [104]

$$I = \int \frac{d^d p}{(2\pi)^d} \frac{1}{(p^2 + m^2)^A} = \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(A - d/2)}{\Gamma(A)} \frac{1}{(m^2)^{A-d/2}}, \quad (3.72)$$

where d is the number of dimensions, and Γ denotes the Gamma function with $\Gamma(z) = \int_0^\infty dt t^{z-1} e^{-t}$ which for positive integer arguments satisfies $\Gamma(n) = (n-1)!$. Setting $A = -1/2$ and $d = 3 - 2\epsilon$, isolates the divergence into a $1/\epsilon$ pole [104]

$$f_0(m) = -\frac{m^4 \mu^{-2\epsilon}}{64\pi^2} \left(\frac{1}{\epsilon} + \ln \frac{\mu^2}{m^2} + \frac{3}{2} + \ln 4\pi - \gamma_E + \mathcal{O}(\epsilon) \right), \quad (3.73)$$

where μ is an arbitrary renormalisation scale parameter. We can cure this divergence by splitting the bare parameters of the Lagrangian into renormalised parameters and counterterms

$$\mathcal{L} \supset = \mu^2 \phi^2 - \lambda \phi^4 = (\mu_R^2 + \delta\mu^2) \phi^2 - (\lambda_R + \delta\lambda) \phi^4, \quad (3.74)$$

where the latter subtract the divergences and give a finite result in total. This gives the standard result, known as the Coleman-Weinberg potential [112]

$$f_{\text{CW}}(m) = \sum_i \pm \frac{n_i m_i^4(\phi_b)}{64\pi^2} \left(\ln \frac{m_i^2(\phi_b)}{\bar{\mu}^2} - C_i \right). \quad (3.75)$$

Here the positive (negative) sign is for bosons (fermions) and the renormalisation constant C_i is $3/2$ for scalars and fermions and $5/6$ for gauge bosons. The values of the counterterms are found by imposing renormalisation conditions at the energy scale $\bar{\mu}$. Typically, these are chosen such that the contribution from the counterterms

$$f_{\text{ct}} = V_{\text{ct}}(\phi_b) = -\frac{\delta\mu^2}{2} \phi_b^2 + \frac{\delta\lambda}{4} \phi_b^4 \quad (3.76)$$

do not shift the position of the VEV and the mass of the scalar does not change compared to their tree level values, i.e.

$$\partial_\phi (f_{\text{CW}} + f_{\text{ct}}) |_{\phi=v} = 0, \quad (3.77)$$

$$\partial_\phi^2 (f_{\text{CW}} + f_{\text{ct}}) |_{\phi=v} = 0. \quad (3.78)$$

Symmetry restoration and breaking

We now have the ingredients to determine the equilibrium state of the system, which is given by the minimum of the free energy [113]. At zero temperature, this minimum is given by the potential of the background field with the corrections from the particles that obtain mass from it

$$f_{T=0}(\phi_b) = V_0(\phi_b) + f_{\text{ct}}(\phi_b) + f_{\text{CW}}(\phi_b) \quad (3.79)$$

with the minimum unchanged at $\langle \phi_b \rangle = v$. The finite temperature contribution can be written in terms of the thermal functions for bosons (b) and fermions (f)

$$J_{b/f} \left(\frac{m^2}{T^2} \right) = \int_0^\infty dx x^2 \ln \left(1 \mp e^{-\sqrt{x^2 + m^2/T^2}} \right), \quad (3.80)$$

with which we can express the finite temperature contribution to the free energy as

$$f_T(\phi_b, T) = \frac{T^4}{2\pi^2} \left(J_b \left(\frac{m_\phi^2}{T^2} \right) + J_b \left(\frac{m_\varphi^2 + \xi m_A^2}{T^2} \right) + 3J_b \left(\frac{m_A^2}{T^2} \right) - J_b \left(\frac{\xi m_A^2}{T^2} \right) \right) \quad (3.81)$$

We can inspect the effect of the finite temperature on the minimum of the free energy in the high temperature limit $z = m^2/T^2 \ll 1$. Here, the thermal functions can be approximated as

$$J_b(z) \stackrel{z \ll 1}{\approx} -\frac{\pi^4}{45} + \frac{\pi^2}{12}z - \frac{\pi}{6}z^{3/2} - \frac{z^2}{32}(\ln(z) - L_b), \quad (3.82)$$

$$J_f(z) \stackrel{z \ll 1}{\approx} -\frac{7\pi^4}{360} + \frac{\pi^2}{24}z + \frac{z^2}{32}(\ln(z) - L_f), \quad (3.83)$$

with

$$L_f = \frac{3}{2} + 2\ln(\pi) - 2\gamma_E \quad \text{and} \quad L_b = L_f + 2\ln(4). \quad (3.84)$$

The leading order field dependent contributions therefore have the form

$$f_T \stackrel{T \gg m}{\approx} \frac{m^2(\phi_b)T^2}{24} - \frac{m^3(\phi_b)T}{12\pi} \quad (\text{bosons}), \quad (3.85)$$

$$f_T \stackrel{T \gg m}{\approx} \frac{m^2(\phi_b)T^2}{48} \quad (\text{fermions}). \quad (3.86)$$

It is clear that for temperatures larger than the energy scale of the theory v , the terms quadratic in T dominate over $V_0 \supset -\mu^2\phi_b^2/2$ and give the free energy a parabolic shape. This shifts the minimum, and hence the expectation value of the scalar to a vanishing value $\langle \phi_b \rangle_{T \gg v} = 0$, which is known as symmetry restoration. Decreasing the temperature leads then to the dynamic breaking of the symmetry and will be the cause of phase transitions in the early universe.

3.3.2. A note on the connection to zero temperature QFT

In the previous section, we looked at the minimum of the free energy density, the VEV, from the point of view of statistical field theory. The more common perspective is the one from zero-temperature QFT through the means of the so-called *effective action* $\Gamma[\phi_b]$. It can be defined as

$$e^{i\Gamma[\phi_b]} = \int_{\text{restr.}} D\varphi \exp \left(i \int d^4x \mathcal{L}[\varphi + \phi_b] \right). \quad (3.87)$$

This effective action describes only the behaviour of the background field, while the quantum effects of the propagating fields are accounted for by integrating them out. The restriction of the integral comes from the requirement to keep the decomposition into background and propagating field intact, i.e. shifts of the field $\varphi \rightarrow \varphi + \phi_b$ are excluded. We clearly see the similarities to the partition function, only the time integral is Wick rotated and bounded by β . The effective action of the background field has the convenient property that the VEV of the theory, including quantum corrections, is directly given by $\partial_{\phi_b} \Gamma[\phi_b] = 0$. This makes it very convenient to study the vacuum structure of a theory.

The evaluation of the effective action follows along similar lines as the partition function. We again consider the Lagrangian of the simple scalar model eq. (3.51) and split it into a kinetic and potential term $V(\varphi + \phi_b)$. Upon inserting it into the effective action and expanding around the background field, eq. (3.87) becomes

$$e^{i\Gamma[\phi_b]} = e^{i\int_x -\frac{1}{2}\phi_b\Box\phi_b - V(\phi_b)} \int D\varphi e^{i\int_x -\frac{1}{2}\varphi\Box\varphi - \frac{1}{2}\varphi^2 V''(\phi_b) - \frac{1}{3!}\varphi^3 V'''(\phi_b) + \dots} \quad (3.88)$$

$$\approx e^{i\int_x -V(\phi_b)} \int D\varphi e^{i\int_x -\frac{1}{2}\varphi\Box\varphi - \frac{1}{2}\varphi^2 V''(\phi_b)} \quad (3.89)$$

$$= \text{const} \times e^{i\int_x -V(\phi_b)} \frac{1}{\sqrt{\det(\Box + V''(\phi_b))}}, \quad (3.90)$$

with the short hand notation $\int_x = \int d^4x$. The tadpole contribution has been dropped since the effective action is composed of connected diagrams only. Here, we restricted the evaluation to the terms quadratic in the propagating fields. Taking the logarithm of both sides allows to evaluate the functional determinant and we obtain

$$\begin{aligned} i\Gamma[\phi_b] &= -i \int d^4x \left[V(\phi_b) + \frac{1}{2} \int \frac{d^4k_E}{(2\pi)^4} \ln(k_E^2 + m^2(\phi_b)) \right], \\ &\equiv -i \int d^4x [V_0(\phi_b) + V_{1\text{-loop}}(\phi_b)], \end{aligned} \quad (3.91)$$

where we dropped a constant term since it does not affect the minimum of $\Gamma[\phi_b]$ and renamed the second term to $V_{1\text{-loop}}$. We can see, that in order to minimise $\Gamma[\phi_b]$, it is sufficient to minimise the *effective potential*, which we approximated here as the tree-level term V_0 and the next-to-leading-order (1-loop) radiative corrections $V_{1\text{-loop}}$.

We can connect this back to the zero-energy shift of the free energy by using the identity $\int dk_0 1/(k_0^2 + \omega^2) = \omega/2$:

$$V_{1\text{-loop}}(\phi_b) = \frac{1}{2} \int \frac{d^4k_E}{(2\pi)^4} \ln(k_E^2 + m^2(\phi_b)) \quad (3.92)$$

$$= \frac{1}{2} \int dm^2 \int \frac{d^4k_E}{(2\pi)^4} \frac{1}{k_0^2 + k^2 + m^2(\phi_b)} \quad (3.93)$$

$$= \frac{1}{4} \int dm^2 \int \frac{d^3k}{(2\pi)} \frac{1}{\sqrt{k^2 + m^2(\phi_b)}} \quad (3.94)$$

$$= \int \frac{d^3k}{(2\pi)} \frac{\omega}{2}. \quad (3.95)$$

This expression is exactly the temperature independent shift of the free energy density we encountered in the previous section, which gave the Coleman-Weinberg potential

$$V_{\text{CW}} = \sum_a \pm n_a \frac{m_a^4(\phi_b)}{64\pi^2} \left[\ln \frac{m_a^2(\phi_b)}{\bar{\mu}^2} - C_a \right]. \quad (3.96)$$

To interpret this result, it is useful to consider an equivalent way to calculate the effective potential. It consists of summing up the 1-loop diagrams of the propagating fields with n external ϕ_b legs. To see this, we take a closer look at $V_{1\text{-loop}}$:

$$V_{1\text{-loop}}(\phi_b) = \frac{1}{2} \int \frac{d^4 k_E}{(2\pi)^4} \ln(k_E^2 - \mu^2 + \lambda\phi_b^2/2) \quad (3.97)$$

$$= \frac{1}{2} \int \frac{d^4 k_E}{(2\pi)^4} \ln\left(1 + \frac{\lambda\phi_b^2/2}{k_E^2 - \mu^2}\right) \quad (3.98)$$

$$= -\frac{i}{2} \int \frac{d^4 k}{(2\pi)^4} \ln\left(1 - \frac{\lambda\phi_b^2/2}{k^2 + \mu^2 + i\varepsilon}\right) \quad (3.99)$$

$$= i \sum_{n=1}^{\infty} \int \frac{d^4 k}{(2\pi)^4} \frac{1}{2n} \left[\frac{\lambda\phi_b^2/2}{k^2 + \mu^2 + i\varepsilon} \right]^n \quad (3.100)$$

$$= \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \dots \quad (3.101)$$

Here, we neglected all ϕ_b independent terms and used an inverse Wick rotation from the second to third line. We can see that the fourth line represents the sum of 1-loop integrals with $2n$ legs of the background field with zero momentum, connected to the propagating field φ . For n vertices, the diagrams contain n propagators $i(k^2 + \mu^2 - i\varepsilon)^{-1}$ and require a symmetry factor of $1/(2n)$, which is consistent with the Feynman rules one obtains from the Lagrangian (3.55). The Coleman-Weinberg term therefore encodes changes in the free energy due to virtual fluctuations around the background field value at zero temperature.

The switch back to finite temperature boils down to a simple replacement rule. Any integral over the four momentum of a function containing fields is replaced by a sum over the Matsubara frequencies

$$\int \frac{d^4 k_E}{(2\pi)^4} f(k_E) \rightarrow T \sum_n \int \frac{d^3 k}{(2\pi)^3} f(\omega_n, k) = \oint \frac{d^3 k}{(2\pi)^3} f(\omega_n, k). \quad (3.102)$$

With this replacement rule, we, for example, regain the thermal contributions as

$$V_{1\text{-loop}}(\phi_b) \rightarrow \frac{1}{2} \oint \frac{d^3 k}{(2\pi)^3} \ln(\omega_n^2 + k^2 + m^2) \quad (3.103)$$

$$= \frac{1}{2} \oint \frac{d^3 k}{(2\pi)^3} \int dm^2 \frac{1}{\omega_n^2 + k^2 + m^2} \quad (3.104)$$

$$= \int \frac{d^3 k}{(2\pi)^3} \left(\frac{\omega}{2} + T \ln(1 \pm e^{-\beta\omega}) \right). \quad (3.105)$$

Hence, we can identify the finite temperature effective potential with the free energy $V_{\text{eff}}(\phi_b, T) = f(\phi_b, T)$.

3.3.3. Resummation

So far, we have also neglected the interactions between the particles in the computation of the free energy. This is a good approximation of the true result if we can perturbatively expand the partition function – usually in the couplings. However, at finite temperature we have two energy scales, the mass (or the VEV) and the average kinetic energy of the particles, the temperature. We will see that this leads to a breakdown of perturbativity and requires to re-organise the perturbation expansion, i.e. resum diagrams.

Let us inspect the following contribution to the self-energy of a spin-0 particle coming from a $\lambda\phi^4$ term in the high-temperature limit $T \gg m$:

$$\begin{aligned} \Pi(T, m) &= \text{diagram} = \frac{\lambda}{2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\omega_n^2 + k^2 + m^2} \\ &= \frac{\lambda}{2} \int \frac{d^3k}{(2\pi)^4} \left(\frac{1}{2\omega} + \frac{1}{\omega} \frac{1}{e^{\beta\omega} - 1} \right) = \frac{\lambda}{2} \left(\frac{T^2}{12} - \frac{mT}{4\pi} + \mathcal{O}\left(\frac{m}{T}\right) \right), \end{aligned} \quad (3.106)$$

where the first term is UV-divergent and will be cancelled by the counterterms introduced in the previous section. The second term gives a finite result, which to leading order is $\Pi(T) \propto \lambda T^2$, called the *hard thermal mass*. Adding n loops on top of the main loop gives in the high temperature limit

$$\begin{aligned} \Pi^{(n)} &= \text{diagram} = T \int \frac{1}{(\omega_n^2 + k^2 + m^2)^{n-1}} \times \left[\lambda \int \frac{1}{\omega_n^2 + k^2 + m^2} \right]^n \\ &\sim \frac{\lambda T^3}{m} \left(\frac{\lambda T^2}{m^2} \right)^{n-2}. \end{aligned} \quad (3.107)$$

For zero temperature perturbation theory, we usually assume that the coupling $\lambda < 1$, but here we get a temperature enhancement. Therefore, we additionally have to require $\lambda T^2/m^2 < 1$, such that higher orders do not give larger contributions. However, around the phase transition we often have $T \sim m$ and our organisation of the perturbative expansion does not work anymore. To treat this, we have to incorporate these thermal enhancements into our calculation. This is done by resumming the propagator with any number of hard loops, which can be pictured diagrammatically as

$$\text{diagram} = \text{diagram} + \text{diagram} + \text{diagram} + \dots \quad (3.108)$$

In terms of the propagator, these diagrams translate into the series

$$\frac{1}{p^2 - m^2} + \frac{\Pi(T)}{(p^2 - m^2)^2} + \frac{\Pi^2(T)}{(p^2 - m^2)^3} + \dots = \frac{1}{p^2 - m^2 - \Pi(T)}, \quad (3.109)$$

which follows by virtue of the geometric series. Therefore, the resummation boils down to the simple replacement rule

$$m^2(\phi) \rightarrow m^2(\phi) + \Pi(T). \quad (3.110)$$

This *dressing* of the propagator restores the perturbative expansion. Note that the fermion propagators do not need to be resummed. This can be seen by inspecting the second term in the self-energy eq. (3.106) from a different perspective. At high temperatures, the infrared modes of bosonic degrees of freedom become highly occupied. This enhances the effective loop expansion parameter for modes with energies smaller than the temperature $E \ll T$ [114]:

$$\lambda \rightarrow \lambda n_b = \frac{\lambda}{e^{E/T} - 1} \stackrel{E \ll T}{\approx} \frac{\lambda T}{E}. \quad (3.111)$$

The culprit here is the Matsubara zero mode, which has $\omega_0 = 0$. All the other modes come with $\omega_n = 2\pi T n$, preventing the IR-enhancement. Since fermions come with frequencies

$\omega_n = (2n+1)\pi T$ there is no IR-divergence in the high temperature limit, or equivalently, the effective coupling does not receive a temperature enhancement

$$y_f \rightarrow y_f n_f = \frac{\lambda}{e^{E/T} + 1} \stackrel{E \ll T}{\approx} y_f. \quad (3.112)$$

Hence, fermions do not require resummation and can be treated perturbatively instead.

A popular method for resummation was developed by Arnold and Espinosa [115], where only the mass of the problematic zero-Matsubara mode is replaced with $m^2 \rightarrow m^2 + \Pi(T)$

$$V_T^{1\text{-loop}}(\phi_b, T) = \frac{1}{2} \sum_{n \neq 0} \frac{d^3 k}{(2\pi)^3} \ln(\omega_n + k^2 + m^2) + \frac{T}{2} \int \frac{d^3 k}{(2\pi)^3} \ln(k^2 + m^2 + \Pi(T)). \quad (3.113)$$

Adding back a zero to restore the sum over the full Matsubara frequencies, we obtain

$$V_T^{1\text{-loop}}(\phi_b, T) = \frac{1}{2} \sum_{n \neq 0} \frac{d^3 k}{(2\pi)^3} \ln(\omega_n + k^2 + m^2) \quad (3.114)$$

$$+ \frac{T}{2} \int \frac{d^3 k}{(2\pi)^3} \{ \ln(k^2 + m^2 + \Pi(T)) - \ln(k^2 + m^2) \}. \quad (3.115)$$

The first term gives the usual Coleman-Weinberg term plus thermal functions. The second term can be evaluated by differentiating and integrating w.r.t. the masses:

$$\frac{T}{2} \int \frac{d^3 k}{(2\pi)^3} \{ \ln(k^2 + m^2 + \Pi(T)) - \ln(k^2 + m^2) \} \quad (3.116)$$

$$= 4\pi \frac{T}{2} \int_0^\infty \frac{dk}{(2\pi)^3} k^2 \int dm^2 \left\{ \frac{1}{k^2 + m^2 + \Pi(T)} - \frac{1}{k^2 + m^2} \right\}. \quad (3.117)$$

Using $k^2/(k^2 + x) = 1 - x/(k^2 + x)$ and $\int_0^\infty dk x/(k^2 + x) = \pi\sqrt{x}/2$, this becomes

$$V_{\text{daisy}} = 4\pi \frac{T}{2} \int_0^\infty \frac{dk}{(2\pi)^3} k^2 \int dm^2 \left\{ \frac{1}{k^2 + m^2 + \Pi(T)} - \frac{1}{k^2 + m^2} \right\} \quad (3.118)$$

$$= -\frac{T}{12\pi} \left[(m^2 + \Pi(T))^{3/2} - m^3 \right]. \quad (3.119)$$

Another approach by Parwani [116], dresses all Matsubara modes

$$V_{1\text{-loop}}(m^2) \rightarrow V_{1\text{-loop}}(m^2 + \Pi), \quad (3.120)$$

which gives equivalent results, is however more challenging to implement since the counterterms then also obtain a temperature dependence.

3.4. Dynamics of a first-order phase transition

Now that we have the full daisy resummed free energy at 1-loop order under control, we can inspect its dynamics in more detail. We write the free energy in terms of the effective potential with the following contributions

$$V_{\text{eff}}^{1\text{-loop}}(\phi_b, T) = V_{\text{tree}}(\phi_b) + V_{\text{CW}}(\phi_b) + V_{\text{ct}}(\phi_b) + V_T(\phi_b, T) + V_{\text{daisy}}(\phi_b, T), \quad (3.121)$$

with

$$V_{\text{CW}} = \sum_a \pm \frac{n_a m_a^4(\phi_b)}{64\pi^2} \left[\ln \frac{m_a^2(\phi_b)}{\bar{\mu}^2} - C_a \right], \quad (3.122)$$

$$V_T = \frac{T^4}{2\pi^2} \sum_a \pm n_a J_{b/f} \left(\frac{m_a^2(\phi_b)}{T^2} \right), \quad (3.123)$$

$$V_{\text{daisy}} = -\frac{T}{12\pi} \sum_l n_l^L \left[(m_l^2(\phi_b) + \Pi_l(T))^{3/2} - m_l^3(\phi_b) \right]. \quad (3.124)$$

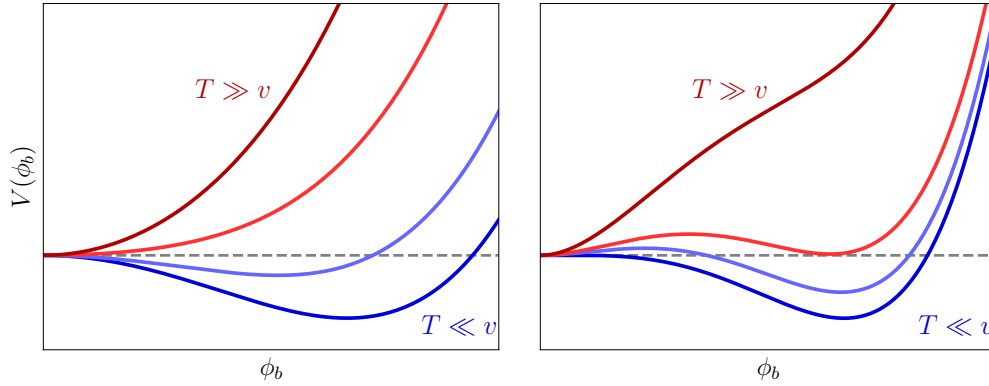


Figure 3.1.: Symmetry restoration through the thermal contributions from low temperature (blue) to high temperature (red). Left panel: Continuous transition between broken symmetry and restored symmetry. Right panel: Discontinuous transition between broken and restored symmetry due to the presence of a barrier.

Here, n_l^L are the bosonic degrees of freedom without the transversal degrees of freedom for gauge bosons, since they do not acquire a Debye mass.

With this potential, we can examine the temperature dependent behaviour of the vacuum for the example model eq. (3.56), shown in fig. 3.1 for two scenarios. In the left panel, going from high temperature (red) to low temperature (blue), the shift of the minimum is continuous, which is known as a *cross-over transition*. The right panel shows a qualitatively different behaviour; with decreasing temperature a local minimum develops, which at smaller temperatures becomes the global minimum, separated by a potential barrier from the symmetric minimum.

The evolution of the *order parameter*, the expectation value of the background field $\langle \phi_b \rangle$, of this phase transition is shown in fig. 3.2 for the two cases. In the left panel, we can see the continuous increase of ϕ_b with decreasing temperature and in the right panel, we see the discontinuity in the order parameter. A transition that exhibits such a discontinuity is called a *first-order phase transition* and is of great interest from the cosmological point of view. The decay of the symmetric phase (also called false vacuum) to the broken phase (true vacuum) comes with the release of vacuum energy that can source GWs as we will see in the last section of the chapter.

3.4.1. False vacuum decay and bubble nucleation

In the previous section, we have seen that the free energy can develop two coexisting minima separated by a potential barrier. Analogous to the case of quantum mechanics, where a particle can tunnel out of a potential well, also the background field can decay to the minimum of lower free energy.

To understand this, we go back to the definition of the partition function, which we computed by the method of steepest descent around a static background field with $\partial_\mu \phi_b = 0$. This formed a trivial saddle point of the Euclidean action $\delta S_E[\phi_b]/\delta \phi_b = 0$. Callan and Coleman showed that a second, non-trivial saddle point exists if a second minimum of the free energy is present in the zero temperature case [117], which was generalised by Linde to finite

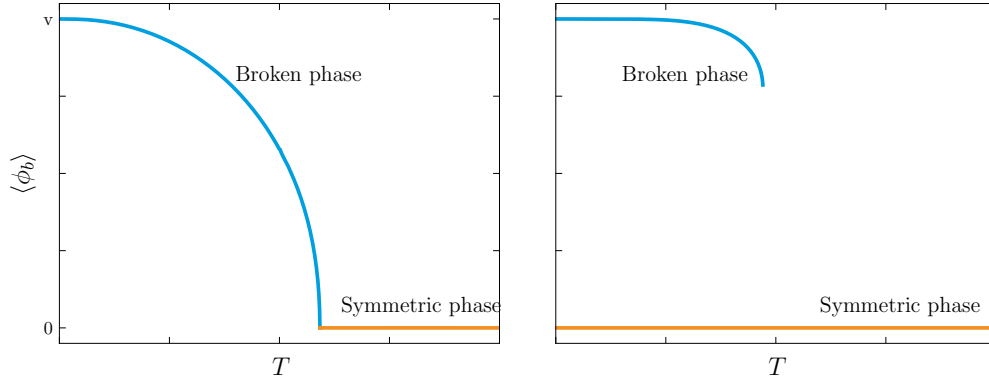


Figure 3.2.: Background field value ϕ_b of the minimum of the free energy for the two cases of fig. 3.1. *Left panel:* Continuous transition from a vanishing (orange) to a non-vanishing (blue) background field value. *Right panel:* Discontinuous change in the background field value.

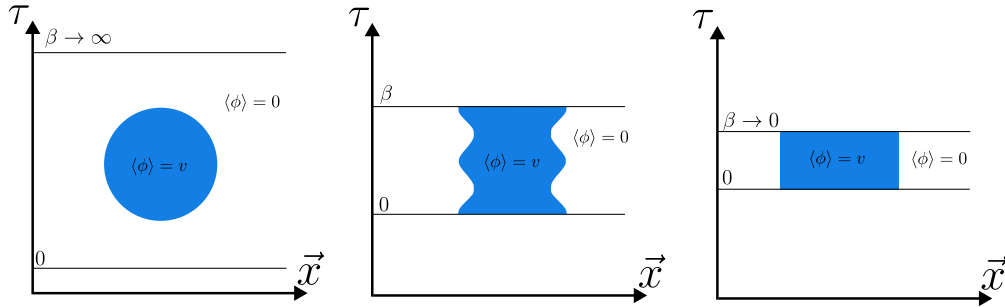


Figure 3.3.: Sketch of the instanton solution for different values of the temperature. The left panel has the hierarchy $v \ll \beta$ in the low temperature limit, the right panel $v \gg \beta$ in the high temperature limit and the middle panel interpolates between the two cases.

temperatures [118, 119]. This saddle point has to satisfy the same boundary conditions as the trivial one

$$\frac{\delta S_E}{\delta \phi_b} = 0, \quad \phi_b(0, x) = \phi_b(\beta, x), \quad \lim_{x \rightarrow \infty} \phi_b(\tau, x) = 0, \quad (3.125)$$

and has been shown to give an imaginary contribution to the free energy, indicating a decay probability. Assuming that a non-trivial solution ($\phi_b \neq 0$) exists, we can expect that it minimises the Euclidean action when it obeys the rotational symmetries of

$$S_E[\phi_b] = \int_0^\beta d\tau \int d^3x \left(\frac{1}{2} \left(\frac{d\phi_b}{d\tau} \right)^2 + \frac{1}{2} (\nabla \phi_b)^2 + V_{\text{eff}}(\phi_b, T) \right). \quad (3.126)$$

In the low temperature limit, the time direction becomes identical to the space directions since $\beta \rightarrow \infty$ and the solution minimising the action is expected to obey a $O(4)$ rotational symmetry as shown in the left panel of fig. 3.3. Increasing the temperature squeezes the time direction, and the second boundary condition affects the shape of the solution as seen in the middle panel. In the high-temperature limit, we can factor out the time coordinate and the solution obeys an $O(3)$ symmetry as shown in the right panel. The equations of motion of

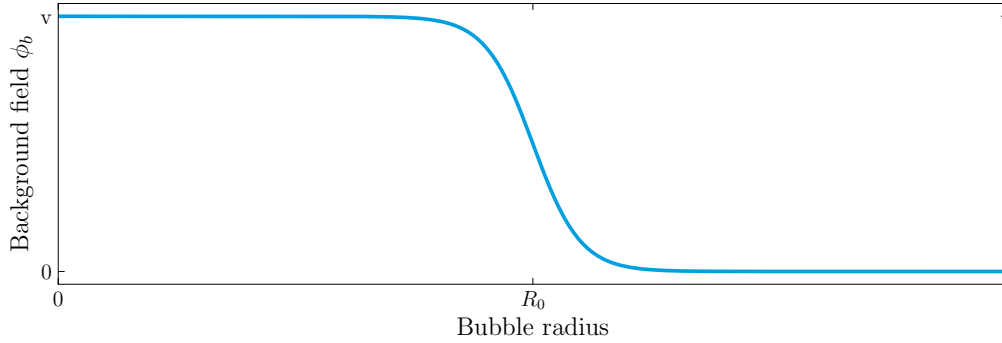


Figure 3.4.: Non-trivial field configuration that obeys the boundary conditions $\phi'(0) = 0$ and $\phi(r \rightarrow \infty) = 0$ and contributes a saddle point to the free energy density. It interpolates between the false vacuum at $r > R_0$ and the true vacuum at $r < R_0$. Also known as an instanton.

the field following from the action eq. (3.126) can be written with the rotational symmetries as

$$\frac{d^2\phi_b}{dr^2} + \frac{d-1}{r} \frac{d\phi_b}{dr} = \frac{d}{d\phi_b} V(\phi_b), \quad (3.127)$$

where $d = 4$ ($d = 3$) and the radial coordinate is $r = \sqrt{\tau^2 + \vec{x}^2}$ ($r = |\vec{x}|$) for the $O(4)$ ($O(3)$) symmetry. An example for the solution of this equation is sketched in fig. 3.4. At the origin, the background field takes the value of the non-vanishing minimum and interpolates around R_0 to the vanishing background field value as required by the boundary condition. Since this field configuration is $O(4)$ ($O(3)$) symmetric, it is also called a bubble. Let us now inspect the dynamics of this bubble after it nucleates. Assuming that the bubble wall (the region that interpolates the true and false vacuum) is small compared to the initial bubble radius, one can derive the equations of motion for the bubble radius from the action eq. (3.126) (after going back to real time) [120]:

$$\frac{d^2 R}{dt^2} + \frac{d-1}{R} \left(1 - \frac{dR}{dt}\right) = \frac{\Delta V}{\sigma} \left(1 - \frac{dR}{dt}\right)^{3/2} \quad \text{with} \quad \sigma = \int_{\text{wall}} d\phi_b \sqrt{2V(\phi)}. \quad (3.128)$$

The dynamics of the bubble depends here on the pressure difference $\Delta V = V(\phi_b = 0) - V(\phi_b = v)$ compared to the surface tension created by the bubble wall σ , where the integration domain is restricted to the region around the bubble wall [120]. Since the initial bubble radius corresponds to a stationary solution of eq. (3.126), the wall velocity vanishes $\dot{R} = 0$, and the initial radius corresponds to the critical radius $R_0 = R_c = (d-1)\sigma/\Delta V$ for which $\ddot{R} = 0$. However, this is not a stable solution and small fluctuations in R_0 determine if the bubble expands or shrinks: If $R_0 < (d-1)\sigma/\Delta V$ the surface tension causes the bubble to implode and vanish ($\ddot{R} < 0$), but for $R_0 > (d-1)\sigma/\Delta V$ the driving pressure ΔV overcomes the surface tension and the bubble will accelerate ($\ddot{R} > 0$).

The rate at which these bubbles are formed is determined by the decay rate of the false vacuum and can be computed analogous to the quantum mechanical case as the imaginary part of the free energy [117, 119, 121]

$$\Gamma \simeq -2\text{Im}F = \left(\frac{S_E}{2\pi}\right)^{d/2} \left| \frac{\det'(-\partial^2 + V''(\phi_b))}{\det(-\partial^2 + V''(0))} \right|^{-1/2} e^{-S_E[\phi_b]}, \quad (3.129)$$

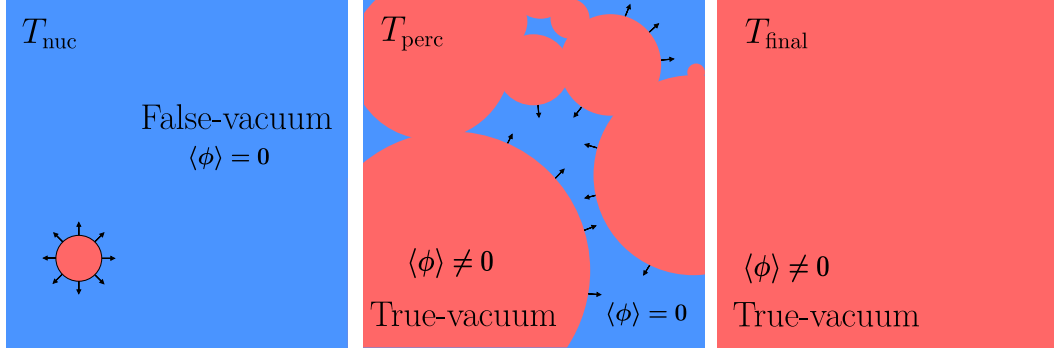


Figure 3.5.: Sketch of the nucleation history of a first-order phase transition. At the nucleation temperature, one bubble per Hubble volume has nucleated (left), at percolation a connected web of bubbles spans the universe (middle) and at the completion temperature the universe is (almost) completely in the new phase (right).

where the functional determinant $\det'$ denotes that the zero eigenvalues are omitted. This prefactor captures the fluctuations around the saddle point and for the high temperature case can be estimated on dimensional grounds: The fluctuations are given by the only energy scale, which is the temperature T and the nucleation rate hence becomes

$$\Gamma \simeq T^4 \left(\frac{S_3}{2\pi T} \right)^{3/2} e^{-S_3/T}. \quad (3.130)$$

3.4.2. Nucleation history

In the early universe, the temperature of the thermal bath is a decreasing function of time due to the Hubble expansion. At early times (high temperatures), the free energy density only has the symmetric minimum, and at some later point a second minimum forms. The critical temperature (time) is defined as the point at which the two minima are degenerate. From here on, the tunneling becomes energetically possible. As temperature decreases, the probability increases and we can define the onset of the phase transition as the point in time when, on average, one bubble has nucleated per Hubble volume [122]. This is called the nucleation time t_n (temperature T_{nuc}) given by the condition [123]

$$\int_0^{t_n} dt \frac{\Gamma(t)}{H^3(t)} \frac{a^3(t')}{a^3(t_n)} = 1, \quad (3.131)$$

where the scale factor ratio accounts for the expanding background. After the first bubble, more and more bubbles will nucleate and expand into the false vacuum. To track this volume fraction, we can define the fraction of the universe in the true vacuum as [119, 124]

$$\bar{P}_t(t) = \int_0^t dt' \Gamma(t') \frac{a^3(t')}{a^3(t)} V(t, t'), \quad (3.132)$$

$$\text{with } V(t, t') = \frac{4\pi}{3} r^3(t, t') = \frac{4\pi}{3} \left(\int_{t'}^t d\bar{t} \frac{a(\bar{t})}{a(t)} v_w \right)^3. \quad (3.133)$$

This accounts for the volume of spherical bubbles which nucleated and expanded with velocity v_w . However, this expression misses to account for the space already converted into the true vacuum, which is no longer available for the nucleation of new bubbles or existing ones to expand into. The non-overlapping fraction is given by [122]

$$P_t(t) = \int_0^t dt' (1 - P(t')) \Gamma(t') \frac{a^3(t')}{a^3(t)} V(t, t'), \quad (3.134)$$

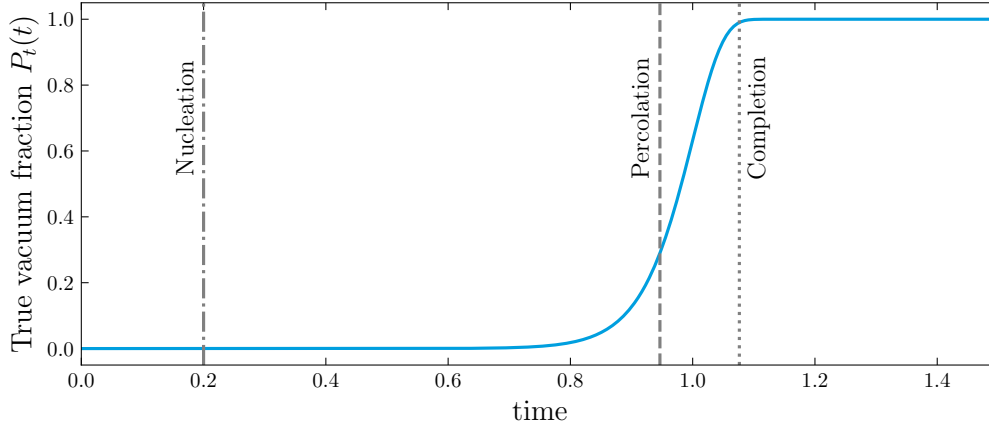


Figure 3.6.: Evolution of the true vacuum fraction from nucleation to percolation and completion. The completion time is here defined as $P_t(t_f) = 0.99$.

which has the solution

$$P_t(t) = 1 - P_f(t) = 1 - \exp \left(- \int_0^t dt' \Gamma(t') \frac{a^3(t')}{a^3(t)} V(t, t') \right). \quad (3.135)$$

Here, usually the time dependence of the velocity of the bubbles is neglected since it is expected that they very quickly reach an equilibrium velocity or accelerate to the speed of light $v_w \rightarrow 1$. The next milestone of the transition is the percolation time (temperature T_{perc}), which is reached when a Hubble volume is permeated by a connected web of bubbles. This has been shown to happen at a true vacuum fraction of $P_t(t_{\text{perc}}) \simeq 0.2895$ [125]. Since the true vacuum fraction only approaches one asymptotically, the definition of the completion time is somewhat arbitrary. Usually it is defined as $P(t_f) = 1 - \varepsilon$ with $\varepsilon \ll 1$. This nucleation history of a first-order phase transition is sketched as a slice through a Hubble volume in fig. 3.5. At nucleation (left panel), the first bubble nucleated at a random location in the Hubble volume. Percolation (middle panel) is reached when enough bubbles have nucleated and expanded to form a connected web spanning the Hubble volume. The phase transition is completed (right panel) when all of the universe is in the new phase. This evolution of the broken phase is also shown in terms of the true vacuum fraction in fig. 3.6. Before the true vacuum fraction vanishes $P_t = 0$, while around percolation the majority of the conversion from false to true vacuum occurs.

3.5. Gravitational waves from cosmological phase transitions

We have now studied the decay of the false vacuum, the bubble nucleation, and the evolution of the true vacuum fraction during the phase transition. In the process of the conversion of false to true vacuum, the energy stored in the potential is freed and can act as a source of GWs. Primarily, there are three different mechanisms that play a role. As the bubbles expand, one part of the released energy is stored in the field gradient, one part reheats the plasma, and another part turns into the kinetic energy of fluid shells around the bubbles. After the collision, the fluid shells around the bubbles form long lived sound waves that also source GWs. These fragment and decay, generating GWs from magnetohydrodynamic (MHD) turbulence. To understand the regimes where the different contributions become important, we first review the hydrodynamics of a bubble expanding in the primordial plasma, which gives the energy budget for the sound waves and turbulence. After that, we review the case

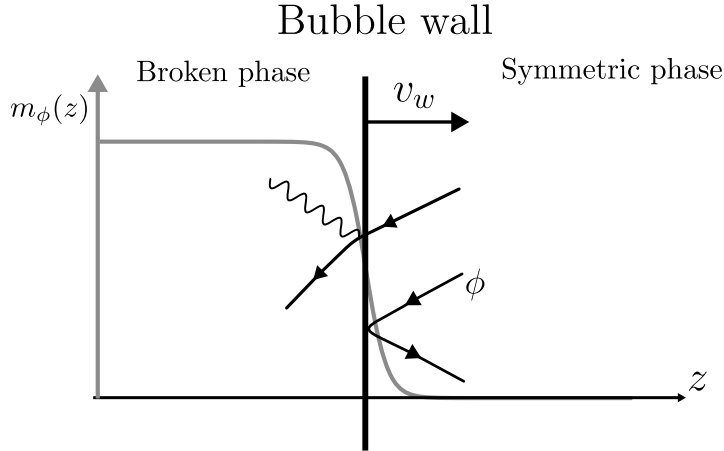


Figure 3.7.: A sketch of a bubble wall moving through the plasma into the z direction. Across the bubble wall the background field ϕ_b interpolates the true $\phi_t \neq 0$ and false $\phi_f = 0$ vacua and creates a position dependent mass of the particles. If the centre of mass energy of the particles and the bubble wall is smaller than the mass difference, the particles get reflected. Particles that enter the bubble can emit transition radiation.

where no equilibrium solution of the expanding bubbles sets in before the collision and the bubble walls run away. In this case, most of the released energy will go into the acceleration of the bubble walls. Lastly, we discuss gravitational wave spectra and templates for each mechanism.

3.5.1. Hydrodynamics of expanding bubbles

In sec. 2.4.3, we saw that the energy density of GWs is determined by the time derivative of the reduced quadrupole moment of the source. For cosmological phase transitions, this source is typically the motion of the plasma driven by the expansion of the bubbles. After the bubble collisions, the initially spherical fluid shells form sound waves and give a time-dependent anisotropic contribution to the reduced quadrupole moment. Here, in order to quantify the energy in these sound waves and later in turbulence, we review the energy budget of a single bubble following [126–128].

We start by considering a single bubble expanding into the plasma. Its expansion is driven by the pressure difference between the two vacua $P_{\text{drive}} = \Delta V$. Upon entering the bubble, the plasma particles obtain a background field dependent mass or get reflected if the centre of mass energy between bubble wall and particle is smaller than the mass difference in the two phases, as sketched in fig. 3.7. This transfers momentum from the bubble wall into the plasma and sets the fluid into motion, creating friction on the bubble expansion [129]. Additional friction can arise through transition radiation of particles entering the bubble [130]. Once the friction and driving pressure balance out, the expansion reaches a steady state which is typically reached very quickly compared to the bubble size at collision.

To proceed, we will examine the equilibrium profiles of different expansion types of the bubbles with the goal of extracting the fraction of the released energy that will end up in sound waves. The starting point for the hydrodynamics of a scalar field interacting with the plasma is the

energy-momentum (EM) tensor. The EM tensor for the scalar background field ϕ_b with the potential $V(\phi_b, T)$ reads

$$T_\phi^{\mu\nu} = \partial^\mu \phi \partial^\nu \phi - g^{\mu\nu} \left(\frac{1}{2} \partial_\alpha \phi \partial^\alpha \phi - V(\phi, T) \right), \quad (3.136)$$

where we drop the subscript b for brevity. The contribution to the EM tensor from the plasma particles can be written as moments of the phase-space distribution functions $f_i(p, x)$

$$T_f^{\mu\nu} = \sum_i \int \frac{d^3p}{(2\pi)^3 E_i} p^\mu p^\nu f_i(p, x). \quad (3.137)$$

Note that, due to the expanding bubbles, the distribution functions are generally not homogeneous here. Typically, the presence of the expanding bubble wall drives the particle species out of equilibrium, which can be described as perturbations around the equilibrium distribution

$$f_i(p, x) = f_i^{\text{eq}}(T(x)) + \delta f_i(p, x). \quad (3.138)$$

In the case where the mean free path of the particles is much shorter than the bubble wall width, local thermal equilibrium (LTE) ($\delta f_i = 0$) is a good approximation and the plasma can be described through the equilibrium distributions with a spatially dependent temperature $T(x)$. Then the EM tensor reduces to that of a perfect fluid

$$T_{f,\text{eq}}^{\mu\nu} = \sum_i w(T) u^\mu u^\nu - p(T) g^{\mu\nu}, \quad (3.139)$$

with $u_\mu = \gamma(v)(1, \vec{v})^T$ denoting the fluid four velocity in the plasma frame and the Lorentz factor $\gamma(v) = 1/\sqrt{1-v^2}$. The pressure and enthalpy of the fluid are given by

$$p = \pm \sum_i n_i \int \frac{d^3p}{(2\pi)^3} \ln[1 \pm \exp(-E_i/T)], \quad (3.140)$$

$$w = T \frac{\partial p}{\partial T}. \quad (3.141)$$

The symmetry breaking inside the bubbles gives the particles different masses, which leads to different plasma properties. These can be related to the properties outside the bubble through the conservation of energy and momentum across the bubble wall

$$T^{\mu\nu}_{;\mu} = (T_\phi^{\mu\nu} + T_f^{\mu\nu})_{;\mu} = 0. \quad (3.142)$$

If we assume that the bubble wall is planar and propagating in the z direction with velocity v_w , by integrating across the bubble wall we obtain

$$T_+^{zz} - T_-^{zz} = 0, \quad \text{and} \quad T_+^{tz} - T_-^{tz} = 0, \quad (3.143)$$

the subscript $+$ ($-$) denotes here the outside (inside) of the bubble. This gives rise to the matching conditions between the plasma inside and outside the bubble

$$w_+ \tilde{\gamma}_+^2 \tilde{v}_+ = w_- \tilde{\gamma}_-^2 \tilde{v}_-, \quad (3.144)$$

$$w_+ \tilde{\gamma}_+^2 \tilde{v}_+^2 + p_+ = w_- \tilde{\gamma}_-^2 \tilde{v}_-^2 + p_-. \quad (3.145)$$

Here, the velocities are understood to be in the *wall frame*, denoted by the tilde ($\tilde{v}, \tilde{\gamma}$), where the bubble wall is at rest. Rearranging yields the conditions

$$\tilde{v}_+ \tilde{v}_- = \frac{p_+ - p_-}{e_+ - e_-} \quad \text{and} \quad \frac{\tilde{v}_+}{\tilde{v}_-} = \frac{e_- + p_+}{e_+ + p_-}. \quad (3.146)$$

Instead of proceeding by computing the pressure and energy density directly from the effective potential, we can use a simplified equation of state that encodes the microphysics and captures the qualitative behaviour. In the cosmological case, often a good approximation can be made with the bag model [131]

$$e_+(T) = a_+ T^4 + \epsilon_+, \quad p_+ = \frac{1}{3} a_+ T^4 - \epsilon_+, \quad (3.147)$$

$$e_-(T) = a_- T^4 + \epsilon_-, \quad p_- = \frac{1}{3} a_- T^4 - \epsilon_-, \quad (3.148)$$

which describes vacuum energy $\epsilon_+ - \epsilon_- = \Delta V$ and pure radiation, with $a_{\pm}$ accounting for the degrees of freedom

$$a_{\pm} = \frac{\pi^2}{30} \sum_i \left(g_i^b + \frac{7}{8} g_i^f \right). \quad (3.149)$$

This model is accurate in the high-temperature regime $T \gg m$, as can be seen from the high-temperature expansions of the thermal functions that we encountered before (cf. eqs. (3.82) and (3.83)). The matching relations become

$$\tilde{v}_+ \tilde{v}_- = \frac{1 - (1 - 3\alpha_+) r}{3 - 3(1 + \alpha_+) r}, \quad \frac{\tilde{v}_+}{\tilde{v}_-} = \frac{3 + (1 - 3\alpha_+) r}{1 + 3(1 + \alpha_+) r}, \quad (3.150)$$

with the definitions

$$\alpha_+ \equiv \frac{\epsilon_+ - \epsilon_-}{a_+ T_+^4}, \quad r \equiv \frac{a_+ T_+^4}{a_- T_-^4}. \quad (3.151)$$

These quantities correspond to the energy released by the vacuum conversion compared to the radiation energy (α_+) and the ratio of enthalpy in the two phases (r). With these two matching conditions, we can now relate the temperature and wall velocity inside the bubble to those outside. To relate these quantities to the nucleation temperature of the bubble and the wall velocity, we additionally need equations governing the fluid profile in front and behind the bubble wall. These equations are obtained projecting the continuity eq. (3.142) along the fluid flow $u^\mu = \gamma(1, \vec{v})$ and the perpendicular direction $\bar{u}^\mu = \gamma(v, \vec{v}/v)$. This yields the two equations [126, 132]

$$0 = u_\mu \partial_\nu T^{\nu\mu} = -\partial_\mu (w u^\mu) + u_\mu \partial^\mu p, \quad (3.152)$$

$$0 = \bar{u}_\mu \partial_\nu T^{\nu\mu} = w \bar{u}_\mu u^\nu \partial_\nu u^\mu + \bar{u}_\mu \partial^\mu p. \quad (3.153)$$

Since the bubbles are spherical, we can reduce the spatial dependence to the radial coordinate, and since there is no scale involved in the problem, switch to the self-similar coordinate $\xi = r/t$. With this, we get the equations in the *plasma rest frame*

$$2 \frac{v}{\xi} = \gamma^2 (1 - v\xi) \left(\frac{\mu^2(\xi, v)}{c_s^2} - 1 \right) \partial_\xi v, \quad (3.154)$$

$$\partial_\xi \omega = \omega \left(1 + \frac{1}{c_s^2} \right) \gamma^2 \mu(\xi, v) \partial_\xi v, \quad (3.155)$$

with the definition of the speed of sound $c_s^2 = dp/de$ and $\mu(\xi, v) = (v - \xi)/(1 - \xi v)$ denoting the Lorentz transformed fluid velocity. The left panel of fig. 3.8 shows the general solutions profiles to these equations that have a fixed point at $\xi = c_s = 1/\sqrt{3}$ and $v = 0$. The grey shaded area excludes unphysical solutions, as in the upper left corner, the solutions would violate causality. For different initial conditions (bubble wall velocity v_w) we obtain three different solution profiles.

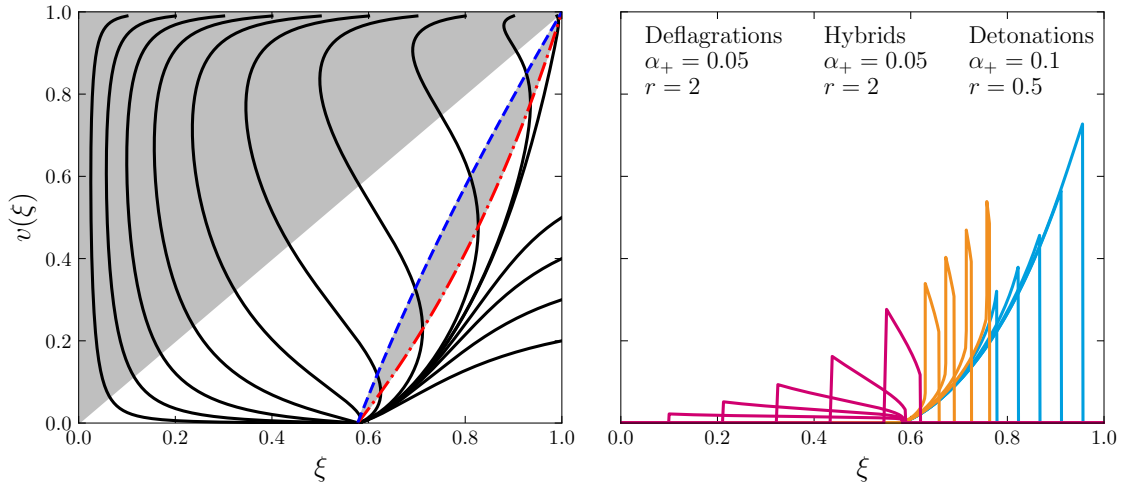


Figure 3.8.: Left: General solutions plane for the velocity profile eq. (3.154). The equation has a fixed point at $(v, \xi) = (0, c_s)$ with $c_s^2 = 1/3$. Physical solutions are found in the white area, the upper left grey shaded region is excluded by causality. Right: Physical velocity profiles for deflagration (purple), hybrid (orange) and detonation (blue) solutions for different initial conditions of (v_w, α_+, r) .

Deflagrations

The first class of solution consists of expanding bubbles moving with subsonic speed $v_w < c_s$. The plasma behind the bubble wall is at rest ($\tilde{v}_- = v_w$ in the wall frame), while the advancing bubble wall sets the plasma in front of the bubble in motion. Outside the bubble, the fluid velocity decreases until a shock front is reached in front of which the fluid is at rest. The velocity profile of this type of bubble expansion is shown in purple in the right panel of fig. 3.8 for the strength $\alpha_+ = 0.05$ and enthalpy ratio $r = 2$.

Detonations

Another class of solutions exists for bubble walls expanding with supersonic velocity $v_w > c_s$, for which the fluid in front of the wall remains unperturbed ($\tilde{v}_+ = v_w$ in the wall frame). Behind the bubble wall, the fluid velocity must be slower than the bubble wall, which leads to the upper bound on v_- shown as the red dashed dotted line in the left panel of fig. 3.8. Inside the bubble, the fluid forms a rarefaction wave and slows down until it comes to rest at $\xi = c_s$. The velocity profiles of these detonation solutions are shown in blue in the right panel of fig. 3.8 for the strength $\alpha_+ = 0.1$ and enthalpy ratio $r = 0.5$.

Hybrid

The last class of solutions are hybrids between the previous two solutions and must have $v_w > c_s$. Both inside and outside the bubble the fluid velocity is non-vanishing, which requires the fluid velocity outside the bubble to be finite in the wall frame $\tilde{v}_+ > 0$, as otherwise the plasma is not set into motion in front of the bubble. This condition gives the lower bound shown as the blue dashed line in the left panel of fig. 3.8. The right panel shows such hybrid velocity profiles obtained for $\alpha_+ = 0.05$ and $r = 2$ in orange.

3.5.2. Energy budget of expanding bubbles

In a first-order phase transition (FOPT), the fluid profiles discussed above build up in the early universe until the bubbles collide. After the collision, the fluid shells propagate further

as sound waves with the necessary anisotropy and time-dependence to source GW. Eventually, the sound waves fragment and decay, which additionally sources GWs from magnetohydrodynamic (MHD) turbulence. To later determine the GW signal, it is convenient to parameterise the fraction of the energy released in the transition that ends up in each type of source.

Sound waves

The kinetic energy in the motion of the plasma can be computed as the difference of the energy density in the plasma motion compared to the unperturbed plasma

$$e_{\text{kin}} = T^{00}(v) - T^{00}(v=0) = \gamma^2 v^2(\xi) w(\xi). \quad (3.156)$$

From this, we can define the efficiency of converting the energy released from the false vacuum conversion to energy in the bulk fluid motion as [122, 126]

$$\kappa_{\text{sw}} \equiv \frac{E_{\text{kin}}}{E_{\text{vac}}} = \frac{1}{4\pi\Delta V v_w^3/3} \int_{\text{bubble}} d^3\xi w v^2 \gamma^2, \quad (3.157)$$

where the integration is restricted to the extent of the fluid profile of the bubble.

Magnetohydrodynamic turbulence

Turbulence is expected to develop at late stages after the bubble collisions and to drain energy from the sound waves as they decay and fragment. Due to the large hierarchy in scales (from the bubble wall width to the separation of bubbles), it is however numerically challenging to evolve a system long enough to see this onset of turbulent motion in the plasma [69, 133]. Simulations have found that at most 5–10% of the fluid motion ends up in vorticity [134], but these were limited to only a fraction of the lifetime of the turbulent motion and hence are not expected to have entered a steady regime yet. Simulations initialised with an already fully developed MHD turbulence spectrum in the fluid velocity suggest that the contribution can be dominant if the initial sound waves decay quickly into turbulent motion [135]. For these reasons, a common approach is to heuristically estimate the kinetic energy fraction in turbulence as a fraction of the energy in the fluid motion

$$\kappa_{\text{turb}} = \varepsilon \kappa_{\text{sw}} = \varepsilon \frac{E_{\text{kin}}}{E_{\text{vac}}}, \quad (3.158)$$

with a common choice of $\varepsilon = 0.05$ [69, 133].

3.5.3. Bubble collisions

So far, we have considered the case that the bubble expansion quickly reaches a steady state and a sizeable amount of the released vacuum energy ends up in the fluid motion. Besides this, there exists also a second regime, where the driving pressure is always larger than the friction, leading to run-away bubbles that keep accelerating before colliding. This typically requires a vacuum dominated universe, such that the driving pressure becomes very large compared to the energy density in the plasma, weak couplings between particles and the background field, or the absence of massive gauge bosons that would give rise to a friction term proportional to the bubble wall Lorentz factor [130].

Considering such an accelerating bubble, we can express the energy density in the bubble wall as the vacuum energy released inside the bubble minus the energy lost to friction [136]

$$E_{\text{wall}} = \frac{4\pi}{3} \int_0^R dr R^2 (\Delta V - P_{\text{LO}} - P_{\text{LL}}). \quad (3.159)$$

The leading order pressure (P_{LO}) on the bubble walls in the limit of highly relativistic bubble walls is given by the squared mass difference of the particles in the two vacua [129]

$$P_{\text{LO}} \approx \frac{\Delta m^2 T^2}{24} \quad \text{with} \quad \Delta m^2 \equiv \sum_i c_i n_i (m_{i,t}^2(\phi_t) - m_i^2(\phi_f))^2, \quad (3.160)$$

with $c_i = 1$ for bosons $c_i = 1/2$ for fermions and n_i denoting the degrees of freedom. This can be interpreted as the friction on the bubble wall by the particles gaining the mass difference Δm^2 . The third term (P_{LL}) accounts for the next-to-leading order effect – radiation of soft gauge bosons known as transition radiation. This leading-logarithm resummed term was shown to be [137–139]

$$P_{\text{LL}} \simeq \gamma_w g_v^2 \Delta m T^3 \ln\left(\frac{v}{T}\right) \quad \text{with} \quad g^2 \Delta m = \sum_v g_v^2 n_v (m_v(\phi_t) - m_v(\phi_f)), \quad (3.161)$$

where the sum runs only over the gauge bosons that obtain mass when they enter the bubble. This term is proportional to the Lorentz factor of the bubble wall $\gamma_w = 1/\sqrt{1 - \dot{R}^2}$ and hence grows for an accelerating bubble. From the equations of motion of the bubble wall eq. (3.128) it can be shown that it obeys [120]

$$\frac{d\gamma_w}{dR} + 2\frac{\gamma_w}{R} = \frac{p}{\sigma} \Rightarrow \gamma_w(R) = \frac{2R}{3R_0} + \frac{R_0^2}{R^2} - \frac{pR_0^3}{3\sigma R^2}, \quad (3.162)$$

with the initial condition $\gamma_w(R_0) = 1$ and R denoting the bubble radius. The driving force is here the ratio between total pressure p and the surface tension of the wall σ given by

$$p = \Delta V - P_{\text{LO}} - P_{\text{LL}}, \quad \text{and} \quad \sigma = \int_{\text{wall}} d\phi \sqrt{2V(\phi)}. \quad (3.163)$$

Since the initial bubble radius R_0 is usually very small compared to the radius at collision $R_0 \ll R_*$, the Lorentz factor is well approximated by $\gamma_w(R) \simeq 2R/(3R_0)$. As long as this equilibrium value is not yet reached, all the energy goes into the acceleration of the bubble wall, i.e.

$$\frac{E_{\text{wall}}}{E_{\text{vac}}} = \frac{\Delta V - \Delta P_{\text{LO}}}{\Delta V}. \quad (3.164)$$

In case the wall reaches an equilibrium state before collision, the acceleration stops and the energy is instead given by the energy that went into the acceleration up to the equilibrium bubble radius R_{eq} , plus the increase in energy stored in the surface tension from that point on:

$$\frac{E_{\text{wall}}}{E_{\text{vac}}} = \frac{(\Delta V - \Delta P_{\text{LO}})R_{\text{eq}}^3}{\Delta V R_*^3} + \frac{3\gamma_{\text{eq}}\sigma(R_*^2 - R_{\text{eq}}^2)}{\Delta V R_*^3}. \quad (3.165)$$

The bubble radius where acceleration stops can be simply inferred from the equilibrium condition $p = 0$ as $R_{\text{eq}} = 3\gamma_{\text{eq}}R_0/2$. With the Lorentz factor of the wall at this equilibrium radius

$$\gamma_{\text{eq}} = \frac{\Delta V - \Delta m^2 T^2/24}{g^2 \Delta m T^3 \ln(v/T)}, \quad (3.166)$$

we can finally define the efficiency factor of turning the vacuum energy into energy carried in the bubble wall in the different regimes as [136, 140]

$$\kappa_{\text{col}} = \frac{E_{\text{wall}}}{E_V} = \begin{cases} 1 - \frac{P_{\text{LO}}}{\Delta V} & \text{if } \gamma_* < \gamma_{\text{eq}} \quad (\text{runaway walls}) \\ \frac{\gamma_{\text{eq}}}{\gamma_*} \left(1 - \frac{P_{\text{LO}}}{\Delta V} \left(\frac{\gamma_{\text{eq}}}{\gamma_*} \right)^2 \right) & \text{if } \gamma_{\text{eq}} \leq \gamma_* \quad (\text{walls with large terminal } v_w) \\ 0 & \text{else (non-relativistic walls).} \end{cases} \quad (3.167)$$

3.5.4. From bubble collisions to gravitational wave spectra

In order to compute the gravitational wave signal emerging after the bubble collisions, in principle, one has to place and evolve the fluid profiles on a lattice and compute the signal numerically. This proves to be computationally very expensive and instead matching templates have been developed. These templates capture the scaling of the GW amplitude with characteristic phase transition parameters and the spectral shape of the signal observed in the simulations. Here, we will first look at the two main parameters necessary to characterise the signal and then turn to the templates for the three different sources.

Phase transition strength

Most important for the strength of the GW signal is the amount of energy released by the false vacuum decay. As we saw in the study of the bubble expansion, this strength determines the energy in the fluid motion and the bubble wall. It can be defined in terms of the pseudo trace of the combined fluid and scalar field EM tensor [127, 128]

$$\bar{\theta}_i(T) = \left(\rho_i(T) - \frac{p_i(T)}{c_{s,i}^2(T)} \right), \quad (3.168)$$

where $i = (t, f)$ labels either vacuum and $c_{s,i}(T)$ is the speed of sound in the respective phase. In the relativistic case ($c_{s,i}^2 = 1/3$) it reduces to the usual trace. The strength of the phase transition can then be defined as the difference in the pseudo-trace of both phases at the percolation temperature compared to the enthalpy in the false vacuum

$$\alpha = \frac{\bar{\theta}_f(T_{\text{perc}}) - \bar{\theta}_t(T_{\text{perc}})}{3w_f(T_{\text{perc}})}. \quad (3.169)$$

This definition allows to write the kinetic energy fraction in terms of the efficiency factors from the previous section

$$K \equiv \frac{\rho_{\text{kin}}}{\rho_f(T_{\text{perc}})} = \kappa \frac{\alpha}{1 + \alpha}, \quad (3.170)$$

which conveniently parameterises the energy density of the source of GWs.

Length scale

The most important quantity that determines the frequency of the GW signal is the characteristic length scale of the process. The self-similar bubble profiles inspected in the previous section grow with the bubble radius and hence the characteristic length scale for cosmological phase transitions is given by the mean bubble separation at percolation, which is when the majority of the collisions occur. We can compute this quantity from the number density of bubbles [122]

$$n(T) = \int_{t_{\text{init}}}^t dt' \Gamma(t') (1 - P_t(t')) \left(\frac{a(t')}{a(t)} \right)^3, \quad (3.171)$$

which allows to compute the mean separation of bubbles as

$$R_{\text{sep}}(T) = \frac{1}{n(T)^{1/3}}. \quad (3.172)$$

A common approximation of this can be made by defining the transition speed through the derivative of the nucleation rate (cf. eq. 3.130)

$$\beta \equiv \frac{d}{dt} \ln \Gamma(t) \Big|_{t_{\text{perc}}} \approx HT \frac{d}{dT} \left(\frac{S_3}{T} \right), \quad (3.173)$$

where the last step uses the approximate time-temperature relation $dT/dt = -HT$ valid for a purely radiation dominated universe. In the literature, this is often mapped to the mean bubble separation via¹ [122]

$$R_{\text{sep}} \approx \left(\frac{8\pi}{1 - P_t(t_{\text{perc}})} \right)^{1/3} \frac{\max(v_w, c_s)}{\beta}, \quad (3.174)$$

which holds for fast phase transitions, but breaks down for slow transitions, as we will show in sec. 4.4.

Frequency redshift

Due to the expansion of the universe, the characteristic length scale will be redshifted by a scale factor ratio of $R_0 = (a_0/a_*)R_*$, where the subscript $*$ denotes the emission time. The frequency scales inversely to the length scale of the source, so the observed frequency today f_0 , in terms of the emitted frequency f_* is

$$f_0 = \frac{a_*}{a_0} f_* = f_* R_* \left(\frac{a_* H_*}{R_* H_*} \right) \quad (3.175)$$

where we set $a_0 = 1$ in the last step. Here, it is convenient to express the redshift factor $a_* H_*$ in terms of the temperature after the phase transition T_* . By using entropy conservation $\partial_t(a^3 s) = 0$, we obtain

$$a_* H_* = 11.2 \text{ nHz} \left(\frac{T_*}{100 \text{ MeV}} \right) \left(\frac{g_*}{10} \right)^{1/2} \left(\frac{10}{h_*} \right)^{1/3}. \quad (3.176)$$

Here, g_* (h_*) denotes the total effective energy (entropy) degrees of freedom at the emission time.

Amplitude redshift

The energy density of GWs redshifts as radiation, as they travel from the early universe to us today. It is commonly expressed as the fractional energy density $\Omega_{\text{GW}} = \rho_{\text{GW}}/\rho_{\text{crit}}$, which receives the redshift factor [77]

$$\mathcal{R}h^2 \equiv \left(\frac{a_*}{a_0} \right)^4 \left(\frac{H_*}{H_0} \right)^2 = \frac{\Omega_\gamma h^2}{D^{4/3}} \left(\frac{h_0}{h_*} \right)^{4/3} \frac{g_*}{g_\gamma}. \quad (3.177)$$

The first term is the usual redshift of radiation, while the second term accounts for the evolution of the critical energy density. The second step then follows from expressing the Hubble rate today in terms of the energy density in photons $\Omega_\gamma h^2 = 2.473 \cdot 10^{-5}$ [8] and the energy and entropy degrees of freedom $g_\gamma = 2$ and $h_0 = 3.91$. The possibility of entropy injection from e.g. decaying DM is accounted for by the dilution factor $D = S_{\text{SM}}^0/S_{\text{tot}}^{\text{init}}$ with S_{SM}^0 being the SM comoving entropy density today and $S_{\text{tot}}^{\text{init}}$ being the total comoving entropy density just before the transition [141].

3.5.5. Sound wave spectrum

The GW spectrum from sound waves has been computed by numerous numerical simulations of the fluid response to expanding and colliding bubbles [134, 142]. The results were interpreted with the sound shell model [143, 144]. This model assumes that after the collision, the sound waves propagate linearly and maintain the form of the radial fluid profile of the

¹The factor $(1 - P_t(t_{\text{perc}}))^{-1/3} \approx 1.51$ is often neglected in the literature.

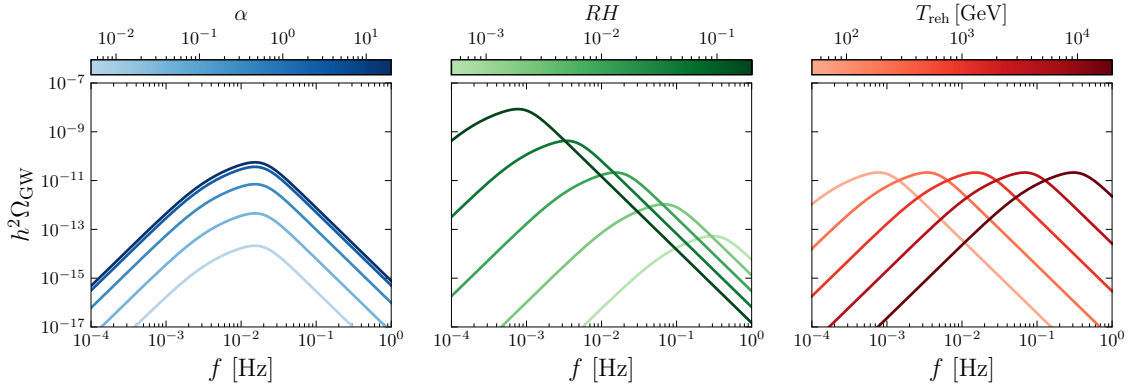


Figure 3.9.: Spectral shape of GWs from sound waves and their scaling with transition strength α , mean bubble separation RH , and reheating temperature T_{reh} . Here, we set $\kappa_{\text{sw}} = 1$ and the parameters to $\alpha = 1$, $RH = 10^{-2}$, and $T_{\text{reh}} = 10^3$ GeV (unless varied).

expanding bubbles. This leads to a second characteristic length scale besides the typical bubble size, the fluid shell thickness and the predicted GW spectrum is found to be a double broken power law [145, 146]

$$S_{\text{sw}}(f) = N \left(\frac{f}{f_{\text{sw},1}} \right)^3 \left[1 + \left(\frac{f}{f_{\text{sw},1}} \right)^2 \right]^{-1} \left[1 + \left(\frac{f}{f_{\text{sw},2}} \right)^4 \right]^{-1}, \quad (3.178)$$

where the frequency breaks occur at

$$f_1 \simeq 0.2 \frac{a_* H_*}{RH}, \quad f_2 \simeq \frac{0.5 a_* H_*}{\Delta_w RH} \quad \text{with} \quad \Delta_w = \frac{|v_w - c_s|}{\max(v_w, c_s)}. \quad (3.179)$$

The second frequency break is determined by the fluid shell thickness Δ_w . If the bubble wall velocity is comparable to the speed of sound, the fluid shell thickness becomes small compared to the mean bubble separation RH (cf. fig. 3.8) and gives a separate length scale that is resolved in the GW spectrum. As shown in fig. 3.9, at small frequencies ($f \ll f_1$) the signal has a causality tail and rises as f^3 . Between the frequency breaks ($f_1 \ll f \ll f_2$) the signal grows linearly in f and decreases after the second frequency break ($f \gg f_2$) with f^{-5} .

The amplitude of the signal primarily depends on the kinetic energy fraction K_{sw} , the mean bubble separation RH at percolation and the lifetime of the source $\mathcal{Y}_{\text{sw}}$ [147]

$$h^2 \Omega_{\text{GW,sw}}(f) = \mathcal{R} h^2 A_{\text{sw}} K_{\text{sw}}^2(RH) \mathcal{Y}_{\text{sw}} S_{\text{sw}}(f), \quad (3.180)$$

with

$$\mathcal{Y}_{\text{sw}} = \min(1, \tau_{\text{sh}} H) \simeq \min \left(1, \sqrt{\frac{\Gamma}{K_{\text{sw}}}} RH \right). \quad (3.181)$$

The source lifetime is either determined by the Hubble time itself or by the time it takes the sound waves to decay into turbulence, quantified by the shock formation time $\tau_{\text{sh}} H \simeq \sqrt{\Gamma/K_{\text{sw}}} RH$. Here, the mean adiabatic index is $\Gamma = 4/3$ for a radiation fluid [133]. The overall normalisation factor A_{sw} is determined by matching to numerical simulations and found to be $A_{\text{sw}} \simeq 0.11$. The kinetic energy fraction was also found to receive a dampening factor in the efficiency of producing bulk fluid motion in the multi-bubble scenario compared to the single bubble case [145] and is here $K_{\text{sw}} = 0.6 \kappa_{\text{sw}} \alpha (1 + \alpha)$.

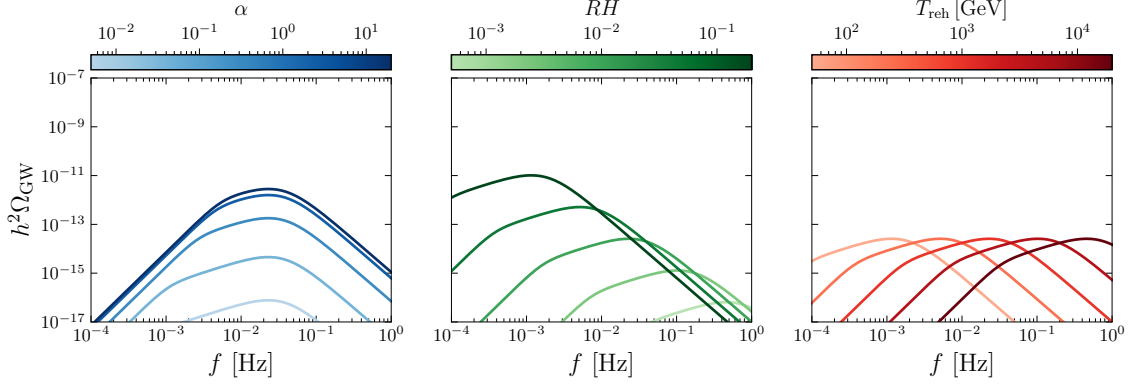


Figure 3.10.: Gravitational wave spectrum from turbulence after a FOPT. The scaling with α , RH and T_{reh} is shown from left to right. Here we set $\kappa_{\text{turb}} = 1$ and the parameters to $\alpha = 0.1$, $RH = 10^{-2}$, and $T_{\text{reh}} = 10^3$ GeV (unless varied).

The scaling of the GW signal with the parameters α , RH and T_{reh} is shown in fig. 3.9. For $\alpha \ll 1$, the amplitude scales quadratically with the transition strength, which saturates for $\alpha > 1$, where the kinetic energy fraction $K \propto \alpha/(1 + \alpha)$ approaches one. The mean bubble separation affects both the peak frequency and the amplitude, which scale as RH^{-1} and RH^2 respectively (as long as the shock formation time is smaller than the Hubble time $\tau_{\text{sh}}H < 1$, see eq. (3.181)). Finally, the reheating temperature shifts the frequency through the amount of redshift received.

3.5.6. Magnetohydrodynamic turbulence spectrum

Due to the large hierarchy of scales, the formation of MHD turbulence is very difficult to model numerically. As discussed in sec. 3.5.2, usually a heuristic parameter ε is introduced to parameterise the fraction of kinetic energy in the sound waves that is converted into turbulence [133]. Simulations initialised with already fully developed MHD turbulence give the following shape of the GW spectrum [135, 148]

$$S_{\text{turb}}(f) = \left(\frac{f}{a_* H_*}\right)^3 \left[1 + \left(\frac{f}{f_{\text{turb},1}}\right)^{2.15}\right]^{-7.9} \begin{cases} \ln^2\left(1 + \frac{a_* H_*}{2\pi f_{\text{turb},3}}\right) & \text{for } f \leq f_{\text{turb},2} \\ \ln^2\left(1 + \frac{a_* H_*}{2\pi f}\right) & \text{for } f > f_{\text{turb},2} \end{cases} \quad (3.182)$$

with the characteristic frequencies

$$f_{\text{turb},1} = 2.2 \frac{a_* H_*}{RH} \quad \text{and} \quad f_{\text{turb},2} = \frac{a_* H_*}{4\pi H_* \tau_e} = \frac{\sqrt{3K_{\text{turb}}}}{4} \frac{a_* H_*}{RH}. \quad (3.183)$$

The first frequency is set by the initial scale of the perturbations, which is determined by the mean bubble separation. The second frequency comes from the eddy turn-over time τ_e , i.e. the time it takes the fluid to complete a turbulent structure (e.g. a vortex), which is here approximated through the characteristic length scale compared to the fluid velocity $\tau_e \simeq R/(2\pi v_f)$, with $v_f^2 \approx 3/4K_{\text{turb}}$ [135, 147, 149]. The amplitude in this parameterisation is given by

$$h^2 \Omega_{\text{GW,turb}}(f) = \mathcal{R} h^2 A_{\text{turb}} K_{\text{turb}}^2 (RH)^3 S_{\text{turb}}(f), \quad (3.184)$$

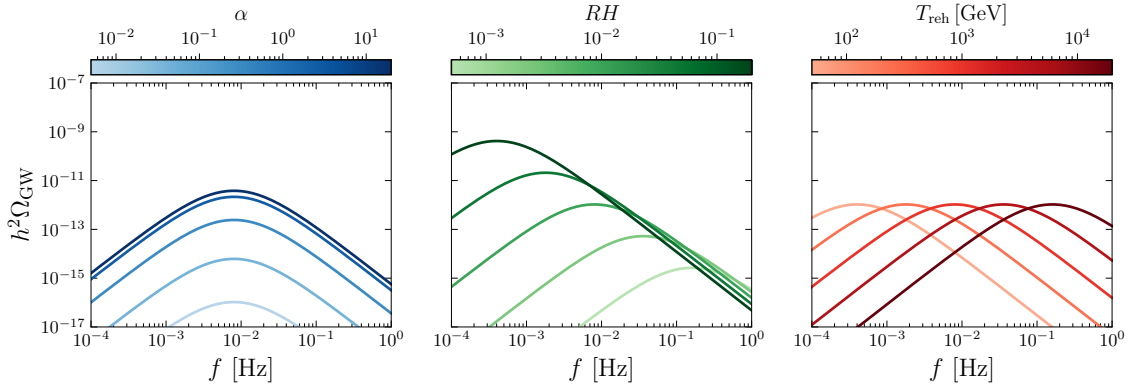


Figure 3.11.: Gravitational wave spectra from bubble collisions and their scaling with α , RH and T_{reh} . Here we set $\kappa_{\text{col}} = 1$ and the parameters to $\alpha = 1$, $RH = 10^{-2}$, and $T_{\text{reh}} = 10^3$ GeV (unless varied).

with the overall normalisation factor $A_{\text{turb}} = 0.255$. Note that the amplitude appears to scale with $(RH)^3$. This is not the case, as can be seen from approximating the logarithms in the spectral shape as $(a_* H_*/2\pi f_{\text{turb},2})^2 [1 + (f/f_{\text{turb},2})^4]^{-1/2}$, which gives the spectral scaling

$$S_{\text{turb}}(f) \propto \frac{1}{RH} \left(\frac{f}{f_{\text{turb},2}} \right)^3 \left[1 + \left(\frac{f}{f_{\text{turb},1}} \right)^{2.15} \right]^{-7.9} \left[1 + \left(\frac{f}{f_{\text{turb},2}} \right)^4 \right]^{-1/2} \quad (3.185)$$

that cancels the extra power in RH . The resulting GW spectra are shown in fig. 3.10 for different values of α , RH and T_{reh} in the left, middle, and right panel respectively. The spectrum shows the causal tail, proportional to f^3 for $f \ll f_{\text{turb},2}$, a frequency break at the scale of the turbulence, given by the eddy turn-over time τ_e (at $f_{\text{turb},2}$) and the peak at the initial scale of the perturbation at $f_{\text{turb},1}$ given by the mean bubble separation RH . Notably, the separation between the two characteristic frequencies depends on the transition strength α , which determines the fluid velocity and hence, on which scales the turbulent structures form.

3.5.7. Bubble collision spectrum

The GW spectrum from the energy stored in the scalar field has been studied extensively both numerically [150–152] and analytically [153, 154]. In the regime of highly relativistic bubble walls, where this signal becomes relevant, the bubble walls widths are highly Lorentz contracted, such that only one length scale – the mean bubble separation – is relevant. Therefore, the spectral shape is given by a single broken power law [147]

$$S_{\text{col}}(f) = \left(\frac{f}{f_{\text{col}}} \right)^{2.4} \left[\frac{1}{2} + \frac{1}{2} \left(\frac{f}{f_{\text{col}}} \right)^{1.2} \right]^{-4} \quad \text{with} \quad f_{\text{col}} = 0.49 \frac{a_* H_*}{RH} \quad (3.186)$$

with the frequency peak at f_{col} . We note here that the low frequency behaviour deviates from what would be expected from causality, as the signal rises with $f^{2.4}$ for $f \ll f_{\text{col}}$, instead of the expected f^3 behaviour from uncorrelated sources [155]. This is due to the simulations on which the spectrum is based not accounting for cosmic expansion. The exact impact of including the expansion on the low frequency part of the spectrum is however not yet clear [156]. The amplitude of the signal is given by

$$h^2 \Omega_{\text{GW}}(f) = \mathcal{R} h^2 A_{\text{col}} K_{\text{col}}^2 \frac{(RH)^2}{\max(c_s, v_w)^2} S_{\text{col}}(f). \quad (3.187)$$

Analogous to the previous two cases, the amplitude here scales quadratically in both the kinetic energy fraction as well as the mean bubble separation as can be seen in the left and middle panels of fig. 3.11. The overall normalisation found by numerical simulations is $A_{\text{col}} = 0.0026$ [147]. Note that we absorbed a factor of $((1 - P_f)/8\pi)^{2/3}$ into the normalisation compared to ref. [147], in order to express the amplitude in terms of RH instead of β/H .

Part II.

First-order phase transitions and gravitational waves from dark sectors

TransitionListener: A numerical tool for cosmological first-order phase transitions

This chapter is based on the publication [157]. I contributed to all aspects of this work.

4.1. Introduction

The prediction of a gravitational wave spectrum from a particle physics model poses the challenge to solve a multi-scale problem that spans many orders of magnitude in energy and length scale. These steps, depicted in fig. 4.1, begin at the microscopic particle description of the free energy density through the effective potential, which one has to compute and explore as a function of temperature to obtain the vacuum structure of the theory. Then one has to determine the decay rate of the false vacuum [117, 119] and to solve the hydrodynamics of the expanding bubbles [126, 158, 159] and the evolution of the true-vacuum fraction [160, 161]. Finally, these results have to be related to the GW spectra obtained from numerical simulations [134, 142, 145–147, 155, 162–166], redshifted through the cosmic history and compared to the sensitivity of (planned) detectors.

In general, these computational steps cannot be performed analytically. Instead, we have to resort to numerical methods. Tools that address this or parts of this computational pipeline exist: **BSMPT** [167–169] implements the whole pipeline and specialises in extended Higgs sectors and the electroweak phase transition, **PhaseTracer** [170, 171] provides robust multi-field phase tracing, **ELENA** [172] offers efficient single-field evolution with PTA likelihood interfaces, and **PT2GWFinder** [173] delivers a Mathematica-based workflow. Despite the numerous tools and progress on the computations, gaps in the modelling remain, particularly in the modelling of the thermodynamics during strong supercooling and the handling of multi-field potentials.

A large part of the work presented in this thesis was enabled by the development of the numerical tool **TransitionListener** (TL) [157], that addresses these limitations in several areas. It is built on the existing tool **CosmoTransitions** [174], which implements the exploration of the phase structure and the computation of the bounce action. We extended this by improving the numerical stability of these algorithms and implementing the computational steps that take us from the bounce action to the observability of the GW signals as described

in chapter 3. The code implements a self-consistent treatment of the true-vacuum fraction evolution, including the backreaction on the Hubble rate, and accounts for the reheating in the broken phase during percolation by considering local energy conservation at the bubble wall. It works with general multi-field effective potentials and automatically implements the one-loop corrections, computes bubble wall velocities in the local thermal equilibrium approximation [175, 176] and predicts the GW spectra using the latest simulation-calibrated templates [147]. Furthermore, the framework evaluates the sensitivity of current and planned detectors across twelve orders of magnitude in frequency for the GW signals and provides an interfaces to *PTArcade* [103] for pulsar timing likelihoods and enables Bayesian parameter inference through integration with the nested sampling tool *UltraNest* [177].

This chapter is structured as follows. First, we review the algorithms that were already implemented in the original tool *CosmoTransitions* [174] and that we use for the calculation of the bounce action (sec. 4.2). Next, we describe our treatment of the thermodynamics with two coexisting phases and present an efficient algorithm to compute the true-vacuum evolution in secs. 4.3 and 4.4. The details of the calculations of the phase transition parameters are then described in sec. 4.5. In sec. 4.6, we validate our computations with the established tool *BSMPT* and, finally, we discuss the validity of the results (sec. 4.7), before concluding with a summary in sec. 4.8.

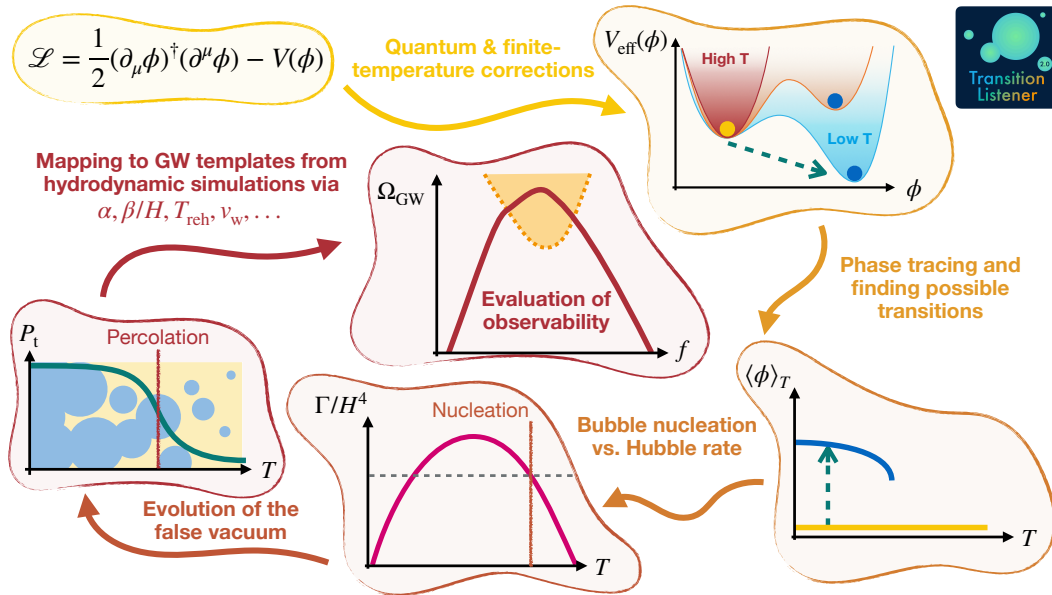


Figure 4.1.: Computational steps to go from a particle physics model to the evaluation of the observability of the predicted GWs from a first-order phase transition. This illustration was kindly provided by C. Tasillo.

4.2. Computation of the bubble nucleation rate

The implementation of the bounce action computation is based on the original program *CosmoTransitions* [174]. In the reference, the author developed the so-called path-deformation algorithm to compute the bounce action in multi-field potentials and implemented an algorithm to trace the temperature-dependent minima of a potential. In *TransitionListener*

the original routines of the path-deformation and shooting algorithm as well as the phase-tracing algorithm were only slightly modified for better numerical stability. Here, we will briefly review these algorithms for completeness.

4.2.1. Effective potential

As we have seen in chapter 3, the dynamics of the phase transition is encoded in the free energy of the thermodynamic system. For a general multi-scalar $\phi = (\phi_1, \phi_2, \dots)$ with the Lagrangian

$$\mathcal{L} \supset \frac{1}{2} (\partial_\mu \phi) (\partial^\mu \phi) - V_0(\phi), \quad (4.1)$$

the free energy, usually labelled as the effective potential, computed up to 1-loop corrections and with the ring diagrams resummed, reads

$$V(\phi, T) = V_0(\phi) + V_{\text{CW}}(\phi) + V_{\text{ct}}(\phi) + V_{\text{T}}(\phi, T) + V_{\text{daisy}}(\phi, T) + V_{\text{rad}}(T) - V_{T=0}(\mathbf{v}). \quad (4.2)$$

The first term is the temperature-independent tree-level part V_0 that receives quantum corrections through the Coleman-Weinberg potential [112]

$$V_{\text{CW}}(\phi) = \sum_i \pm \frac{n_i}{64\pi^2} m_i^4(\phi) \left[\ln \left(\frac{m_i^2(\phi)}{\bar{\mu}^2} \right) - C_i \right]. \quad (4.3)$$

Here, the sum runs over the particle species i that interact with the scalar fields, the sign is positive (negative) for bosons (fermions), n_i are the degrees of freedom, $\bar{\mu}$ is an arbitrary renormalisation scale and C_i is 3/2 for scalars and fermions and 5/6 for gauge bosons. As the quantum corrections come with UV divergences, the introduction of counterterms that cancel these is required, giving another contribution V_{ct} . At finite temperature, these corrections become temperature dependent and add an additional term to the effective potential

$$V_{\text{T}}(\phi, T) = \sum_i \pm \frac{n_i T^4}{2\pi^2} J_{\text{b/f}} \left(\frac{m_i^2(\phi)}{T^2} \right), \quad J_{\text{b/f}}(z^2) = \int_0^\infty dx x^2 \ln \left(1 \mp e^{-\sqrt{x^2+z^2}} \right), \quad (4.4)$$

which is given in terms of the thermal functions $J_{\text{b/f}}$ for bosons (b) and fermions (f). Infrared divergences of these corrections have to be cured by resumming the longitudinal, bosonic Matsubara zero-modes, which we implement by default in the Arnold-Espinosa scheme. This resummation gives the additional term [115]

$$V_{\text{daisy}}(\phi, T) = -\frac{T}{12\pi} \sum_{i \in B_{\text{L}}} n_i \left[(m_i^2(\phi) + \Pi_i(T))^{3/2} - m_i^3(\phi) \right]. \quad (4.5)$$

Alternatively, the Parwani resummation scheme [116] can be used that replaces the mass $m_i^2 \rightarrow m_i^2 + \Pi_i$ for all bosonic Matsubara modes in V_{T} . Finally, we have added two field-independent terms $V_{\text{rad}}(T) - V_{T=0}(\mathbf{v})$ to the potential. These are required to consistently relate the effective potential to the free energy in our thermodynamic treatment. The first term allows for additional degrees of freedom that are not coupled to ϕ , but still contribute to the free energy. The second term is a normalisation constant, ensuring that the energy density and pressure vanish at the global minimum $\phi = \mathbf{v}$ for $T = 0$.

4.2.2. Phase tracing algorithm

The prerequisite for the calculation of the dynamics of a vacuum decay is knowing the temperature-dependent vacuum structure of the system. In sec. 3.3 we have seen that this is given by the minimum of the free energy, i.e. the effective potential. Any minimum of

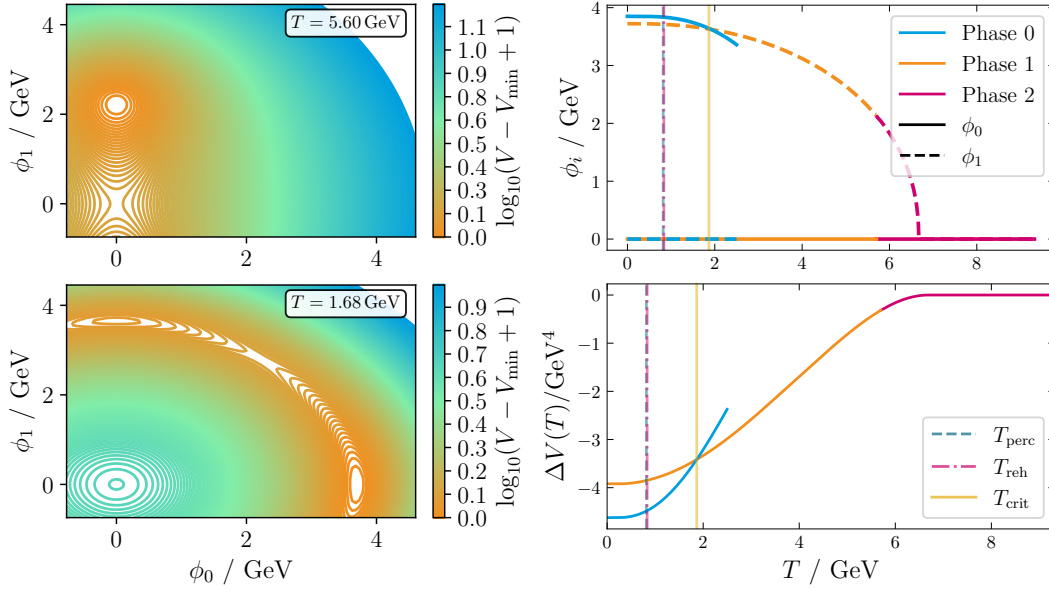


Figure 4.2.: *Left panels:* A two-field example potential at two different temperatures. At $T = 5.60$ GeV the potential has only one minimum at the ϕ_1 axis, at $T = 1.68$ GeV the potential developed an additional minimum on the ϕ_0 axis. *Right panels:* Phase structure obtained from the tracing algorithm for the two-field potential shown in the left panels. The model will be discussed in detail in sec. 5.3.2.

the potential satisfies $\partial V(\phi_{\min})/\partial \phi_i = 0$ for each scalar field direction ϕ_i . This minimum is temperature-dependent, so differentiating this condition yields

$$\frac{\partial^2 V}{\partial \phi_i \partial \phi_j} \frac{d\phi_{\min,j}}{dT} + \frac{\partial^2 V}{\partial \phi_i \partial T} = H_{ij}(\phi, T) \frac{d\phi_{\min,j}}{dT} + \frac{\partial^2 V}{\partial \phi_i \partial T} = 0, \quad (4.6)$$

where the repeating indices are summed over and H_{ij} denotes the Hessian matrix of the potential. As long as $\phi_{\min}(T)$ remains a minimum, the Hessian matrix is positive definite and by inverting H_{ij} , the equation can be solved for

$$\frac{d\phi_{\min,i}}{dT} = -H_{ij}^{-1} \frac{\partial^2 V}{\partial \phi_j \partial T}. \quad (4.7)$$

For a given minimum, the tracing algorithm uses this expression as a first prediction for the minimum ($\phi_{\min}^{\text{approx}}(T + \Delta T)$) after a temperature step ΔT . Then a gradient-free minimiser determines the precise location of the minimum $\phi_{\min}(T + \Delta T)$, by using $\phi_{\min}^{\text{approx}}$ as a starting point. The difference between these is used to adapt the step-size of the following point. These steps repeat to trace the minimum up in temperature until the maximum tracing temperature is reached or the phase vanishes, which is indicated by the Hessian obtaining a zero (or negative) eigenvalue. In practice, it is numerically more stable to set a bound on the ratio between maximal and minimal eigenvalue below which the Hessian is treated as singular. Once the vanishing of a phase is detected, the algorithm takes a small jump in temperature, minimises the potential to find a new minimum and appends it to the list of minima to trace. To ensure the full extent of the phase is found, the phase is then traced down in temperature, using the same procedure. These steps are repeated for all zero-temperature minima and minima found after a phase vanished. With all phases traced, redundant phases are then merged by comparing the distance in field space within a threshold and cross-over transitions are identified for phases terminating in saddle points.

To illustrate the phase tracing algorithm, we show an example two-field potential at two different temperatures in the left panel of fig. 4.2. At high temperatures, the field has only

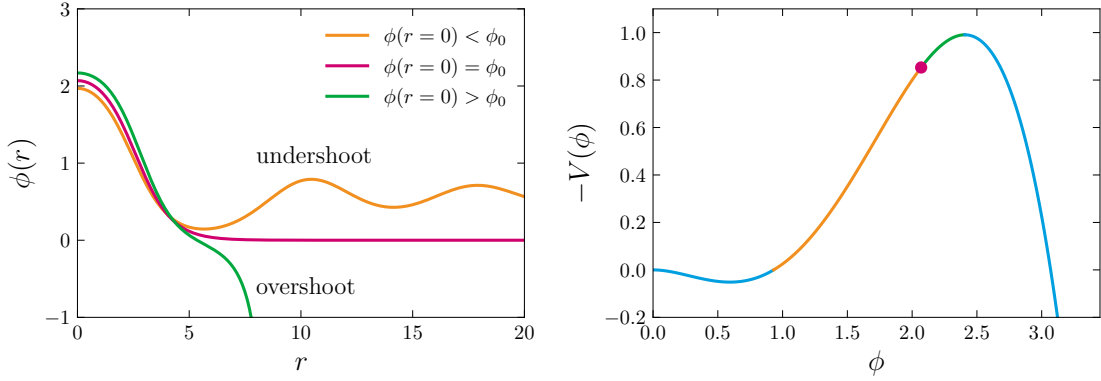


Figure 4.3.: *Left panel:* Solutions of the bounce eq. (3.127). The boundary condition $\phi(r \rightarrow \infty) = 0$ is overshoot by the green and undershoot by the orange solution. The purple solution satisfies the boundary condition. *Right panel:* Inverted potential. The field values of the orange region give undershoot solutions, the green overshoot solutions, while the purple dot marks the release point ϕ_0 that satisfies the desired boundary condition.

one minimum on the ϕ_1 axis, and at lower temperatures, it develops a second minimum on the ϕ_0 axis. The details of the model will be introduced in the next chapter (sec. 5.3.2). The result of the phase tracing algorithm is shown for this potential in the right panels of fig. 4.2. At high temperatures $T \gtrsim 2.5$ GeV only one phase is present, which has a cross-over transition into the ϕ_1 field direction (red dashed line). A very weak and fast first-order transition from phase 2 (red) to phase 1 (orange) around $T \approx 5.7$ GeV is treated as a crossover transition. At lower temperatures a local minimum develops in the ϕ_0 direction, which becomes the global minimum at the critical temperature. From here on the first-order phase transition can proceed, since the phase 0 (blue) is now energetically favoured, as shown in the bottom panel by the potential difference $\Delta V = V(\phi_i, T) - V(\phi = 0, T)$.

4.2.3. Path deformation algorithm

The determination of the decay rate of one phase to another requires the evaluation of the bounce action, as we saw in sec. 3.4. In the case of a one-dimensional effective potential, the bounce action can be solved using a shooting algorithm. The bounce equation has the analogy of a ball rolling down a hill described by the inverted potential with a friction term. Here, the release point ϕ_0 , where the field reappears after the tunneling, corresponds in this picture to the starting point from where the ball has to roll down so that it stops on top of the hill at $\phi = 0$. If the initial point is chosen too far up the hill $\phi > \phi_0$ the field rolls too far, overshooting the solution. This is shown as the green solution in the left panel of fig. 4.3, which corresponds to the green line segment in the potential values in the right panel. If the initial point is chosen too small $\phi < \phi_0$, the field will roll back to the minimum of $-V$ (orange line), undershooting the solution. The desired boundary condition $\phi(r \rightarrow \infty) = 0$ is only recovered for the correct release point ϕ_0 , shown as the purple dot in the potential.

The generalisation to a multi-field potential case was first developed in the code `CosmoTransitions` [174]. In this method, an initial guess for the tunneling path (a straight line) is parameterised as $\phi(x)$ with the normalisation $|\mathrm{d}\phi/\mathrm{d}x| = 1$. This parameterisation allows to split the bounce equation into a parallel and perpendicular part to the tunneling path

$$\frac{\mathrm{d}^2 x}{\mathrm{d} r^2} + \frac{2}{r} \frac{\mathrm{d} x}{\mathrm{d} r} = \frac{\partial}{\partial x} V(\phi(x), T) \quad \text{and} \quad \frac{\mathrm{d}^2 \phi}{\mathrm{d} x^2} \left(\frac{\mathrm{d} x}{\mathrm{d} r} \right)^2 = \nabla_{\perp} V(\phi, T), \quad (4.8)$$

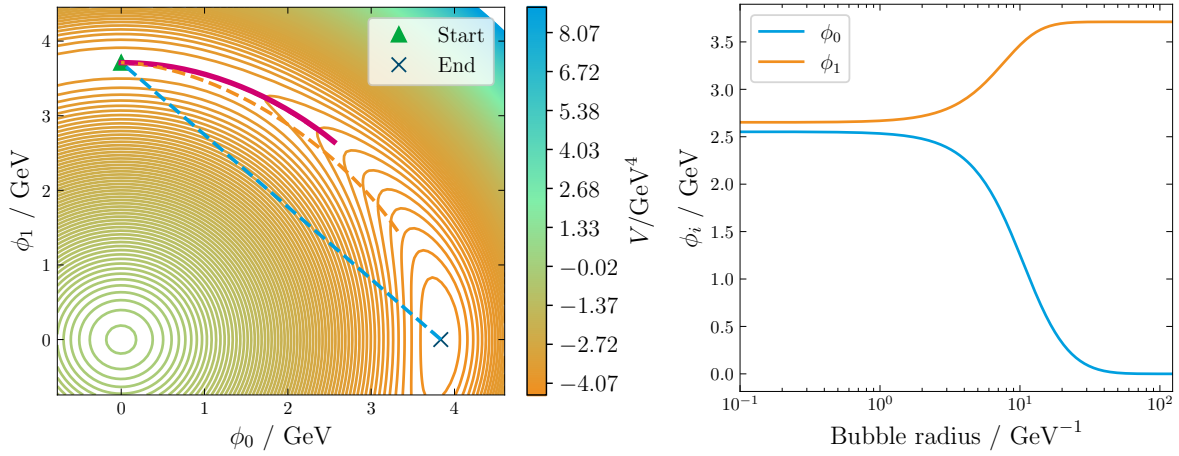


Figure 4.4.: *Left panel:* Path deformation algorithm for the tunneling in a two-dimensional potential. The initial guess (blue dashed line) is deformed in two steps to the final tunneling path (purple line). *Right panel:* Resulting bounce profile of the two fields. The model is discussed in detail in sec. 5.3.2.

where $\nabla_{\perp}$ denotes the perpendicular component of the derivative along the tunneling path x . The bounce equation is then solved along the path, giving $\phi(x(r))$. With this solution, the normal force on the tunneling path is computed through

$$\mathbf{N} = \frac{d^2\phi}{dx^2} \left(\frac{dx}{dr} \right)^2 - \nabla_{\perp} V(\phi, T). \quad (4.9)$$

To satisfy the perpendicular part of the bounce equation, the tunneling path is then deformed until the normal force vanishes, $\mathbf{N} = 0$. Using the new path, the bounce equation is solved again and the path is again deformed. These two steps are repeated until the path converges. An example of this is shown for a two-dimensional potential in the left panel of fig. 4.4. The initial guess of the tunneling path, connecting the false minimum (triangle) to the true minimum (cross) through a straight line (dashed blue line) is deformed in the first step to the dashed orange line and converges in a second step to the purple line. The resulting bounce profile of the two scalar fields along this tunneling path is shown in the right panel of the figure. Finally, using the field profile $\phi(r)$, the $O(3)$ symmetric bounce action, corresponding to thermal tunneling, is computed through

$$S_3(T) = 4\pi \int_0^{\infty} dr r^2 \left[\frac{1}{2} \sum_i \left(\frac{d\phi_i}{dr} \right)^2 + V(\phi, T) - V(\phi_f, T) \right], \quad (4.10)$$

where ϕ_f are the field values of the false-vacuum, i.e. the starting point of the tunneling. The computation of the nucleation rate is implemented as [119]

$$\Gamma(T) = T^4 \left(\frac{S_3(T)}{2\pi T} \right)^{3/2} \exp \left[-\frac{S_3(T)}{T} \right]. \quad (4.11)$$

4.3. Thermodynamics of two phases

The focus of the tool is the treatment of slow phase transitions, which are the first ones that will be probed by future experiments and where typical assumptions start to break down. To obtain an accurate description of the phase transition temperature and the subsequent redshift of the GW amplitude, it is critical to have an accurate description of the universe in the presence of two distinct phases. Here, we describe how we treat the evolution of the Hubble parameter and the energy densities during the phase transition.

4.3.1. Energy density from the effective potential

From the effective potential in eq. (4.2) and the phase structure obtained by the tracing algorithm, we can derive the thermodynamic properties of the early universe plasma as a function of temperature. Within a given phase $\phi_{\min}(T)$, the pressure p , entropy density s , and energy density ρ are obtained as

$$p = -V(\phi_{\min}, T), \quad (4.12)$$

$$s = \frac{\partial p}{\partial T} = -\frac{\partial V(\phi_{\min}, T)}{\partial T}, \quad (4.13)$$

$$\rho = Ts - p = V(\phi_{\min}, T) - T \frac{\partial V(\phi_{\min}, T)}{\partial T}. \quad (4.14)$$

Let us now compute the energy density in a given phase, which contains a few subtleties. First, we split the potential into a temperature-independent part $V_{T=0} = V_0 + V_{\text{cw}} + V_{\text{ct}}$ and temperature-dependent components ($V_{\text{T}}, V_{\text{daisy}}, V_{\text{rad}}$). With this, the energy density splits into the different terms

$$\rho(\phi, T) = \underbrace{V_{T=0}(\phi) - V_{T=0}(v)}_{\rho_{\text{vac}}} + \underbrace{V_{\text{T}} - T \partial_T V_{\text{T}}}_{\rho_{\text{rad}}} + \underbrace{V_{\text{rad}} - T \partial_T V_{\text{rad}}}_{\rho_{\text{rad,ext}}} + \underbrace{V_{\text{daisy}} - T \partial_T V_{\text{daisy}}}_{\rho_{\text{int}}} \quad (4.15)$$

$$= \rho_{\text{vac}} + \frac{\pi^2}{30} g_{\text{eff}}(T) T^4 + \frac{\pi^2}{30} g_{\text{eff}}^{\text{ext}}(T) T^4 + \rho_{\text{int}}. \quad (4.16)$$

These different components offer an intuitive interpretation. The first term accounts for the potential energy stored in the scalar field. The second term is the radiation energy of a non-interacting plasma, where we rewrote the thermal functions in terms of the effective degrees of freedom we encountered in sec. 2.3.3. In the third term, we collected the energy density of the particles that do not obtain a mass from the scalar fields and the last term contains the energy stored in plasma interactions mediated by the gauge bosons and scalars. This last term can be written as

$$\rho_{\text{int}} = \frac{T^2}{8\pi} \sum_{i \in B_{\text{L}}} (m_i^2(\phi) + \Pi_i(T))^{1/2} \frac{\partial \Pi_i(T)}{\partial T}. \quad (4.17)$$

Since the squared mass m_i and thermal mass Π_i scale quadratically with the couplings to the scalars, $m_i^2 \propto g^2 \phi_{\min}^2$ and $\Pi_i \propto g^2 T^2$, this plasma energy is typically suppressed with g^3 compared to the other contributions. Additionally, the thermal masses are typically computed in the hard thermal mass approximation $T \gg m$, resulting in $\Pi_i \propto T^2$. If a transition is supercooled ($\phi_{\min} \gg T$) this leads to an unphysical scaling of the energy density in the broken phase of $\rho_{\text{int}} \propto m T^2$, as this approximation is used outside the range of validity. Here, the thermal mass should be computed without the high-temperature approximation. Taking the example of the self-energy of a scalar field from a $\lambda \phi^4$ term (cf. eq. (3.106)), the thermal part can be written as [104]

$$\Pi(T, m) = \frac{\lambda m T}{2 \pi^2} \sum_{n=1}^{\infty} \frac{1}{n} K_1 \left(\frac{nm}{T} \right) = \begin{cases} \frac{\lambda}{2} \frac{T^2}{12} & \text{for } T \gg m \\ \frac{\lambda}{2} \left(\frac{m T^3}{2 \pi^3} \right)^{1/2} e^{-m/T} & \text{for } T \ll m \end{cases} \quad (4.18)$$

where K_1 is the modified Bessel function of the first kind. We see here that in the non-relativistic limit, the thermal self-energy receives the Boltzmann suppression factor $e^{-m/T}$. For these reasons, we neglect ρ_{int} in the computation of the energy density.

Radiation energy density and degrees of freedom

Within TL we compute the radiation energy density in terms of the thermal functions (eq. (3.80)) that can be tabulated, allowing for an efficient evaluation

$$\rho_{\text{rad}} = - \sum_a n_a \left(\frac{3T^4}{2\pi^2} J_{\text{b/f}}(z_a) - \frac{m^2 T^2}{\pi^2} \frac{d}{dz_a} J_{\text{b/f}}(z_a) \right). \quad (4.19)$$

Another subtlety comes from the gauge sector. Its contribution to the thermal corrections of the potential in the R_ξ gauge has the following form, as we saw in sec. 3.3,

$$V_{\text{T}}^{\text{gauge}} = \frac{T^4}{2\pi^2} \sum_g \left[3J_b \left(\frac{m_g^2}{T^2} \right) - J_b \left(\frac{\xi m_g^2}{T^2} \right) \right]. \quad (4.20)$$

In the Landau gauge $\xi = 0$, the second term gives a field-independent (pure radiation) contribution, which is often neglected. We include this term in the effective potential to ensure the correct number of degrees of freedom from gauge and Goldstone bosons in the true- and false-vacua when computing the pressure and energy densities.

4.3.2. Hubble expansion with two distinct phases

The defining feature of a cosmological first-order phase transition is the coexistence of two separate phases with different thermodynamic properties. In a fast transition with $\beta \gg H$, the expansion of the universe can be safely neglected in the analysis. However, we saw in sec. 3.5 that the signals with large amplitudes, i.e. the signals that will be probed first, come from slow transitions. In these transitions, the influence of the expansion can be significant and common approximations that neglect this effect start to break down.

To account for the Hubble expansion during the phase transition, a first step is to derive the evolution of the true-vacuum energy density and temperature. We will do this here by assuming that the bubbles containing the new phase are statistically homogeneous in their distribution and we define the volume-averaged energy density and pressure using the true-vacuum fraction $P_{\text{t}}(t)$ (eq. (3.135))

$$\bar{\rho} = P_{\text{t}}\rho_{\text{t}} + (1 - P_{\text{t}})\rho_{\text{f}} \quad \text{and} \quad \bar{p} = P_{\text{t}}p_{\text{t}} + (1 - P_{\text{t}})p_{\text{f}}. \quad (4.21)$$

Here, the pressure and energy density in the true- $\phi_{\text{t}}(T)$ and false-vacuum $\phi_{\text{f}}(T)$ are derived from $V(\phi_{\text{t/f}}, T)$ using eqs. (4.12) and (4.14). Assuming additionally that the overdensities are small, we can write the Friedman and continuity equation as

$$H^2 = \frac{8\pi G}{3} \bar{\rho} \quad \text{and} \quad \frac{d\bar{\rho}}{dt} = -3H(\bar{\rho} + \bar{p}). \quad (4.22)$$

With these assumptions, we can now turn to derive the evolution of the true-vacuum energy density. We begin by writing the continuity equation for the volume averaged quantities, that have to satisfy

$$\bar{T}^{\mu\nu}_{;\mu} = \frac{d\bar{\rho}}{dt} + 3H(\bar{\rho} + \bar{p}) = 0, \quad (4.23)$$

This can be split into equations for the components of the two phases

$$(T_{\text{f}})^{\mu\nu}_{;\mu} = \frac{d\rho_{\text{f}}}{dt} + 3H(\rho_{\text{f}} + p_{\text{f}}) = \Phi_{\text{f}}, \quad (4.24)$$

$$(T_{\text{t}})^{\mu\nu}_{;\mu} = \frac{d\rho_{\text{t}}}{dt} + 3H(\rho_{\text{t}} + p_{\text{t}}) = \Phi_{\text{t}}, \quad (4.25)$$

where we allowed energy fluxes $\Phi_{f/t}$ between both phases. With this, we can rewrite the volume averaged equation as

$$\bar{T}^{\mu\nu}_{;\mu} = (1 - P_t)\Phi_f + P_t\Phi_t + \dot{P}_t(\rho_f - \rho_t) = 0, \quad (4.26)$$

where the last term describes the conversion of false to true-vacuum. If the phase transition is sufficiently strong, we can assume that the bubble expansion occurs with a detonation profile (cf. sec. 3.5.1), where the false-vacuum outside the bubbles remains unperturbed. For these cases, no heat transfer from the true- to the false-vacuum occurs and we have $\Phi_f = 0$. However, the conversion of false-vacuum into true-vacuum releases latent heat, therefore, we have $\Phi_t \geq 0$. In total, we get

$$\bar{T}^{\mu\nu}_{;\mu} = P_t\Phi_t + \dot{P}_t(\rho_f - \rho_t) = 0 \quad (4.27)$$

$$\Rightarrow \Phi_t = \frac{\dot{P}_t}{P_t}(\rho_f - \rho_t). \quad (4.28)$$

Hence we have the evolution of the separate energy densities

$$\frac{d\rho_f}{dt} + 3\frac{\dot{a}}{a}(\rho_f + p_f) = 0, \quad (4.29)$$

$$\frac{d\rho_t}{dt} + 3\frac{\dot{a}}{a}(\rho_t + p_t) = \frac{\dot{P}_t}{P_t}(\rho_f - \rho_t). \quad (4.30)$$

From the first equation, we recover the usual entropy conservation equation of the false vacuum $d/dt(sa^3) = 0$.

For slow transitions, the constant vacuum energy density leads to a slower redshift of the false-vacuum energy density compared to the true-vacuum. In the conversion of false- to true-vacuum, this difference in the energy density leads to a reheating of the true-vacuum and creates entropy in the process, which is captured by the right hand side of the second equation. In fig. 4.5, we show an example of the evolution of the energy density in both phases. In this example, the total energy density in the false vacuum (solid blue line) is dominated by the vacuum energy (dashed-dotted blue line) before percolation, which slows down the redshift of the total energy density, shown in purple. Around percolation, the majority of the conversion from false- to true-vacuum occurs and the redshift of the true-vacuum determines the evolution of the total energy density again.

In this derivation, we have assumed that the energy density in each bubble is homogeneous and that every bubble shares the same temperature, regardless of the time it nucleated. Additionally, we assumed a detonation profile such that there is no energy flux from the true-vacuum to the false-vacuum. We, however, expect the impact of this to be small, since only a finite fluid shell around the bubble is set into motion and reheated by the bubble expansion. A detailed analysis of these effects would require to solve the expansion and reheating in a lattice simulation.

4.4. True vacuum evolution

With an expression for the evolution of the energy densities during the phase transition, we can turn to the arguably most challenging equation to solve, the true-vacuum fraction. We saw that it is given in terms of time as (cf. sec. 3.4.2)

$$1 - P_t(t) = e^{-I(t)} = \exp\left(-\frac{4\pi v_w^3}{3} \int_{t_{\text{init}}}^t dt' \Gamma(t') \frac{a^3(t')}{a^3(t)} \left[\int_{t'}^t dt'' \frac{a(t)}{a(t'')}\right]^3\right). \quad (4.31)$$

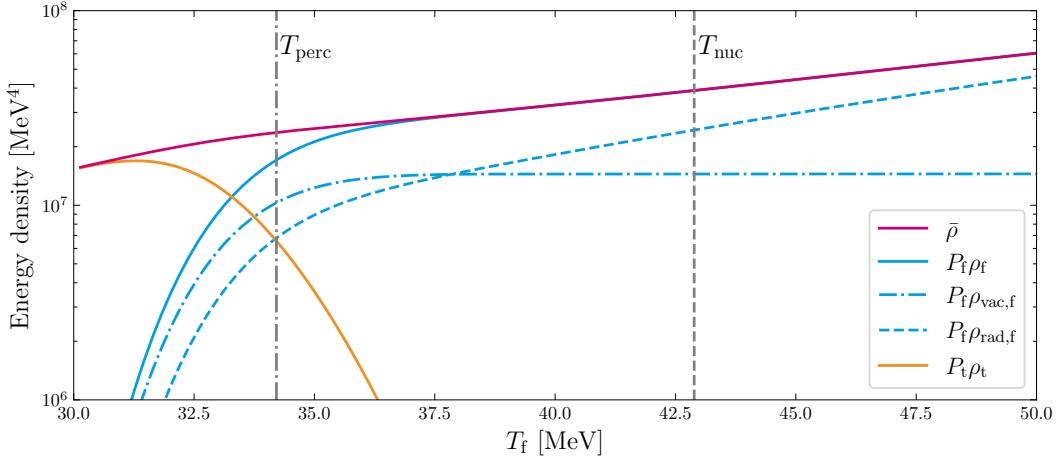


Figure 4.5.: Example of the evolution of the energy density in a first-order phase transition. The total energy density is composed of the vacuum energy density ρ_{vac} that dominates over the radiation energy density in the false vacuum ρ_f from nucleation on. Around percolation, where the majority of the false vacuum is converted into the true-vacuum, the vacuum energy reheats the true-vacuum.

In practice, it is more convenient to express it in terms of the false-vacuum temperature. This can be done by using the continuity eq. (4.29) and expressing it as [122]

$$\frac{dT_f}{dt} = -3H \frac{\rho_f + p_f}{\partial \rho_f / \partial T_f} = -3HT_f c_{s,f}^2, \quad \text{where} \quad c_{s,f}^2 = \frac{\partial_T V_f}{T_f \partial_T^2 V_f}. \quad (4.32)$$

The speed of sound in terms of the effective potential follows directly from expressing $c_s^2 = dp/d\rho$ through eqs. (4.12) and (4.14). With this, the percolation integral $I(T)$ in terms of temperature becomes

$$I(T) = \frac{4\pi}{3} v_w^3 \int_T^{T_{\text{init}}} \frac{dT'}{H(T')T'} \frac{\Gamma(T')}{3c_s^2(T')} \frac{a^3(T')}{a^3(T)} \left[\int_T^{T'} \frac{dT''}{H(T'')T''} \frac{1}{3c_s^2(T'')} \frac{a(T)}{a(T'')} \right]^3. \quad (4.33)$$

Here, the difficulties become apparent. The integral depends recursively on itself through the Hubble rate that depends on the true-vacuum fraction, see eqs. (4.21) and (4.22). Additionally, the evaluation of the bounce action S_3 in the nucleation rate is numerically costly and the integration boundary (usually $T = T_{\text{perc}}$) is a priori unknown. That makes it difficult to choose a well suited integration step-size to straightforwardly integrate eq. (4.33) up to the percolation or final temperature. In the code, we implement two approaches to deal with this problem.

4.4.1. Algorithm I: Fixed step-size integration

The first approach addresses the problem of the unknown integration boundary by finding a numerically cheap approximation of the percolation temperature. This is based on the realisation that the false-vacuum fraction is the exponential of a rapidly changing function, where the main contribution to the function comes from a small temperature range around the percolation temperature. This indicates that we can make a saddle point approximation of the integral, as shown by refs. [178, 179].

Therefore, we approximate the nucleation rate as an exponential function around the percolation time

$$\ln \Gamma(t) = \ln \Gamma(t_{\text{perc}}) \left(1 + \frac{d}{dt} \ln \Gamma(t) \Big|_{t_{\text{perc}}} (t - t_{\text{perc}}) + \mathcal{O}((t - t_{\text{perc}})^2) \right) \quad (4.34)$$

$$\Rightarrow \Gamma(t) \approx \Gamma_{\text{perc}} e^{\beta(t-t_{\text{perc}})} \quad \text{with} \quad \beta \equiv \frac{d}{dt} \ln \Gamma \Big|_{t_{\text{perc}}} . \quad (4.35)$$

By additionally neglecting the expansion factors $a(t')/a(t)$ for the moment, we can compute $I(t)$ analytically as [178]

$$I(t) \approx \frac{4\pi}{3} v_w^3 \int_{-\infty}^t dt' \Gamma_{\text{perc}} e^{\beta(t'-t_{\text{perc}})} (t - t')^3 = \frac{8\pi}{\beta^4} v_w^3 \Gamma_{\text{perc}} e^{\beta(t-t_{\text{perc}})} , \quad (4.36)$$

where we additionally send the lower integration boundary to $-\infty$. We can express this in terms of temperature as

$$I(T) \approx \frac{8\pi v_w^3}{\beta/H^4} \frac{\Gamma(T)}{H^4} . \quad (4.37)$$

From this, we can devise a percolation criterion using $I_{\text{perc}} = \ln(0.71)$ and use a simple root finding algorithm to solve for T_{perc} , by requiring the following to vanish

$$C_{\text{perc}}(T) = \frac{1}{\beta/H} \left(\frac{\Gamma(T)}{H^4(T)} \right)^{1/4} \left(\frac{8\pi v_w^3}{I_{\text{perc}}} \right)^{1/4} - 1 . \quad (4.38)$$

Note here that the evaluation of this criterion requires the computation of the bounce action at two points, at $\Gamma(T)$ and at $\Gamma(T + \Delta T)$ to obtain β/H through a numerical derivative. Using this approximate value for the percolation temperature, we choose a step-size in the integration of eq. (4.33) that balances accuracy and computational cost. Note that this algorithm relies on the crucial assumption that we can approximate the nucleation rate as an exponential, i.e. a monotonically increasing function of temperature.

For the scenario where the effective potential has a non-vanishing potential barrier at zero temperature, this however does not hold anymore. At zero temperature, S_3 will be a constant and hence S_3/T will increase as $T \rightarrow 0$. Here, the approximate transition speed can become zero or even negative $\beta \leq 0$ which is unphysical. Instead, the nucleation rate should be modelled around the minimum of S_3/T as a Gaussian

$$\Gamma \approx \Gamma_{\text{perc}} e^{-\frac{\alpha}{2}(t-t_{\text{perc}})^2} \quad \text{with} \quad \alpha \equiv \frac{d^2}{dt^2} \ln \Gamma \Big|_{t_{\text{perc}}} , \quad (4.39)$$

which allows to derive a similar criterion to eq. (4.38). The finite difference evaluation of the second derivative of Γ , however requires three bounce evaluations [180]. This increases the numerical cost to find an approximate value for the percolation temperature by a factor of 3/2. Therefore, we adopt a different strategy in the second algorithm.

4.4.2. Algorithm II: Adaptive integration

The second approach is based on the realisation that the integral eq. (4.33) can be reformulated into a system of differential equations. It is of the general form

$$J_n(T) \equiv \int_T^{T_{\text{max}}} dT' \gamma(T') R(T, T')^n , \quad \text{with} \quad R(T, T') \equiv \int_T^{T'} d\tilde{T} \nu(\tilde{T}) . \quad (4.40)$$

Remembering the Leibniz integral rule, the derivative of $R(T, T')$ is simply $\partial_T R(T, T') = -\nu(T)$ and the derivatives of J_n become

$$\frac{\partial J_n(T)}{\partial T} = \begin{cases} -\gamma(T) & \text{if } n = 0, \\ -n \nu(T) J_{n-1}(T) & \text{if } n \geq 1. \end{cases} \quad (4.41)$$

For the percolation integral we have $I(T) = 4\pi/3 v_w^3 J_3(T)$,

$$\gamma(T) \equiv \frac{a^3(T)\Gamma(T)}{3c_s^2(T)H(T)T}, \quad \text{and} \quad \nu(T) \equiv \frac{1}{3c_s^2(T)H(T)Ta(T)}. \quad (4.42)$$

This allows the use of an ODE integration scheme with adaptive step-size and error control to integrate these 4 coupled equations (J_0, J_1, J_2, J_3) until the percolation or final temperatures are reached. This method does not require the a priori knowledge of the percolation temperature and allows for control over the desired accuracy. We find this algorithm to work well in the cases of strong supercooling. There, the initial cost of finding a suitable step-size is balanced out by the larger steps the integrator can take in the region between critical temperature and percolation, where $P_t \approx 0$ and $\dot{P}_t \approx 0$.

4.4.3. Iterative solution

With the solution methods at hand, we can sketch the full algorithm to solve the true vacuum fraction as depicted in fig. 4.6.

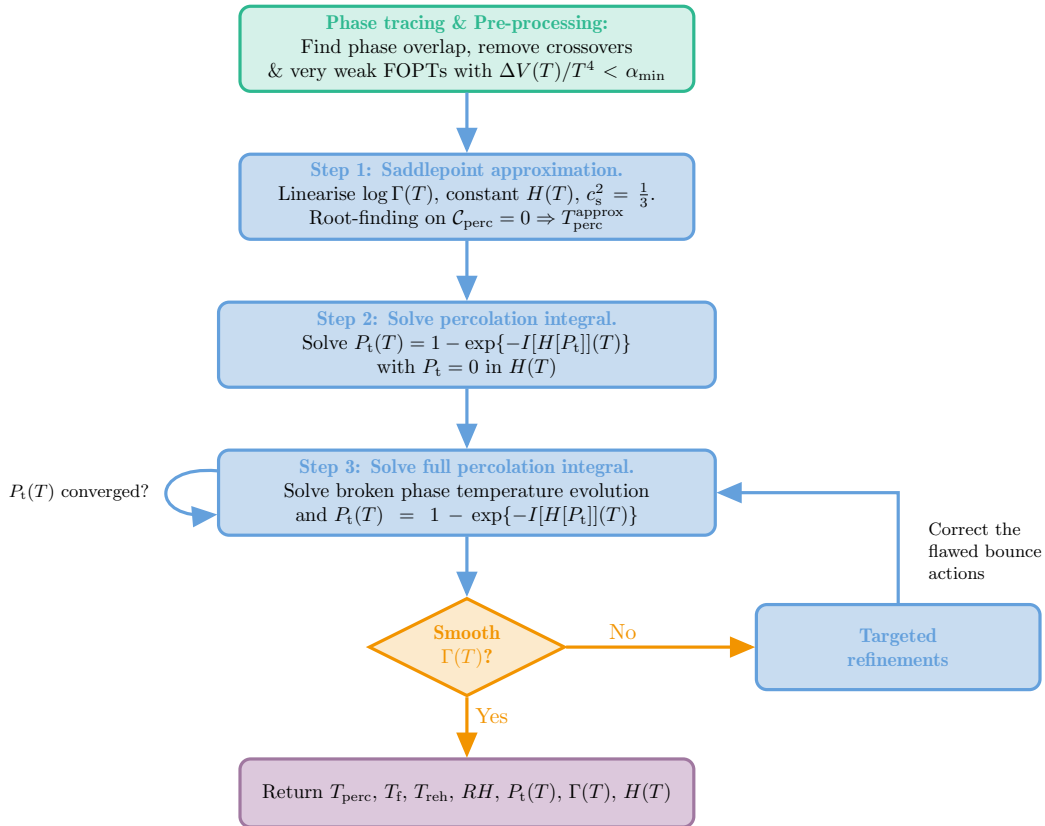


Figure 4.6.: Flowchart of the structure of the percolation algorithm.

Phase tracing and pre-processing:

The first step is the phase tracing and identification of suitable phase transitions. Typically, phase transitions that occur over a very small fraction of the Hubble time and only release a

small amount of energy are of less interest from the viewpoint of GW emission. To save computational costs, we implement an optional threshold that can filter out very weak transitions. If the approximate transition strength lies below a certain value $\max_T(\Delta V(T)/T^4) < \alpha_{\min}$, we treat the transition as cross-over and do not compute the GW signal. Here, $\max_T$ denotes the maximal value the argument takes over the coexistence of the two phases.

Step 1: Saddlepoint approximated T_{perc} :

In the case of the fixed step-size approach, we first determine the approximate percolation temperature through criterion eq. (4.38). The step-size is then determined by the distance in temperature to the critical temperature and the number of desired action evaluations $\Delta T = (T_{\text{crit}} - T_{\text{perc}}^{\text{approx}}) \cdot w/N_{\text{action}}$. Here, the weighting factor w determines how many steps should approximately lie before and after percolation.

Step 2: Solution of the simplified percolation integral:

With the temperature step-size determined, we integrate the percolation integral either with the fixed step-size or through the formulation as an ODE with an adaptive step-size. In a first approximation, we use $P_t(T) = 0$ in the Hubble rate. In this step, we cache all the bounce action evaluations for later reuse.

Step 3: Solution of the full percolation integral:

With the first approximation of the percolation and final temperatures and the false vacuum fraction, we can refine the Hubble rate by recomputing it with the true-vacuum fraction obtained in the previous step, $H(T, P_t(T))$. We solve again the percolation integral, now with the updated Hubble rate. This is numerically very cheap, since we can reuse the cached bounce action evaluations from the previous step. We repeat this refining of the false-vacuum fraction until the change in percolation and final temperature converge below a threshold.

Bounce action accuracy control:

In some cases, the path-deformation or tunneling accuracy settings do not give a sufficiently smooth bounce action, which leads to jumps in the nucleation rate. To catch these cases, the algorithm fits a quadratic polynomial through $\log_{10} \Gamma/H^4$ around the percolation temperature. If any points deviate more than a threshold (a factor of 10), they are recomputed with increased accuracy settings.

Result:

The resulting true-vacuum fraction computed with this algorithm is shown in the right panel of fig. 4.7 for an ultra-slow transition ($(\beta/H)_{RH} = 3.3$, see next section eq. (4.45)). The dashed blue line shows the first approximation of the false-vacuum fraction, which sets $P_t = 0$ in the Hubble parameter. The subsequent iterations with $P_t \neq 0$ lead to a less rapid expansion, since the radiation (matter) energy density in the true-vacuum redshifts with a^4 (a^3), while the false-vacuum energy density is dominated by constant vacuum energy. This reduces the Hubble expansion and leads to an earlier completion and larger final temperature compared to the first approximation.

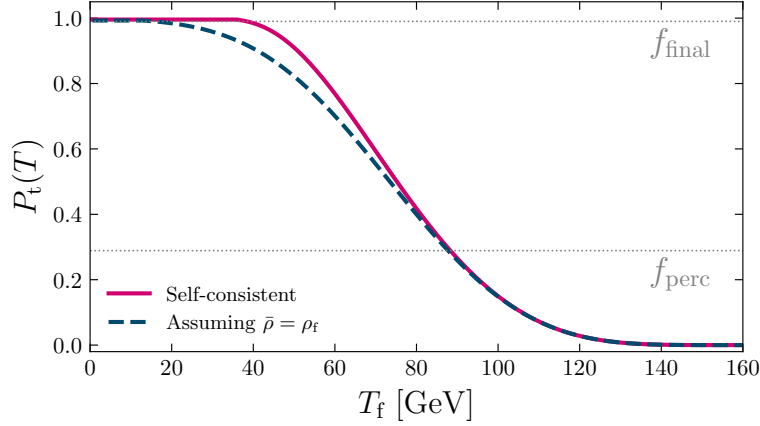


Figure 4.7.: Approximate (dashed line) and self-consistent (solid line) solution of the true vacuum fraction for an ultra-slow transition with $(\beta/H)_{\text{RH}} = 3.3$ and $\alpha = 10$ in the example $U(1)'$ model (app. B.1). The corresponding parameter point is $g = 1.237, \lambda = 0.039$ and $v = 1$ TeV.

4.4.4. Transition temperature

We solve the percolation integral until the final temperature is reached, here defined through $P_t(T_f) = 0.99$. From the resulting true-vacuum fraction, we can extract the nucleation temperature through the criterion that the number of bubbles per Hubble volume is 1. This is given by

$$N(T_{\text{nuc}}) = \frac{4\pi}{3} \int_{t_{\text{init}}}^{t_{\text{nuc}}} dt \frac{\Gamma(t)(1 - P_t(t))}{H^3(t)} = 1. \quad (4.43)$$

The next transition milestone, the percolation temperature, is then similarly obtained by solving $P_t(T_{\text{perc}}) \simeq 0.28957$ [122, 125] for T_{perc} .

4.5. Computation of the phase transition parameters

In this section, we give more details on the computation of the phase transition parameters and compare them to common approximations found in the literature. To demonstrate the differences between the implemented calculations and the common approximations we use an example model consisting of a scalar and a gauge boson charged under a $U(1)'$ symmetry, that we describe in app. B.1.

Mean bubble separation:

Using the true-vacuum fraction, we can compute the mean bubble separation using eqs. (3.172) and (3.171), expressed in terms of temperature

$$R_{\text{sep}}(T) = \frac{1}{n(T)^{1/3}} = \left[\int_T^{T_{\text{max}}} dT' \frac{\Gamma(T')}{H(T')T'} \frac{1 - P_t(T')}{3c_s^2(T')} \left(\frac{a(T')}{a(T)} \right)^3 \right]^{-1/3}. \quad (4.44)$$

It is convenient to express the mean bubble separation as a fraction of the Hubble radius at percolation, which we define as $RH \equiv R_{\text{sep}}(T_{\text{perc}})H(T_{\text{perc}})$. To keep comparability with the literature, we additionally define the mapping to the transition speed as

$$\left(\frac{\beta}{H} \right)_{RH} \equiv \left(\frac{8\pi}{f_{\text{perc}}} \right)^{1/3} \frac{\max(v_w, c_s)}{RH}. \quad (4.45)$$

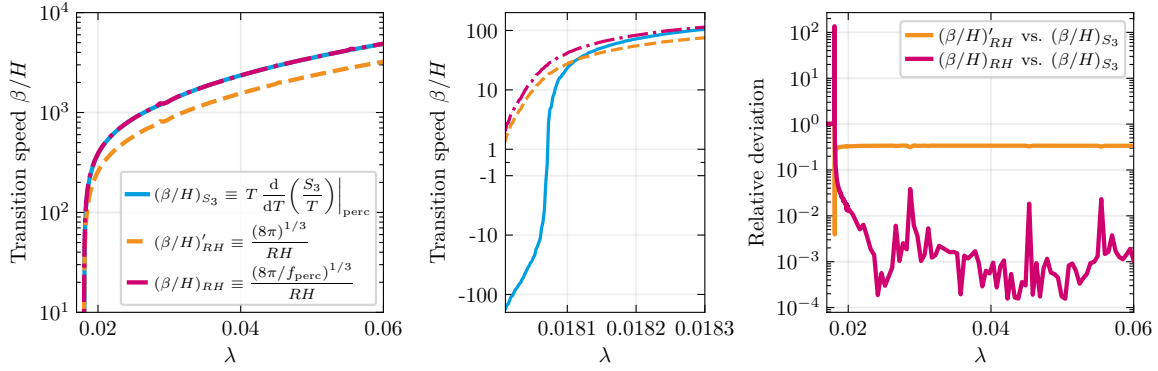


Figure 4.8.: Transition speed for the example $U(1)'$ example model (app. B.1) that exhibits strong supercooling with smaller self-coupling. Here, the gauge coupling and VEV are fixed to $g = 1$ and $v = 100$ MeV.

Note that the factor f_{perc} is usually omitted in the literature and leads to a deviation of $1/f_{\text{perc}}^{1/3} \simeq 1.51$. We derive the origin of this factor in app. B.3. In order to compare this to the commonly used definition of the transition speed, we also define

$$\left(\frac{\beta}{H} \right)_{S_3} \equiv T \frac{d}{dT} \left(\frac{S_3}{T} \right) \Big|_{\text{perc}}, \quad (4.46)$$

as found in the literature [122].

Fig. 4.8 shows the results of the mean bubble separation mapped to the transition speed for a scan over the self-coupling $\lambda \in [0.018, 0.06]$ of the example model, where we fixed $g = 1$ and $v = 100$ MeV. The blue line shows the approximation of $(\beta/H)_{S_3}$ found through the temperature derivative of the bounce action S_3/T and the orange dashed line shows the result of the mapping of RH to β/H , neglecting the factor accounting for the true-vacuum fraction, as often done in the literature. Finally, the purple dashed-dotted line shows the results implemented in TL via eq. (4.45). In the right panel, we see that the blue and purple curves agree well for $\beta/H > 100$, but start to strongly disagree for slower phase transitions, where $(\beta/H)_{S_3}$ even becomes negative. This indicates that the nucleation rate is no longer well approximated as an exponential function here, but should be represented as a Gaussian (cf. eq. (4.39)). The dashed orange curve shows that neglecting the factor $f_{\text{perc}}^{-1/3}$ leads to a systematic underestimation of the transition speed.

Transition strength:

As discussed in sec. 3.5.4, the strength of a phase transition is defined as the difference in the pseudo-trace of the energy-momentum tensor of the two phases

$$\alpha = \frac{\bar{\theta}_f(T_{\text{perc}}) - \bar{\theta}_t(T_{\text{perc}})}{3(\rho_f(T_{\text{perc}}) + p_f(T_{\text{perc}}))} \quad \text{with} \quad \bar{\theta}_i(T) = \left(\rho_i(T) - \frac{p_i(T)}{c_{s,i}^2(T)} \right). \quad (4.47)$$

Here $i = (t, f)$ labels the two vacua and $c_{s,i}(T)$ is the speed of sound in the respective phase. Other definitions of α in the literature, using $\Delta\rho$ or Δp instead of $\Delta\bar{\theta}$ were shown to under- or overestimate the energy available to the GW signal [127, 128]. One other often-used approximation is the assumption of a purely relativistic fluid with $c_{s,i}^2 = 1/3$. Here, the

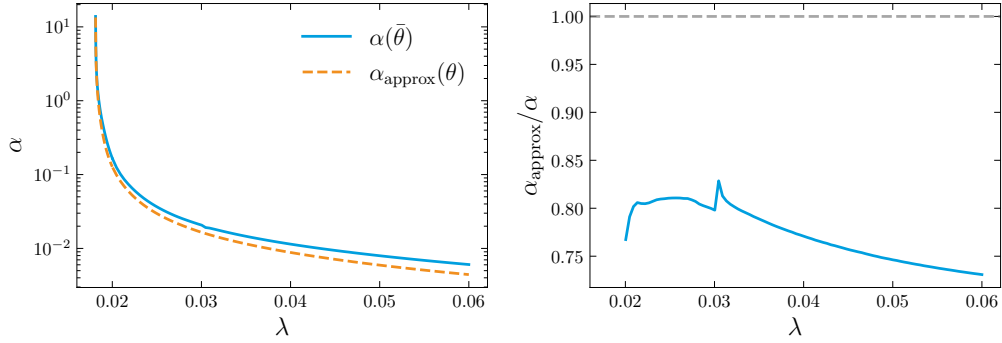


Figure 4.9.: Transition strength α for a scan over the self-coupling $\lambda \in [0.018, 0.06]$ of the $U(1)'$ example model (app. B.1). The other model parameters are fixed to $g = 1$ and $v = 100$ MeV.

pseudo-trace reduces to the trace of the energy-momentum tensor, $\theta = g_{\mu\nu}T^{\mu\nu} = \rho - 3p$, and the definition of α becomes equivalent to

$$\alpha_{\text{approx}} = \left. \frac{\Delta V(T) - \frac{1}{4}T\partial_T\Delta V(T)}{\rho_{\text{f}}^{\text{rad}}(T)} \right|_{T_{\text{perc}}} . \quad (4.48)$$

This approximation can still have a significant impact on the transition strength as we show in fig. 4.9, again for a scan over the self-coupling $\lambda \in [0.018, 0.06]$ of the $U(1)'$ model, while fixing $g = 1$ and $v = 100$ MeV. In the left panel, the transition strength computed from the pseudo-trace eq. (4.47) is shown in blue, while the approximation with $c_s^2 = 1/3$ is shown in orange. Here we can clearly see the differences from taking into account a variable speed of sound. These reach up to 25% as shown in the left panel and come here primarily from the change in the SM effective degrees of freedom, that we assumed to be in kinetic equilibrium with the new model states.

Reheating temperature:

A typical approximation of the temperature after a phase transition can be made by the instantaneous reheating assumption. Here, one assumes that the phase transition is fast compared to the Hubble expansion, such that energy conservation dictates the temperature after the phase transition. This translates to [122]

$$T_{\text{reh}}^{\text{approx}} = T_{\text{perc}} (1 + \alpha)^{1/4} . \quad (4.49)$$

For strong (and slow) transitions, this approximation becomes increasingly inaccurate as it neglects the effect of the cosmic expansion. Instead, we compute the reheating temperature from the evolution of the true-vacuum energy density that we derived in the previous section. We compute it as the true-vacuum temperature at the percolation temperature in the false-vacuum $T_{\text{reh}} = T_{\text{t}}(T_{f,\text{perc}})$. The left panel of fig. 4.10 shows the resulting reheating temperature as a function of the transition strength α (blue line). It approaches a constant with increasing α , as expected: For strong supercooling, the energy density is dominated by the constant vacuum energy density, which sets the reheating temperature and thus the result becomes independent on the percolation temperature. Instead, the reheating temperature computed with the approximation eq. (4.49) shows deviations from this behaviour and rises at strong supercooling $\alpha \gtrsim 10^3$. In this example, the approximation leads to deviations of up to $\mathcal{O}(10\%)$ as shown in the right panel.

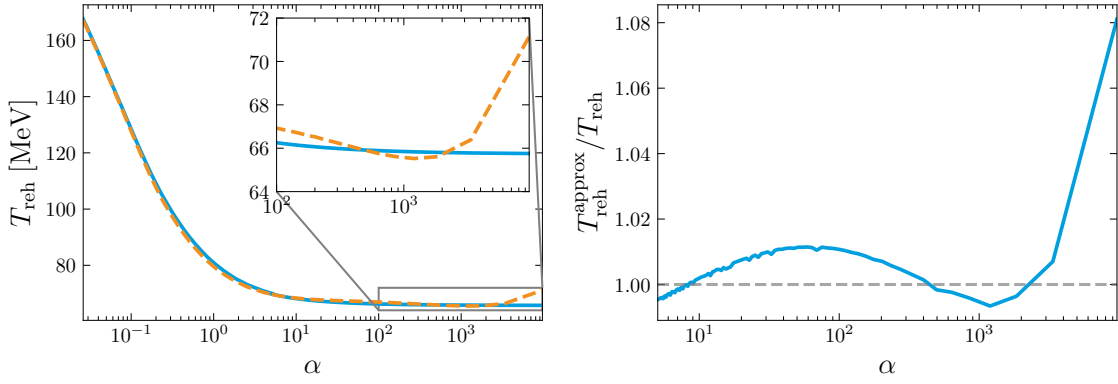


Figure 4.10.: One dimensional scan over the gauge coupling $g \in [0.35, 5]$ of example $U(1)'$ model (app. B.1) with $v = 1 \text{ GeV}$ and $\lambda = 10^{-3}$. *Left:* Reheating temperature (blue) and approximation eq. (4.49) (orange) as a function of the transition strength α . *Right:* Difference between the approximation and the full calculation.

4.5.1. Bubble wall velocity

We saw in sec. 3.5.1, that the energy available to produce GWs depends on the expansion dynamics of the bubbles in the plasma. For a precise description, we require the value of the bubble wall velocity to derive the hydrodynamic profiles. A general computation of the bubble wall velocity would include the solution of the Boltzmann equation to describe the phase space distribution of the particle species around the wall. This integro-differential equation is, in general, very difficult and numerically expensive to solve. Nonetheless, specialised tools exist [159], that solve the relativistic Boltzmann equation in the presence of an advancing bubble wall [159, 181]

$$\left(p^\mu \frac{\partial}{\partial x^\mu} + \left(\frac{\partial}{\partial x_\mu} m_i^2 \right) \frac{\partial}{\partial p^\mu} \right) f_a(p^\mu, x^\mu) = -\mathcal{C}_i[f_a, \dots]. \quad (4.50)$$

These tools then find the pressure on both sides of the bubble wall and solve for a steady-state solution. The second term of the Liouville operator accounts for the change of mass of the particles entering the bubble. The right-hand side of the equation is given by the collision operator, which is an integral over all the distribution functions of the interacting particle species, making it numerically costly to evaluate. However, in the approximation that the mean free path of the particles is much smaller than the bubble wall width, the distribution function will follow local thermal equilibrium as discussed in sec. 3.5.1. In LTE there is no entropy production, leading to an additional matching equation [182]

$$s_+ \gamma_+ v_+ = s_- \gamma_- v_- \Rightarrow T_+ \gamma_+ = T_- \gamma_- . \quad (4.51)$$

Since T_+ is determined by the nucleation temperature of the bubble T_n , there are now three unknowns T_- , v_+ , v_- , that can be solved for using the hydrodynamic equations and matching conditions discussed in sec. 3.5.1 and the one above. This was shown in refs. [176, 182] where they study the wall velocity in the template model [127, 128]. This extends the bag model by allowing for a general, but constant sound speed different from $c_s^2 = 1/3$ in each phase

$$e_f(T) = \frac{1}{3} a_+ (\mu - 1) T^\mu + \epsilon_+ , \quad p_f(T) = \frac{1}{3} a_+ T^\mu - \epsilon_+ , \quad (4.52)$$

$$e_t(T) = \frac{1}{3} a_- (\nu - 1) T^\nu + \epsilon_- , \quad p_t(T) = \frac{1}{3} a_- T^\nu - \epsilon_- . \quad (4.53)$$

The speed of sound enters here through the constants μ, ν , which are defined as

$$\mu = 1 + \frac{1}{c_{s,f}^2} \quad \text{and} \quad \nu = 1 + \frac{1}{c_{s,t}^2}. \quad (4.54)$$

We adapted the code-snippet provided by ref. [176] to compute the wall velocity in LTE in TL, by mapping the temperature, speed of sound, pressure and energy density computed from the effective potential onto $a_{\pm}$, $\epsilon_{\pm}$, μ and ν . From the obtained wall velocity, we compute the sound wave efficiency factor κ_{sw} (eq. (3.157)) by using the fitting functions from ref. [126].

The out-of-equilibrium contributions give additional friction to the bubble wall and hence predict a slower bubble wall velocity, setting the LTE value as an upper limit $v_w \lesssim v_w^{\text{LTE}}$. However, it has been shown that the typical deviation between the LTE value and a full computation that solves the Boltzmann eq. (4.50) including out-of-equilibrium effects leads to an overestimation of around 20% [183]. Special care has to be taken for detonation solutions. Here, the LTE pressure on the bubble wall is a monotonically decreasing function of the wall velocity, leading to an unstable solution in the LTE approximation.

For these cases, the wall velocity is therefore set to $v_w = 1$ in TL. To determine whether the bubble wall runs away or reaches a terminal velocity, we compute the equilibrium Lorentz factor of the wall γ_{eq} from next-to-leading-order (NLO) friction (cf. eq. (3.166)) and compare it to the would-be value at collision γ_* , if we were to neglect the NLO friction. This allows to determine the efficiency factor κ_{col} (cf. eq. (3.167)) from which the kinetic energy fraction in the bubble walls is determined

$$K_{\text{col}} = \kappa_{\text{col}} \frac{\alpha}{\alpha + 1}. \quad (4.55)$$

The remaining released energy, which does not go into the bubble wall, is available for the sound wave and turbulence production [126]. So the kinetic energy fractions become

$$K_{\text{sw}} = \kappa_{\text{sw}}(1 - \kappa_{\text{col}}) \frac{\alpha}{\alpha + 1}, \quad K_{\text{turb}} = \kappa_{\text{turb}}(1 - \kappa_{\text{col}}) \frac{\alpha}{\alpha + 1}. \quad (4.56)$$

We note that there is still debate in the literature under which conditions the LTE solution is taken by expanding bubbles. Real-time simulations of bubbles expanding from their nucleation size show that the steady state-solution is not always reached [184, 185]. Instead, in these simulations it is observed that in some cases during the initial acceleration phase of the expansion, the bubble wall velocity surpasses the velocity that would be reached in LTE. This is due to the fluid profile not being fully developed in this early stages, leading to a lower pressure.

4.5.2. Gravitational wave spectra and observability

We implemented the three gravitational wave spectra from sound waves, MHD turbulence and bubble collisions as recommended by the LISA cosmology working group [147], which we can express as

$$h^2 \Omega_{\text{GW}}(f) = \mathcal{R} h^2 \times \begin{cases} A_{\text{col}} K_{\text{col}}^2 (RH)^2 S_{\text{col}}(f) & \text{for bubble wall collisions,} \\ A_{\text{sw}} K_{\text{sw}}^2 (RH) \mathcal{Y}_{\text{sw}} S_{\text{sw}}(f) & \text{for sound waves, and} \\ A_{\text{turb}} K_{\text{turb}}^2 (RH)^3 S_{\text{turb}}(f) & \text{for turbulence.} \end{cases} \quad (4.57)$$

The details and spectral shapes were discussed in the previous chapter in sec. 3.5. Additionally, we implement the observability of the signals for the current and planned or proposed GW observatories listed in tab. 2.1. To conclude this section, we show the GW spectra for

BP	Model	Description	Model parameters	α	$(\beta/H)_{RH}$	$T_{\text{reh}} [\text{GeV}]$
1	Conformal dark $U(1)'$	sec. 5.3.3	$g = 0.7, y = 0.01, v = 140 \text{ MeV}$.	620	59	1.4×10^{-2}
2	Dark flipflop	sec. 5.3.2	$\lambda_0 = 0.0051, \lambda_1 = 0.0021, \lambda_{12} = 0.0031,$ $v = 3.7 \text{ GeV}, y = 0.97, \gamma = 0.75$.	0.18	1400	5.9×10^{-1}
3	2HDM (Type-I)	app. B.2	$\lambda_1 = 0.29, \lambda_2 = 0.26, \lambda_3 = 5.81,$ $\lambda_4 = -2.2, \lambda_5 = -2.2, \tan \beta = 21,$ $m_{12}^2 = 1.6 \times 10^3 \text{ GeV}^2, v = 246 \text{ GeV}$.	0.60	91	4.4×10^1
4	Dark $U(1)'$	app. B.1	$\tilde{g} = 2.65, \lambda = 1.5 \cdot 10^{-3}, v = 1 \cdot 10^7 \text{ GeV}$.	1.4	810	5.6×10^5

Table 4.1.: Illustrative points used in fig. 4.11 which have not been checked against other constraints.

four benchmark points in fig. 4.11. The corresponding points are listed in tab. 4.1 together with the model, parameters and the phase transition parameters. For each benchmark point, the sound wave spectrum dominates (black lines) while the spectrum from turbulence (purple lines) is orders of magnitude smaller and the spectrum from bubble collisions negligible, since $\kappa_{\text{col}} \approx 0$ for all points.

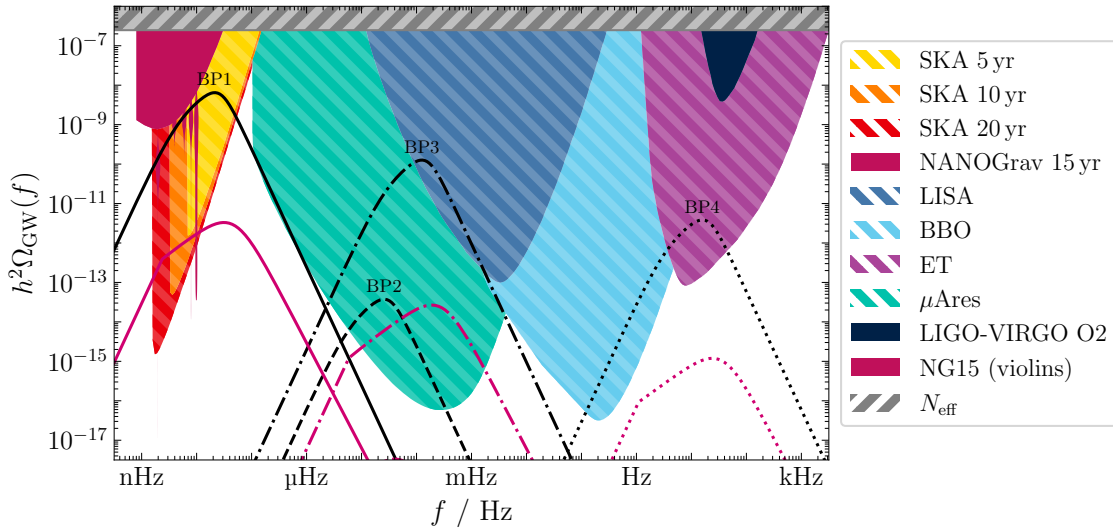


Figure 4.11.: Gravitational wave spectra for four benchmark points listed in tab. 4.1. The spectrum from sound waves is shown in black, while the spectrum from turbulence is shown in purple. Here we set $\kappa_{\text{turb}} = 0.1 \kappa_{\text{sw}}$.

4.6. Comparison with existing software tools

To validate our computations, we compare our results with the established tool **BSMPTv3**. For a non-trivial example, we implement the CP-conserving two Higgs doublet model (2HDM) [28, 186], (see app. B.2 for details on the implementation) and compute the phase transition parameters for a benchmark line scan in the parameter $\lambda_3 \in [5.5, 5.9]$. The other parameters are fixed to the benchmark point given in tab. 4.1. In this comparison, for better comparability, we compute the energy density that enters the Hubble rate from the effective degrees of freedom as done in **BSMPT** (see ref. [169]), instead of deriving it directly from the effective potential. Moreover, we fix the wall velocity in **BSMPT** to $v_w = 1.0$, which is the value we find with **TL** for all of the parameter points. For each of the points we compute $T_{\text{crit}}, T_{\text{nuc}}, T_{\text{perc}}, T_{\text{reh}}, \alpha$ and $(\beta/H)_{RH}$ (using eq. (4.45)). Note that we do not enforce the light Higgs state to

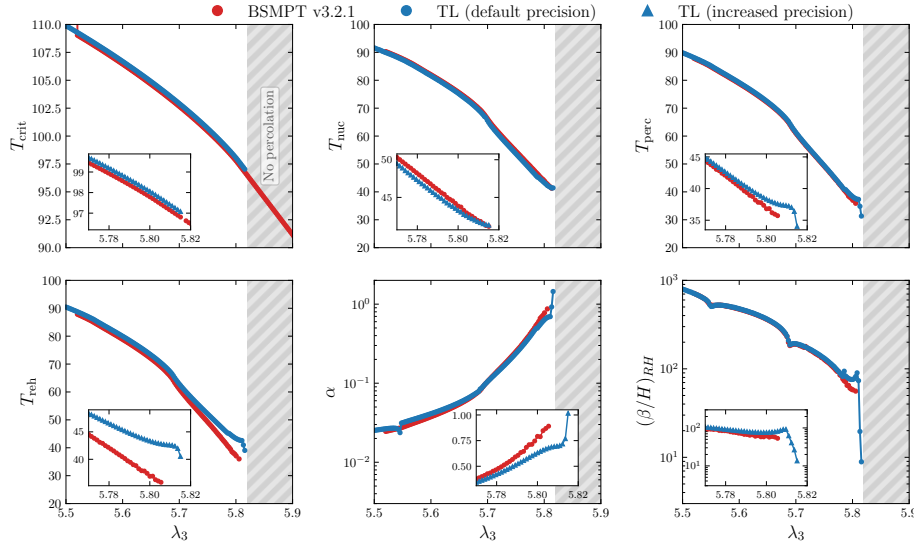


Figure 4.12.: Comparison of a 2HDM benchmark scan between *TransitionListener* v2.0.0 and BSMPT v3.2.1. The shaded region marks the TL exclusion boundary where vacuum trapping occurs.

have the SM value $m_h = 125$ GeV at every point as we want to isolate the behaviour of varying only one parameter. The phase transition parameters obtained from TL (blue line) and BSMPT (red line) are shown in fig. 4.12, while the relative differences $\delta X = (X_{\text{BSMPT}} - X_{\text{TL}})/X_{\text{BSMPT}}$ are presented in fig. 4.13.

In the main scan, we use the default accuracy settings in TL, but as we see some numerical instabilities at large λ_3 values, we perform an extra scan with increased accuracy for $\lambda_3 \in [5.76, 5.82]$. We identified the reason for the numerical noise in the convergence of the path deformation algorithm (cf. sec. 4.2) and tighten the convergence criterion in the extra scan. Here we use the algorithm in TL that solves the ODE formulation of the true-vacuum fraction.

Overall, our implementation of the calculations in TL agrees very well with BSMPTv3. The critical temperature and nucleation match on the sub-percent (T_{crit}) and percent level (T_{nuc}) as can be seen in fig. 4.13. The calculation of the percolation temperature matches at around 0.5%, but starts to disagree at the most supercooled points to up to 5%. We find the difference to come from the time-temperature relation that is used. While TL computes the time-temperature relation from the effective potential (eq. (4.32)), BSMPT approximates it with $dT/dt \approx -HT$, which only holds for $c_s^2 = 1/3$. In the reheating temperature, we see even bigger differences that increase with the degree of supercooling up to 20%. BSMPT uses here the common approximation $T_{\text{reh}} \approx T_{\text{perc}}(1 + \alpha)^{1/4}$, while TL solves the true vacuum energy density evolution according to the continuity equation (cf. sec. 4.4) to extract T_{reh} . This approximation becomes increasingly inaccurate with slower phase transitions, as discussed in the previous section. The transition strength α deviates up to 20% between the two codes. We find this is due to two effects, one is again the approximation of $c_s^2 = 1/3$ in BSMPT, that leads to the approximation of α , see eq. (4.48). Additionally, the percolation temperature enters the transition strength through the radiation energy density $\rho_{\text{rad}} \propto T^4$, such that small differences can be amplified. The transition speed, here computed from the mean bubble separation RH , shows a similar trend to the other parameters. At smaller transition strengths the results agree very well, but disagree up to 40% for stronger supercooling. With the iterative algorithm and the increased precision, TL can resolve the fine tuned region with large λ_3 up to ultra-slow transitions $(\beta/H)_{RH} = \mathcal{O}(10)$.

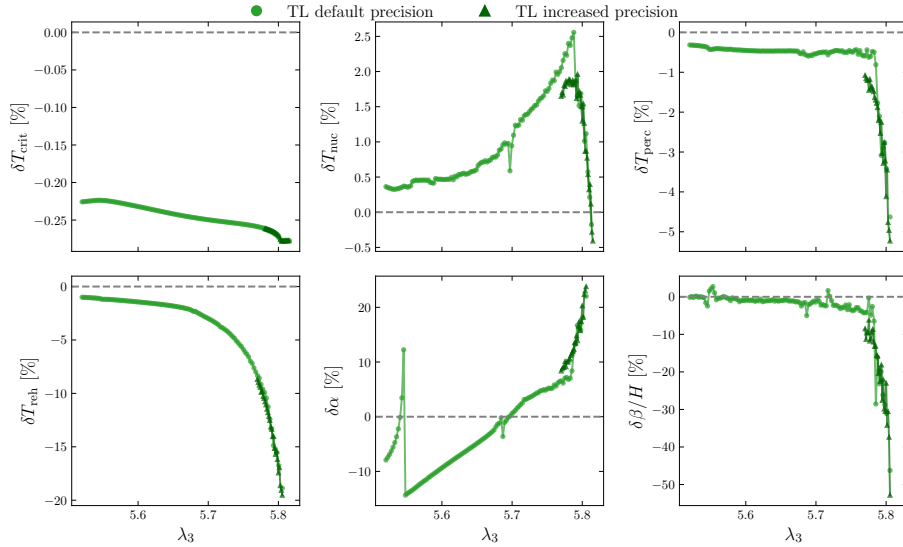


Figure 4.13.: Relative differences between the phase transition parameters obtained for the 2HDM model with BSMPT and TL, see fig. 4.12.

In summary, we conclude that the comparison of the results with BSMPTv3 validates the implementations in TL for weak and intermediate phase transition strengths, where the common approximations of fast transitions hold. In the regime of stronger transitions, we find that the more careful treatment of the reheating dynamics leads to sizable differences.

4.7. Discussion and outlook

The examples in sec. 4.5 have shown that the tool can compute the phase transition parameters up to very large supercooling ($\alpha \gg 1$ and $\beta/H < 10$) where conventional approximations break down. At these points, we saw the differences in the resulting phase transition parameters, that we can expect from e.g. taking the Hubble expansion into account in the computation of the reheating temperature. These refinements propagate into the predicted GW amplitudes and frequency of the signal, giving rise to sizable uncertainties for strongly supercooled transitions.

Nonetheless, while we refined treatment of the strong transitions, we note here that the simulations that underlie the parameterised GW spectra are usually only performed for weak ($\alpha \lesssim 0.5$) and fast transitions [145, 146, 187, 188]. The reason for this is that with increasing transition strength and fewer bubbles, the hierarchy of scales between the bubble wall width, the fluid profiles and the mean bubble separations increases drastically. Additionally, the slower a transition, the longer the simulation has to be run for, which additionally increases the numerical challenge. Thus, it is unclear if the scaling of the GW spectra found for $\alpha \ll 1$ and $\beta \gg 100$ will also hold for strongly supercooled transitions where far fewer bubbles collide. Reference [189] for example studied the impact of the cosmic expansion on the GW signal semi-analytically and found a weaker dependence of the amplitude and frequency for strongly supercooled transition than usually assumed. We also expect the expansion and energy density evolution of the true-vacuum that we derived to not hold up to arbitrarily small transition speeds. If only very few bubbles nucleate, they will have a different temperature depending on when they nucleated and we would expect deviations in the reheating temperature.

Another aspect that we did not address in this work is the validity of the 1-loop daisy-resummed approach. This approach suffers, for example, from a very large renormalisation

scale and gauge dependence, as demonstrated e.g. in refs. [114, 190], that can lead to orders of magnitude of uncertainty in the predicted GW signal. To see this, we can explicitly write out the 1-loop contributions to the effective potential, which can be split into two contributions

$$\begin{aligned}
 V_{1\text{-loop}} &\propto \oint \frac{d^3k}{(2\pi)^3} \ln(\omega_n^2 + k^2 + m^2) \\
 &= \underbrace{T \int \frac{d^3k}{(2\pi)^3} \ln(k^2 + m^2)}_{TJ_{\text{soft}}} + \underbrace{T \sum_{n \neq 0} \int \frac{d^3k}{(2\pi)^3} \ln(\omega_n + k^2 + m^2)}_{J_{\text{hard}}} . \quad (4.58)
 \end{aligned}$$

Explicit evaluation of J_{hard} reveals that it depends on terms proportional to $\ln(\bar{\mu}^2/T^2)$, while J_{soft} contains terms with $\ln(m^2/\bar{\mu}^2)$ [104]. In the high temperature regime, it is not possible to render both terms small. So, we are left with a strong dependence of our potential on the arbitrary renormalisation scale $\bar{\mu}$.

A possibility to improve upon these large uncertainties is given by using the methods of effective field theory (EFT) to compute the effective potential. These methods rely on the separation of scales, which appear with different orders in the coupling. The Matsubara frequencies introduce the hard scale (πT) which we saw in sec. 3.3.3 is perturbative and the soft scale (gT) to which the Matsubara zero-modes belong to, which we had to resum. The ultra-soft scale is introduced by, e.g. transversal gauge boson states, which receive a thermal mass only at the scale g^2T/π . For perturbative couplings, this gives a hierarchy between these scales $g^2T/\pi \ll gT \ll \pi T$ [114] that can be used to alleviate this problem.

At energies around the hard scale, where the dependence on $\ln(\bar{\mu}^2/T^2)$ is small, one can construct an effective Lagrangian by integrating out the non-zero Matsubara modes (including the fermions). Since the sum over the Matsubara frequencies replaced the time integral in equilibrium thermodynamics, this reduces the dimensionality of the effective theory to three. From here, the running of the couplings can then be used to go to the soft scale where the remaining renormalisation scale dependence $\ln(m^2/\bar{\mu}^2)$ is small. This is known as the framework of *dimensional reduction* and has been shown to greatly reduce the theoretical uncertainties in the prediction of the GWs [114, 190–192]. A clear direction for future work is therefore given by incorporating these methods, e.g. by interfacing tools that automate these dimensional reductions to TL.

We note here, however, that while the uncertainties of individual points in the simpler four-dimensional approach are large, the refinement of dimensional reduction typically only slightly shifts the parameter space [190]. To probe the general properties of a model with respect to first-order phase transitions, we therefore view it as sufficient to use the simplified approach.

4.8. Conclusion

In this chapter, we presented the numerical tool **TransitionListener** that enables the exploration of the GW phenomenology of cosmological phase transitions for general dark sector models. We implemented the full analysis pipeline that starts with the effective potential of a model, traces the vacuum structure, computes the phase transition parameters, GW spectra and evaluates the observability and likelihood of the signal for future and existing experiments.

Compared to existing tools, the framework focuses on improving the thermodynamic treatment of the early universe during phase transitions and shows that typical simplifying assumptions lead to uncertainties that are amplified in the predicted GW spectrum. With this

tool, we take a step beyond conventional approximations. These include the assumption of radiation domination, simplified time temperature relations $\dot{T} = -HT$, approximate reheating scaling $T_{\text{reh}} \approx T_{\text{perc}}(1 + \alpha)^{1/4}$ and simplified nucleation criteria $S_3/T \simeq 140$. These approximations break down precisely where GW signals become strong and best testable. Instead, the framework allows for general time-temperature relations computed from entropy conservation and tracks the evolution of the true-vacuum temperature by self-consistently solving $P_t(T)$ that takes the backreaction of the phase transition on the Hubble expansion into account. This allows to directly extract the nucleation, percolation and reheating temperature, as well as the length scale of the transition, the mean bubble separation.

Moreover, we presented two algorithms to efficiently compute the evolution of the true-vacuum during the phase transition. The computation of the true-vacuum fraction requires the integration over the nucleation rate, which is costly to evaluate. We developed two efficient approaches to minimise the required evaluations of the nucleation rate. The first one relied on finding an analytical approximation of the percolation temperature, which enables to choose a integration step size that balances accuracy and speed. In the second algorithm, we reformulated the percolation integral as a system of ordinary differential equations that allows to efficiently integrate these with adaptive step sizes and error controls.

A validation with the established tool **BSMPT** has shown good agreement up to intermediate transition strengths in the CP-conserving 2HDM. For strong phase transitions ($\alpha \gg 1$, $\beta/H \lesssim 100$), we have found expected deviations due to the aforementioned approximations. Since this is precisely the regime that will be probed first by future detectors, as it gives the strongest signals, this work brings us a step closer to robust predictions that will enable us to interpret future data.

This framework now provides a robust and tested analysis pipeline to study gravitational wave backgrounds. Using the built-in interface to **PTArcade** [103] that provides the likelihood of the NANOGrav PTA data, we will employ this tool in the following chapters to explore the possibility to explain the PTA data with dark sector phase transitions.

Dark sector phase transition models for the PTA signal

This chapter is based on the publication [193]. I contributed to all aspects of this work.

5.1. Introduction

In chapter 2, we have discussed the evidence for a stochastic gravitational wave signal measured by the pulsar timing arrays in the nanohertz (nHz) regime. In 2023, the collaborations NANOGrav [3], EPTA & InPTA [4], PPTA [194], CPTA [195], and MPTA [196] (in 2024) all reported evidence for the characteristic Hellings and Downs correlation between pulsars, which is expected from a stochastic GW background. The combination of the data measured by the individual collaborations will be published in an upcoming third data release of the International Pulsar Timing Array (IPTA) [197, 198] with the expectation that a discovery level of significance is achieved. The expected signal from the astrophysical source in this frequency range comes from inspiralling supermassive BHB from galaxy mergers, as discussed in sec. 2.5.2. However the amplitude of the observed signal was found to be significantly larger than what this astrophysical process has so far been estimated to yield [42, 43, 199–201]. Additionally, the tilt of the predicted spectrum from BHB is somewhat in tension with the data [202]. On top of that comes that the mechanism that dissipates enough energy, such that the supermassive BHBs approach a separation at the order of milliparsecs at which the GW emission drives the merging is not fully understood yet. This is also named the *final parsec problem* [44, 45]. In light of these problems, it is intriguing to consider the possibility that at least part of the signal is sourced by a signal of cosmological origin [71]. The possibilities encompass signals from inflation [203], topological defects [204–209], the generation of primordial black holes (PBHs) [210–214] or first-order phase transitions (FOPTs) [46–51].

Here we will focus on the possibility that a cosmological FOPT contributes to the signal. The general requirements for a phase transition that can fit the PTA data were already studied in ref. [49], in terms of the phase transition parameters, but without considering underlying particle physics models and with the previous 12.5 yr NANOGrav data release [46]. In order to obtain the observed nHz frequencies today, the signal produced by a FOPT must originate from temperatures around the MeV scale, where new physics is already tightly constrained [215]. It has been shown that a supercooled electroweak phase transition is

unfeasible at these temperatures [216] and hence it must come from a largely secluded dark sector, that is coupled weakly enough to not have been detected so far, but coupled enough to decay before BBN [217–221] and to not leave imprints in CMB anisotropy observations [8, 222, 223]. This leaves a temperature window at MeV temperatures open, where a dark sector could have a phase transition and subsequently decay before neutrino decoupling [49].

Here, we will study the general requirements on the underlying dark sector particle physics models to create such a cosmological scenario. In particular, we identify three qualitatively different possibilities to generate a potential barrier necessary for a phase transition to become first-order

1. A thermally induced barrier.
2. A two-step transition with a zero-temperature barrier.
3. A loop-induced barrier.

Each of these we realise with a representative model. For the thermally induced barrier, we take the example of an Abelian dark Higgs model, for the two-step transition, we implement a model with two scalar singlets and for the loop-induced barrier, we take the near conformal version of the dark Abelian Higgs model. For each model, we discuss the requirements to obtain a good fit to the PTA data, while obeying the cosmological constraints. We find that while a priori all models can generate a strong FOPT that fits the data, this is not a generic prediction. In the Abelian and flip-flop model significant tuning of the model parameters is necessary, in contrast to the conformal model, which generically predicts a strong and slow enough phase transition to fit the data.

This chapter is structured as follows. First, we study the requirements on the dark sector phase transition data using the NANOGrav 15 yr data set [3] (sec. 5.2). Then, we introduce the three models that realise different ways to achieve a first-order phase transition in sec. 5.3 and study their general FOPT predictions. In sec. 5.4, we compare the models to the data and discuss the constraints on these models. Finally, we discuss the results in sec. 5.5 and conclude in sec. 5.6.

5.2. Model independent analysis for FOPTs

We start our analysis by a general consideration of the requirements on the signal needed to fit the PTA data. Specifically, we focus on the scenario where the GW background is predominantly produced by the FOPT in the dark sector from sound waves. For our purposes here, we can consider the GW signal to depend on three main parameters, which determine its amplitude and frequency. The amount of energy carried in the GW background is proportional to the amount of vacuum energy released in the transition and usually quantified in the transition strength α . The frequency of the signal is determined by the characteristic length scale of the process, here given by the mean bubble separation RH at percolation and expressed in terms of the transition speed β/H . Finally, the reheating temperature T_{reh} sets the scale of the peak frequency through the amount of redshift the signal goes through. As discussed in sec. 3.5.4, in absence of extreme supercooling or in the presence of massive gauge bosons, this is typically the predominant contribution to the GW signal. The spectrum from sound waves is described by [145, 146]

$$h^2 \Omega_{\text{gw}}^{\text{PT}}(f) = \mathcal{R} h^2 A_{\text{sw}} K_{\text{sw}}^2 \mathcal{Y}_{\text{sw}}(RH) S(f), \quad (5.1)$$

where the lifetime of the source is given by $\mathcal{Y}_{\text{sw}} = \min(1, \sqrt{4/(3K_{\text{sw}})} RH)$ and the kinetic energy fraction $K_{\text{sw}} = 0.6 \kappa_{\text{sw}} \alpha / (1 + \alpha)$. For a discussion of further details and the spectral

shape $S(f)$, we refer to sec. 3.5.5. Around the MeV temperatures, we can write the redshifted peak frequency as

$$f_{\text{peak}} \simeq 10 \text{ nHz} \left(\frac{T_{\text{reh}}}{100 \text{ MeV}} \right) \left(\frac{g_{\text{reh}}}{10} \right)^{1/2} \left(\frac{10}{h_{\text{reh}}} \right)^{1/3}. \quad (5.2)$$

As we can see here, the peak frequency is set by the reheating temperature after the phase transition and therefore, we can expect the transition to occur around $\mathcal{O}(10 - 100 \text{ MeV})$ to fit the nanohertz frequency range of the PTA data. From the large amplitude of the PTA signal $h^2 \Omega_{\text{gw}} \sim 10^{-8}$, we can deduce further requirements on the phase transition. The strength of the signal is mainly determined by the transition strength α that enters the kinetic energy fraction K_{sw} and the mean bubble separation RH . To achieve a large amplitude today, we hence require a strong (large α) and slow transition (large RH) as already noted by refs. [47–49, 71, 224–229]. In principle, the bubble wall velocity also impacts the signal, but for strong transitions we expect it to be luminal $v_w \approx 1$, such that we will not treat it as a free parameter. Note that we express the length scale RH through the transition speed $\beta/H = (8\pi/f_{\text{perc}})^{1/3} \max(c_s, v_w)/RH$ in the following to keep comparability with the literature.

To quantify the above statements, we compare the general GW template for sound waves eq. (5.1) to the PTA data. For this, we employ the tool `PTArcade` [103] which uses the `ceffyl` [230] backend to compute the PTA likelihood for the NANOGrav 15 yr data set [3]. For details on the calculation of the PTA likelihood, we refer to app. A.1. As recommended by the NANOGrav collaboration [71], we take here the first 14 Fourier frequency bins into account, which span the frequency range $f \in [2, 28] \text{ nHz}$. To simplify the analysis, we account for the dark sector energy density in the redshift of the signal by adding $g_{\text{eff,DS}} = h_{\text{eff,DS}} = 2$ to the SM energy and entropy degrees of freedom².

The left panel of fig. 5.1 shows the preferred region obtained by comparing the template eq. (5.1) to the 15 yr PTA data in the α and β/H plane and after profiling over T_{reh} for each point. The iso-likelihood 1σ and 2σ -contours are shown by the solid and dashed blue lines respectively. As already anticipated, a good fit requires a specific combination of a large $K_{\text{sw}}(\alpha)$ and small β/H to give the right amplitude at the nHz frequencies. Notably, the faster the transition is, the stronger it has to be. This saturates at $a \gtrsim 10$, as $K_{\text{sw}} \rightarrow 0.6$ for large alpha. For transitions faster than $\beta/H \gtrsim 100$, larger alpha cannot anymore accommodate the large amplitude required. In the same region of large α , transitions slower than $\beta/H \lesssim 6$ instead overshoot the signal. This region of slow transitions generally comes with larger uncertainties, as simulations neglect the effect of cosmic expansion during the phase transition. Since the time between nucleation and percolation is around $10/\beta$ [145], we marked the region $\beta/H \lesssim 10$ with a grey dashed line. Below this line, we expect the GW signal to be overestimated.

The reheating temperature T_{reh} is indicated by the colour scale and takes values between 10 MeV and a few 100 MeV. We see that transitions with larger amplitude (smaller β/H) come with a larger reheating temperature. This can be understood by inspecting the right panel of the figure, showing the NANOGrav data in Fourier bins with the uncertainty represented by the Bayesian spectrograms as the red violins. A signal with larger amplitude can be shifted to higher frequencies (larger T_{reh}) to maintain a good fit with the rising part of the spectrum. Generally, the reheating temperatures are larger than previously found by studies that used the 12.5 yr data set [49]. The reason for this is that the previous dataset preferred a fit with the peak of the signal instead of the rising slope. The larger reheating temperature generally

²Note that a change in the DS degrees of freedom can always be absorbed here into a small shift of the reheating temperature. Therefore, this has no qualitative effect on the result shown in fig. 5.1.

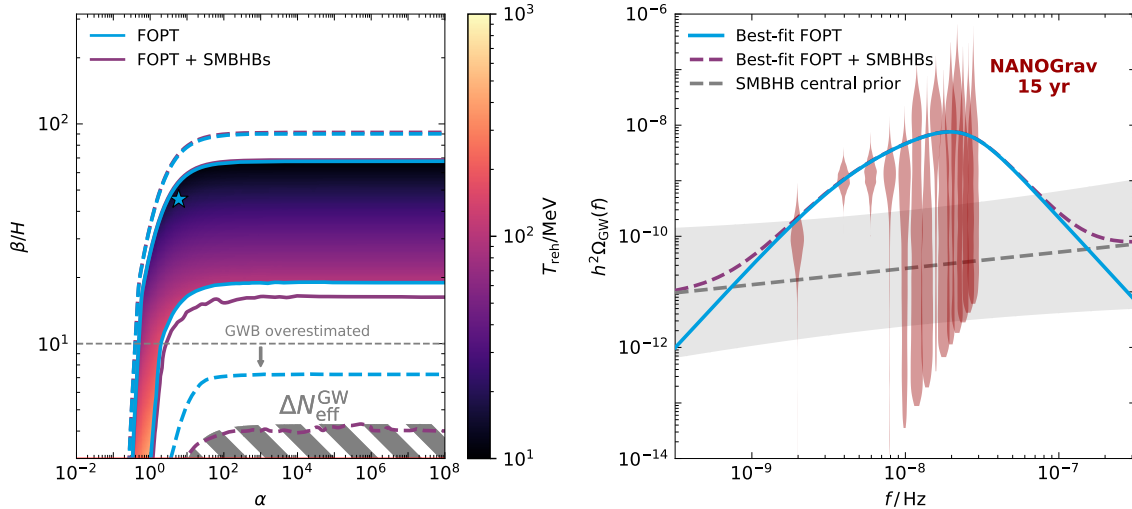


Figure 5.1: *Left panel:* Fit of the sound wave GW template to the PTA data in the plane of transition strength α and speed β/H . The reheating temperature is shown in the colour coding. The 1σ and 2σ best-fit regions are shown in the solid and dashed curves respectively. *Right panel:* GW spectra of the best-fit points of a signal from a FOPT only (blue line) and a combined signal from FOPT and BHB (dashed purple line). The grey area indicates the effect of varying the amplitude and slope of the BHB contribution within the 1σ expectation [71].

relaxes cosmological constraints, as it leaves more time for the dark sector states to decay before BBN.

To test the impact of our previous assumption of luminal bubble wall velocities, we have explicitly rerun this profile-likelihood analysis with a slower bubble wall speed of $v_w = 0.7$. This showed only a minor effect on the results, namely, it allowed slightly smaller values of β/H . Another implicit assumption is the initial thermal equilibrium between the dark sector (DS) and SM, as we assumed equal temperature of the dark and visible sector. The effect of assuming an initially hotter dark sector with $T_{\text{DS}} > T$ is that the fit allows slightly smaller values of α : we find for a DS with double the SM temperature $T_{\text{DS}} = 2T$, that the lower limit on the transition strength shifts to $\alpha \gtrsim 0.1$ (instead of $\alpha \gtrsim 0.4$). A smaller DS temperature on the other hand, leads to a larger shift towards larger α , as the GW amplitude approximately scales here with $\Omega_{\text{gw}} \propto (T_{\text{DS}}/T)^4$ (see e.g. ref. [141]).

So far, we have not yet accounted for a contribution to the stochastic background coming from inspiralling BHB [42]. We can include these by adding their contribution modelled by a single power law, as discussed in sec. 2.5.2:

$$h^2 \Omega_{\text{gw}}^{\text{BH}}(f) = \frac{2\pi^2}{3H_{100}^2} A^2 \left(\frac{f}{\text{yr}^{-1}} \right)^{5-\gamma} \text{yr}^{-2}, \quad (5.3)$$

with $H_{100} = H_0/h = 100 \text{ km s}^{-1} \text{ Mpc}^{-1}$ and the present day Hubble rate given by $H_0 = 67.8 \text{ km s}^{-1} \text{ Mpc}^{-1}$. We assume that the BHB contribution follows the power law in the relevant frequency range and use a Gaussian likelihood for the amplitude A and spectral index γ with the central values and variance

$$\mu_{A,\gamma} = \begin{pmatrix} -15.615 \\ 4.707 \end{pmatrix} \quad \text{and} \quad \text{cov}_{A,\gamma} = \begin{pmatrix} 0.279 & -0.003 \\ -0.003 & 0.124 \end{pmatrix}, \quad (5.4)$$

as recommended by the NANOGrav collaboration [71] and implemented in PTArcade [103]. We show the 1σ and 2σ contours resulting from profiling over T_{reh} and the nuisance parameters

A and γ in the purple solid and dashed lines respectively, in the left panel of fig. 5.1. This additional contribution generally improves the fit, as it opens up a region with smaller β/H (slower transitions), which we can interpret as follows: The fit of the FOPT background to the lowest frequency bin degrades when moving the peak amplitude to higher frequencies and increasing the overall amplitude. The contribution from the BHBs allows here for a deviation from the pure power law at low frequencies. However, this only very slightly affects the best-fit region of the FOPT only analysis, as can be seen by the best-fit point of the combined signal $\Omega_{\text{gw}}(f) = \Omega_{\text{gw}}^{\text{PT}}(f) + \Omega_{\text{gw}}^{\text{BH}}(f)$ in the right panel of fig. 5.1, shown as the purple dashed line. The addition of the BHB contribution only modifies the fit slightly for the lowest frequency bin, but leaves the rest of the signal unchanged. The BHB signal is shown as the grey dashed line, with the central prior of the BHB contribution indicated as the grey shaded area. From the shape of the central prior it also becomes clear that the slope of the BHB signal makes it hard to achieve a good fit with BHBs alone, even with large amplitudes, only the lowest frequency bins can be fitted well [43]. The addition of the FOPT signal improves this with the larger slope of the rising part of the spectrum, that we see in the data. With the present modelling of the BHB GW background, we can therefore treat the dark sector phase transition contribution as the dominant cause of the PTA signal in our analysis. Since we do not expect the presence of the BHB GW signal to affect the outcome, we will neglect this contribution in the following.

In the above analysis, we have not yet dealt with general constraints on dark sectors that come from CMB and BBN observations. In the left panel of fig. 5.1, we have indicated the constraints on extra radiation from GWs at BBN and CMB through the grey hatching. After the phase transition, we are however not only left with extra radiation energy density in the GW background, but also with the energy density of the dark sector. While we can see in fig. 5.1 that the GW background does not conflict with the constraint $\Delta N_{\text{eff}} < 0.22$ [222], in general, the dark sector has to thermalise with the SM in order to avoid conflicting with the measurement of N_{eff} . We will revisit this assumption of thermal equilibrium for the specific models in the next section.

5.3. Dark sector models

In the general considerations of the phase transition parameters that can produce a signal expected to explain the PTA data, we treated the phase transition parameters as independent. However, for a given model, the strength and the speed of a phase transition are generally correlated by the shape and temperature dependence of the underlying effective potential. For this reason, we will study three concrete particle physics models in detail that exhibit a FOPT. Each model represents a different qualitative way to generate the potential barrier required for the transition to become first order. For the conceptually simplest case of a thermally induced barrier, we consider an Abelian dark sector. The second mechanism we study is a two-step phase transition, realised by a model with two scalar singlets, where a cross-over transition precedes the first-order transition across a zero-temperature barrier. For the third example, we consider the classical conformal limit of the Abelian model where the potential barrier is generated from the radiative corrections. Finally, we discuss the constraints on the models that come from the requirement that the DS depletes sufficiently fast to not affect the CMB and BBN measurements of N_{eff} .

5.3.1. Abelian dark sector

For the first example of a thermally induced barrier, we consider an Abelian dark sector with a $U(1)'$ gauge symmetry [141], described by the Lagrangian

$$\mathcal{L} = |D_\mu \Phi|^2 - \frac{1}{4} F'_{\mu\nu} F'^{\mu\nu} - V(\Phi). \quad (5.5)$$

It consists of a dark photon A'_μ with the field strength tensor $F'_{\mu\nu} = \partial_\mu A'_\nu - \partial_\nu A'_\mu$ and a dark Higgs field Φ with the covariant derivative $D_\mu = \partial_\mu + igA'_\mu$. After expanding the complex scalar into background field ϕ_b , dark Higgs ϕ , and Goldstone boson φ as $\Phi = (\phi_b + \phi + i\varphi)/\sqrt{2}$, we obtain the background field tree-level potential

$$V_0(\phi_b) = -\frac{\mu^2}{2}\phi_b^2 + \frac{\lambda}{4}\phi_b^4, \quad (5.6)$$

and choose the usual renormalisation conditions that fix the VEV and scalar masses to their tree-level expressions when adding the counterterms and the Coleman-Weinberg corrections (cf. eq. (3.122)). The background-field dependent masses are here

$$m_\phi^2(\phi_b) = -\mu^2 + 3\lambda\phi_b^2, \quad m_\varphi^2(\phi_b) = -\mu^2 + \lambda\phi_b^2, \quad m_{A'}^2(\phi_b) = g^2\phi_b^2. \quad (5.7)$$

For more details on the model implementation, see app. B.1.

This model develops a thermal potential barrier for large enough ratios $\tilde{g} \equiv g/\lambda^{1/4} \gtrsim 1$ as e.g. shown in ref. [141]. This parameter describes the ratio between barrier height and potential depth that increases with $\tilde{g}$. Starting from a cross-over transition at $\tilde{g} \simeq 0.8$, increasing $\tilde{g}$ leads to stronger phase transitions and longer trapping in the false vacuum (supercooling) until at $\tilde{g} \gtrsim 3$ false vacuum trapping prevents the phase transition. This minimal model captures the qualitative behaviour of a thermally induced barrier and can be extended to e.g. include a fermionic DM candidate as shown in ref. [38]. These additional matter fields come with an opposite sign in the Coleman-Weinberg potential, and therefore require somewhat larger gauge couplings to prevent an unstable potential for small values of λ , but do not change the qualitatively behaviour.

With these considerations of the parameters in mind, we can study the predictions from the range of parameters shown in the left panel of fig. 5.2, that produce a FOPT. For easier interpretation, we scan over the VEV $v = \sqrt{\mu^2/\lambda}$ instead of the parameter μ , since the VEV directly connects to the energy scale at which the transition takes place and hence sets the scale of the transition temperature. Along similar lines, we also choose to scan over the parameter $\tilde{g} = g/\lambda^{1/4}$, as this parameter controls the phase transition strength. This parameterisation will additionally make it numerically less challenging to find the best-fit region, when we confront the models with the PTA data in sec. 5.4.

To obtain the typical prediction of the model, we randomly sample over the prior ranges of the model parameters and compute the parameters α , β/H , and T_{reh} . This makes it possible to construct a probability distribution for the resulting phase transition parameters (which is dependent on the prior choice of the model parameters). We show the resulting values of α and β/H in the right panel of fig. 5.2. The most likely model prediction for our choice of priors is marked by the blue lines of constant probability that contain 68% and 95% of the predicted values of α and β/H . For comparison, the requirements on these values found in the model-independent PTA fit are indicated by the grey shading. We can see that the typical prediction of the model gives fast transitions $\beta/H \gtrsim 100$ and the resulting 1σ and 2σ contours have no overlap with the PTA-preferred values for α and β/H . Only at the at least 3σ level points fall into the right regime. As we will discuss further in sec. 5.4, this indicates that we require a strong degree of tuning of the model parameters to describe the data with an first-order phase transition induced by a thermal barrier. As a degree of supercooling, we show the (mean) log ratio of the reheating temperature compared to the VEV at each point in the colour scale. This ratio becomes smaller with increasing transition strength, as the supercooling increases. We note here that the prior ranges do not cover the full parameter space where first-order phase transitions can occur. As can be seen in the fig. B.1 of appendix B.1, the phase transition parameters are mainly determined by the ratio $g/\lambda^{1/4}$, so we do not expect new qualitative features from expanding the prior ranges.

Parameter	Range	Prior
$\tilde{g} \equiv g \lambda^{-\frac{1}{4}}$	$[0.8, 3.2]$	lin
λ	$[10^{-5}, 1]$	log
v / MeV	$[1, 1000]$	log

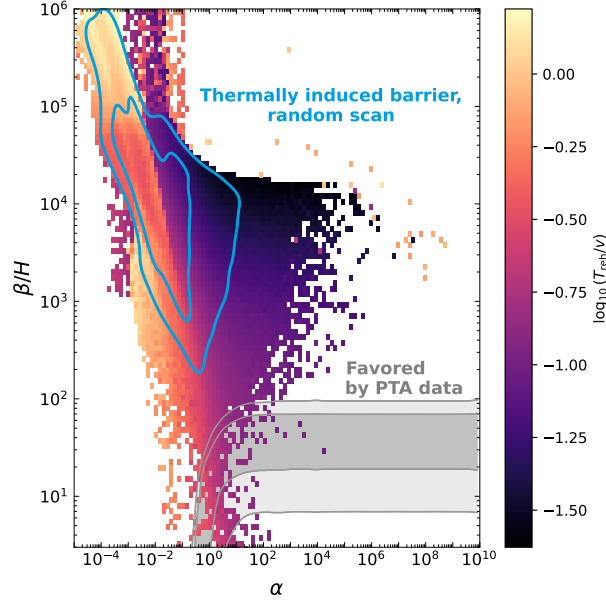


Figure 5.2.: *Left panel:* Prior ranges for the Abelian dark sector model. *Right panel:* Resulting values of α and β . The blue lines show the lines of constant probability that contain 68% and 95% of the predicted values for the prior possibilities assumed. The colour code indicates at each point the ratio of the mean reheating temperature T_{reh} and vev v . For comparison, the grey-shaded area shows the result of the model-independent fit to the PTA data, as displayed in figure 5.1.

The reason for the difficulty of finding parameter points in this model, which give small β/H is further illustrated in fig. 5.3. The panels in the top row show the effective potential for three different values of λ while $g = 1$ and $v = 100 \text{ MeV}$ are fixed, for different temperatures around nucleation. In each case, we can see the potential barrier decreasing with the temperature, leading to larger tunnelling rates, but we can observe that the decrease in the barrier height slows down with smaller values of λ (left to right). This is due to the potential depth decreasing ($V_0(v) = -\lambda v^4/4$), such that the thermal corrections dominate up to smaller temperatures. Therefore, the bubble nucleation rate becomes smaller with smaller values of λ . This is also highlighted in the lower row of the figure. In the left panel, we see that with decreasing λ , the bounce action decreases less and less rapidly with decreasing temperature as the potential barrier persists for longer. Eventually, the potential barrier even approaches a constant as $T \rightarrow 0$ and the bounce action never becomes efficient as $S_3/T > 200$, indicated by the hatched area. The right panel shows the corresponding slope of the nucleation rate (given by β/H) as it crosses the nucleation threshold $S_3/T = 200$ as a function of λ . We can see that only a very small range of values around $\lambda \sim 0.018$ gives the right speed $\beta/H \sim 10 - 100$ for the transition to explain the PTA data. Increasing or decreasing the value slightly leads either to vacuum trapping or to a phase transition that proceeds too fast.

5.3.2. Dark flip-flop model

We realise the second possibility to create a first-order phase transition – a tree-level barrier – in a model with two dark singlets. This model exhibits a two-step (flip-flop) phase transition. The model contains two real scalars ϕ_1 and ϕ_2 as well as a Majorana fermion $\psi = \psi^c$, which only couples to ϕ_1 :

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \phi_1) (\partial^\mu \phi_1) + \frac{1}{2} (\partial_\mu \phi_2) (\partial^\mu \phi_2) + \frac{1}{2} i \bar{\psi} \not{\partial} \psi - \frac{y}{2} \phi_1 \bar{\psi} \psi - V(\phi_1, \phi_2). \quad (5.8)$$

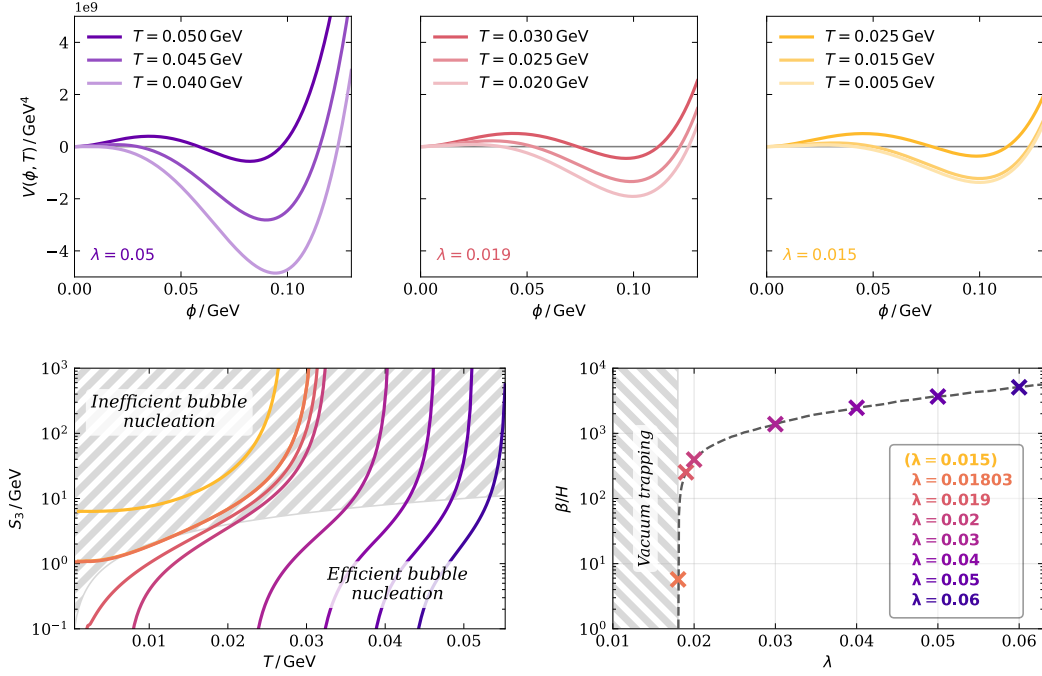


Figure 5.3.: *Upper row:* Effective potential of the Abelian dark sector model at different temperatures, with the parameters fixed to $g = 1$, $v = 100 \text{ MeV}$ and three different values of the self-coupling λ . *Lower left:* Corresponding tunnelling action S_3 as a function of temperature. *Lower right:* Resulting transition speed β/H as a function of the self-coupling λ .

For simplicity, we assume here that the bare Majorana masses are sufficiently small, so that they do not affect the phenomenology of the phase transition discussed below. The tree-level potential of the two scalars can be put into the suggestive form

$$V(\phi_1, \phi_2) = \frac{\lambda_0}{4} (\phi_1^2 + \gamma^2 \phi_2^2 - v^2)^2 - \frac{\lambda_1}{2} v^2 \phi_1^2 + \frac{\lambda_{12}}{2} \phi_1^2 \phi_2^2. \quad (5.9)$$

This tree-level potential is constructed such that it has the four minima located on the ϕ_1 and ϕ_2 axes

$$\langle \phi \rangle_{1,2} = \begin{pmatrix} 0 \\ \pm v_2 \end{pmatrix} \equiv \begin{pmatrix} 0 \\ \pm v/\gamma \end{pmatrix} \quad \text{and} \quad \langle \phi \rangle_{3,4} = \begin{pmatrix} \pm v_1 \\ 0 \end{pmatrix} \equiv \begin{pmatrix} \pm \sqrt{1 + \lambda_1/\lambda_0} v \\ 0 \end{pmatrix}, \quad (5.10)$$

where the tree-level potential becomes

$$V_{\text{tree}}(0, \pm v_2) = 0 \quad \text{and} \quad V_{\text{tree}}(\pm v_1, 0) = -\frac{\lambda_1}{4} \left(2 + \frac{\lambda_1}{\lambda_0} \right) v^4. \quad (5.11)$$

Hence, for $\lambda_1 > 0$, the global minimum is always given by $(v_1, 0)$. We can further assume a small bias term that breaks the $\mathbb{Z}_2$, but otherwise does not play a role and singles out the positive minima to avoid domain walls. Therefore, we restrict our analysis to the positive field-space quadrant ($\phi_1 \geq 0, \phi_2 \geq 0$).

The mass matrix of the scalars takes the form

$$\mathcal{M}^2(\phi_1, \phi_2) = \begin{pmatrix} -v^2(\lambda_0 + \lambda_1) + 3\lambda_0\phi_1^2 + \phi_2^2(\gamma^2\lambda_0 + \lambda_{12}) & 2\phi_1\phi_2(\gamma^2\lambda_0 + \lambda_{12}) \\ 2\phi_1\phi_2(\gamma^2\lambda_0 + \lambda_{12}) & -\gamma^2\lambda_0v^2 + \phi_1^2(\gamma^2\lambda_0 + \lambda_{12}) + 3\gamma^4\lambda_0\phi_2^2 \end{pmatrix}. \quad (5.12)$$

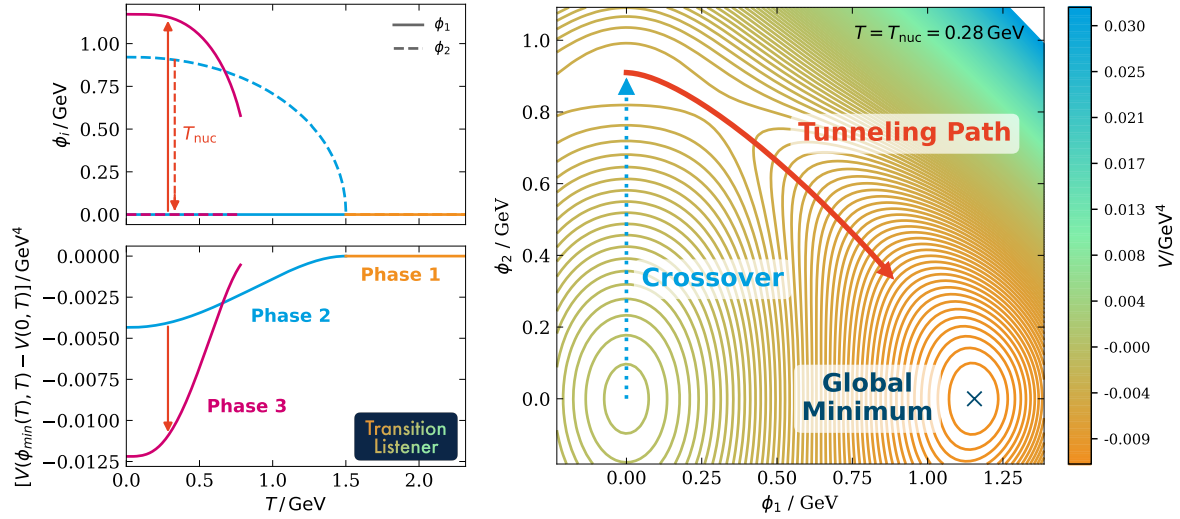


Figure 5.4.: Left panels: Field values ϕ_1 and ϕ_2 of the flip-flop model as a function of temperature (upper panel). At high temperatures, the symmetry is restored to the origin (orange line), while at intermediate temperatures the minimum shifts from the origin to $\phi_1 = 0$ and $\phi \neq 0$ (blue line). At lower temperatures, a local minimum forms on the ϕ_1 axis (red line), which becomes the global minimum. Right panel: Effective potential at the nucleation temperature $T_{\text{nuc}} = 0.28 \text{ GeV}$. The evolution of the minimum in the ϕ_2 direction is shown as the blue dotted arrow until nucleation. The tunneling path from the local minimum is shown as the red arrow, which ends at the release point of the fields. The values of the parameter point are listed in tab. 5.2.

Analogous to the Abelian model, we choose the counterterms such that the tree-level values of the scalar masses and the position of the global VEV do not change upon adding the 1-loop contribution. The counterterm potential that obeys the same $\mathbb{Z}_2$ symmetries as the tree-level potential has the non-vanishing terms

$$V_{\text{ct}} = -\frac{\delta\mu_1^2}{2}\phi_1^2 - \frac{\delta\mu_2^2}{2}\phi_2^2 + \frac{\delta\lambda_1}{4}\phi_1^4, \quad (5.13)$$

where the coefficients are determined by the conditions

$$\delta\lambda_1 = \frac{1}{2v_1^3} \frac{\partial V_{\text{CW}}}{\partial \phi_1} \Big|_{(v_1,0)} - \frac{1}{2v_1^2} \frac{\partial^2 V_{\text{CW}}}{\partial \phi_2^2} \Big|_{(v_1,0)}, \quad (5.14)$$

$$\delta\mu_1^2 = \frac{3}{2v_1} \frac{\partial V_{\text{CW}}}{\partial \phi_2} \Big|_{(v_1,0)} - \frac{1}{2} \frac{\partial^2 V_{\text{CW}}}{\partial \phi_2^2} \Big|_{(v_1,0)}, \quad (5.15)$$

$$\delta\mu_2^2 = \frac{\partial^2 V_{\text{CW}}}{\partial \phi_2^2} \Big|_{(v_1,0)}. \quad (5.16)$$

Finally, the hard thermal masses for the two scalars are

$$\Pi_{\phi_1}(T) = \frac{T^2}{24} (y^2 + 2(3 + \gamma^2)\lambda_0 + \lambda_{12}) \quad \text{and} \quad \Pi_{\phi_2}(T) = \frac{T^2}{12} (\gamma^2\lambda_0 + 3\gamma^4\lambda_0 + \lambda_{12}), \quad (5.17)$$

which are added to the diagonal elements of the mass matrix in eq. (5.12) in the daisy contribution to the thermal potential, cf. eq. (4.5).

We note that the quantum and thermal corrections are invariant under the transformation $\phi_i \rightarrow -\phi_i$ and hence the minima are always located on the two field axes. At very high temperatures, the thermal contributions dominate and restore the symmetry to the origin.

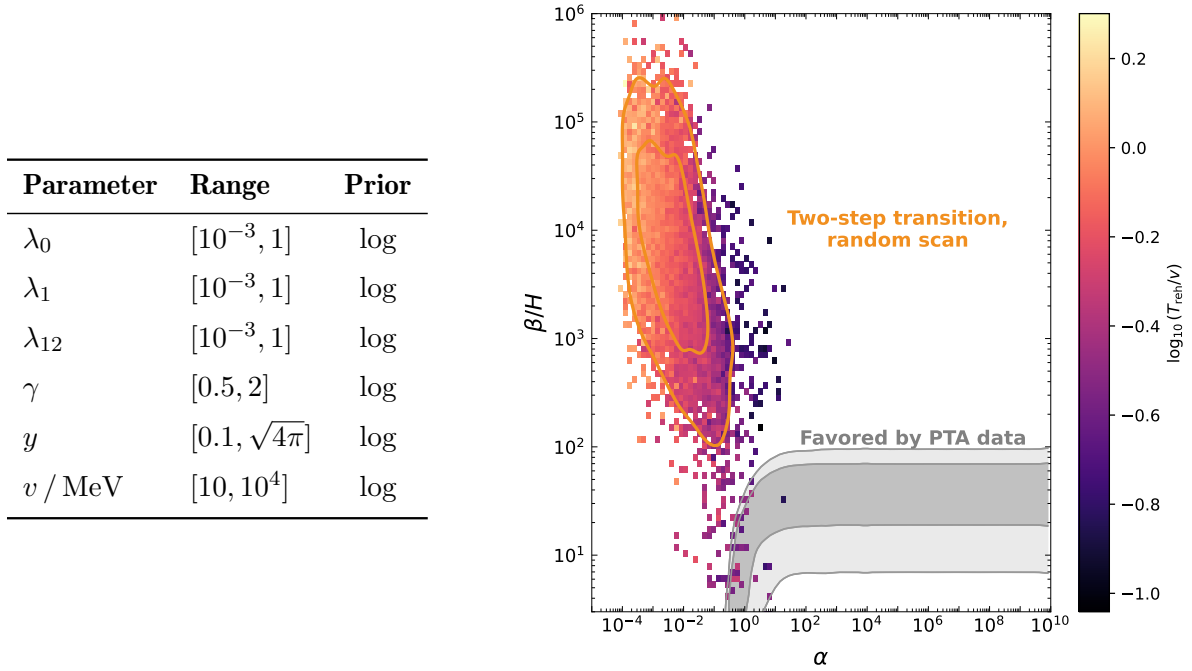


Figure 5.5.: *Left panel:* Prior choices for the flip-flop model to obtain a FOPT around the MeV scale. *Right panel:* Resulting phase transition parameters in the $\alpha - \beta/H$ plane. The orange contours mark the lines of constant probability containing 68% and 95% of the predicted values of α and β/H for the assumed prior probabilities. The colour coding indicates the ratio of the mean reheating temperature and the vev T_{reh}/v for each point. The grey-shaded area corresponds to the result of the model-independent fit to the PTA data, as shown in figure 5.1.

The symmetry breaking can now occur in two possible ways. One way is that the minimum on the ϕ_1 axis appears first and the phase transition occurs through a single step into the zero temperature phase. Since this mechanism is equivalent to the thermal barrier induced case of the Abelian model, we are interested in the second possibility: Here, the minimum in the ϕ_2 direction develops first and the ϕ_1 minimum develops later, changing from a local to the global minimum. This can be achieved by the fermion that couples only to the ϕ_1 field. If it obtains a sufficiently large mass $m_\psi = y \langle \phi_1 \rangle / \sqrt{2}$, the thermal corrections along the ϕ_1 axis are stronger and delay the formation of the minimum compared to the ϕ_2 axis. The amount of supercooling in the transition from $\langle \phi_2 \rangle$ is then controlled by the coupling λ_{12} that induces a tree-level barrier between the two minima. This flip-flop mechanism is shown in the phase structure in the left panels of fig. 5.4 for a benchmark point (cf. tab. 5.2). In the right panel, we can see the steps in field space. First, a smooth cross-over transition in the ϕ_2 direction occurs along the blue dotted arrow, then, at the nucleation temperature, the fields tunnel along the red arrow into the direction of the global minimum and roll from the release point (end of red arrow) to the global minimum (cross).

In order to obtain a picture of the typical prediction for the phase transition parameters in this model, we again randomly sample over the prior ranges summarised in the left panel of fig. 5.5. While the coupling λ_0 determines the overall shape of the potential, the desired two-step transition that we investigate here requires a specific combination between the coupling λ_{12} that controls the height of the tree-level barrier and λ_1 that sets the depth of the global minimum. Additionally, the parameter γ controls the distance in field space between the two minima; choosing $\gamma \ll 1$ brings the minimum on the ϕ_2 -axis close to the origin, and hence

reproduces the case of the thermally induced barrier, choosing it too large ($\gamma \gtrsim 2$) suppresses the nucleation rate and leads to vacuum trapping. The Yukawa coupling y has the effect of increasing the finite-temperature corrections along in the ϕ_1 -axis. Therefore, decreasing the values of this coupling further ($y \lesssim 0.1$) has little effect on the transition dynamics. We note here that, while the chosen prior ranges do not include all of the parameter space where a first-order, two-step transition would be possible, we do not expect a qualitative difference by increasing the ranges.

Since not all parameter combinations produce the desired flip-flop transition, we only include the ones that give a successful two-step transition in the results in the right panel of fig. 5.5. The lines of constant probability constructed from the prior probabilities containing 68% and 95% of the predicted values of α and β/H are shown by the orange contours. We see that this model generally predicts weak ($\alpha < 1$) and fast ($\beta/H > 100$) transitions that lie outside the band of values favoured by the PTA data indicated by the grey contour. Only very few points outside the indicated 1σ and 2σ contours (orange lines) reach small enough values in β/H . The degree of supercooling follows the same trend as in the Abelian model as the mean of $\log(T_{\text{reh}}/v_1)$ in each point in the $\alpha - \beta/H$ plane decreases with increasing α . Compared to the Abelian model, this model predicts overall smaller values of α for similar values of β/H . This can be explained by the increased distance in field-space between the two minima, which increases the bounce action and suppresses the nucleation rate.

5.3.3. Conformal dark sector

As the third example, we consider a model exhibiting a classically conformal symmetry. For this we take the Abelian model from sec. 5.3.1, but without the mass parameter μ

$$\mathcal{L} = |D_\mu \Phi|^2 - \frac{1}{4} F'_{\mu\nu} F'^{\mu\nu} - \lambda (\Phi^* \Phi)^2. \quad (5.18)$$

At the classical level, this exhibits an invariance of the action $S = \int d^4x \mathcal{L}$ under the scaling transformations $x^\mu \rightarrow \alpha x^\mu$, $\Phi(x) \rightarrow \alpha^{-1} \Phi(\alpha x)$ and $A'_\mu(x) \rightarrow \alpha^{-1} A'_\mu(\alpha x)$ with $\alpha > 0$. This symmetry of the model is only broken at the one-loop level through the radiative corrections [112] that induce a non-vanishing VEV. Since the potential at tree-level only has a minimum at the origin, we have to change our renormalisation conditions compared to the previous models. Here, we set the mass of the dark Higgs to vanish at $\phi_b = 0$ and fix the scalar self-coupling at some energy scale to its tree-level value. These conditions translate to

$$\left. \frac{\partial^2 (V_0 + V_{\text{CW}} + V_{\text{ct}})}{\partial \phi^2} \right|_{\phi=0} = 0 \quad \text{and} \quad \left. \frac{\partial^4 (V_0 + V_{\text{CW}} + V_{\text{ct}})}{\partial \phi^4} \right|_{\phi=\Lambda} = 6\lambda. \quad (5.19)$$

The first condition trivially yields $\delta\mu^2 = 0$ and the second one determines the counter term $\delta\lambda$:

$$V_{\text{ct}} = \frac{\delta\lambda}{4} \phi^4 = - \sum_a \frac{\eta_a g_a}{64\pi^2} m_a^4(\phi) \left[\left(\ln \frac{m_a^2(\Lambda)}{\bar{\mu}^2} - C_a \right) - \frac{50}{12} \right]. \quad (5.20)$$

We can combine this with the Coleman-Weinberg potential (eq. (3.122)) to obtain the zero temperature one-loop corrected potential as

$$V_{1\text{-loop}} = \frac{\lambda}{4} \phi^4 + \sum_a \frac{g_a}{64\pi^2} m_a^4(\phi) \left[\ln \frac{m_a^2(\phi)}{m_a^2(\Lambda)} - \frac{50}{12} \right]. \quad (5.21)$$

Here, it is convenient to define the self-coupling λ at the loop-induced VEV of the theory $\Lambda = \langle \phi \rangle = v$, i.e. the minimum of $V_{1\text{-loop}}$. With this, we have the condition at the minimum

$$\left. \frac{\partial V}{\partial \phi} \right|_{\langle \phi \rangle} = \left(\lambda - \frac{32}{3} \sum_a \frac{n_a}{64\pi^2} \lambda_a^4 \right) \langle \phi \rangle^3 = 0, \quad (5.22)$$

Parameter	Range	Prior
g	$[0.5, 2]$	linear
v	$[1, 1000]$ MeV	logarithmic

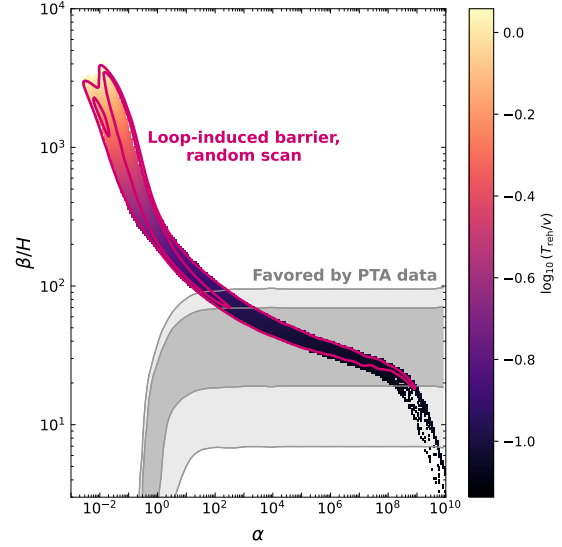


Figure 5.6.: *Left panel:* Prior choices for the conformal dark sector model to obtain a FOPT at the MeV temperature scale. *Right panel:* Resulting phase transition parameters in the $\alpha - \beta/H$ plane. The purple contours mark the lines of constant probability containing 68% and 95% of the predicted values of α and β/H for the assumed prior ranges. The colour coding indicates the ratio of mean reheating temperature T_{reh} and vev v for each point. The grey-shaded area corresponds to the result of the model-independent fit to the PTA data, as displayed in figure 5.1.

which leads to an equation that fixes the self-coupling as a function of g

$$\lambda = \frac{11}{48\pi^2} (10\lambda^2 + 3g^4) . \quad (5.23)$$

This exchange of a dimensionless model parameter (λ) for a dimensionful parameter (v) is also called *dimensional transmutation* [112].

Compared to the Abelian model discussed in sec. 5.3.1, the zero-temperature potential lacks a mass term proportional to $-\mu^2\phi^2$, instead the symmetry breaking is induced by the term $\phi^4\log(\phi^2/v^2)$ from the running of the quartic coupling. This logarithmic effect, together with the quadratic and cubic terms of the thermal contributions lead to potential barrier that persists up to lower temperatures, resulting in stronger phase transitions, see ref. [231]. This logarithmic behaviour propagates into the temperature dependence of the bounce action, and for smaller runnings (smaller g), the bounce action becomes flatter, which results in strong and slow transitions. The two parameters governing the model are the VEV v that sets the energy scale of the transition and the gauge coupling g that affects the strength. In the left panel of fig. 5.6 we summarise the ranges of for these parameters to obtain a FOPT in the right temperature range for the PTA data. For small values of $g \lesssim 0.5$, the potential obtains a zero temperature barrier that lead to vacuum trapping such that the phase transition does not complete (or begin) today. Increasing the gauge coupling, the transition becomes faster and weaker up until $g \approx 2$, where the relation eq. (5.23) does not give real solutions and perturbation theory breaks down.

The results of a random scan over these prior choices are shown in the right panel of fig. 5.6. Again, we mark the constructed probability, for the assumed priors for the model parameters, for α and β/H by the purple contours that contain 68% and 95% of the predicted values. We can clearly see that the transition strength and speed are tightly (anti-) correlated, as expected, since they now only depend on one parameter (g). A large fraction of the typical

values predicted for α and β/H fall into the region preferred by the PTA data. The strong supercooling in this region with $\alpha \gtrsim 10^2$ and $20 \lesssim \beta/H \lesssim 100$ can also be read off the ratio T_{reh}/v as indicated by the colour scale. Here T_{reh} is about an order of magnitude smaller than the mass scale (v).

5.3.4. Constraints

In the above discussions of the GW signals produced by the models from their respective phase transitions, we have assumed thermal equilibrium with the SM during the phase transition and not yet examined the cosmological constraints at MeV temperatures. Generally, the stringent constraints from BBN on ΔN_{eff} require the dark sector to decay sufficiently quickly between the reheating temperature ($T_{\text{reh}} \simeq \mathcal{O}(10 - 100)$ MeV) and the onset of BBN. In the presented DS models, there are two possibilities to couple the DS to the SM in a renormalisable way. These are Higgs portals and kinetic mixing of the dark photon with the SM photon. We will discuss these possibilities here for each model.

Abelian dark Higgs model

The Abelian dark Higgs model could decay via both the kinetic and Higgs mixing through the interactions with the SM

$$\mathcal{L}_{\text{int}} = \frac{\kappa}{2} F'_{\mu\nu} F^{\mu\nu} + \lambda_{H\Phi} |H|^2 \Phi^* \Phi, \quad (5.24)$$

where $F_{\mu\nu}$ is the SM photon field strength tensor. The dark photons in the region of a good fit to the PTA data have typical masses of $10 \text{ MeV} \lesssim m_{A'} \lesssim 2 \text{ GeV}$ (see fig. C.1). As shown in studies of the BBN constraints, in this mass range, dark sector states that decay into electron-positron-pairs are in general required to have a lifetime of $\tau \leq 1 \text{ s}$ [219]. The corresponding values of the kinetic mixing parameter $\kappa \gtrsim 10^{-9} - 10^{-10}$ for the main decay channel $A' \rightarrow e^+ e^-$ are very close to supernova cooling constraints or even in conflict [232, 233], but there exists another window of $10^{-6} \lesssim \kappa \lesssim 10^{-4}$ that will be probed in the future by Belle II [234], NA64 μ [235] and LHCb [236], but also by FASER2 [237], DarkQUEST [238] and SHiP [239]. Heavier dark photon masses open up additional decay channels to e.g. muons, relaxing the lower bounds on κ , as this decreases the lifetime and also weaken supernova bounds as the dark photon becomes too heavy to be produced in supernovae.

For the dark Higgs, we find that its mass is always below the threshold of allowed decays into dark photons $m_\phi < 2m_{A'}$ for the relevant region (fig. C.1) with masses between $2 \text{ MeV} \lesssim m_\phi \lesssim 1 \text{ GeV}$. The dark Higgs population could, in principle, also be depleted via a dark photon mediated decay into charged SM particles. This process is however loop suppressed, leading to an even larger lifetime. Instead, the dark Higgs can also mix with the SM Higgs through the second term in eq. (5.24). After EW symmetry breaking this introduces a mass term $\propto \lambda_{h\Phi} v_{\text{ew}}^2 |\Phi|^2$ that can prevent the symmetry breaking for couplings $\lambda_{h\Phi} \geq m_\phi^2/v_{\text{ew}}^2$. A small enough coupling $\lambda_{h\Phi}$ would lead to a lifetime $\tau_\phi \gg 1 \text{ s}$ for dark Higgs masses below the muon threshold. This can be relaxed by a shift of the tree-level mass parameter to smaller values $-\mu^2$, under the condition not to change the dynamics of the electroweak and dark sector transitions. For this, we simply require positive curvature of the combined Higgs and dark Higgs potential in the ϕ direction at the electroweak scale: $\partial_\phi^2 V_{\text{eff}}(h, \phi, T \sim v_{\text{ew}})|_{\phi=0} > 0$. This ensures two separate phase transitions and leads to the upper bound on the portal coupling $\lambda_{h\Phi} \ll g^2 + \lambda$. Using the mixing angle between the Higgs bosons $\theta = \lambda_{h\Phi} v_{\text{ew}} v / (m_h^2 - m_\phi^2)$, this leads to

$$\sin \theta \ll \left(\frac{v_{\text{ew}}}{v} \right) \left(\frac{m_A^2 + m_\phi^2}{m_h^2} \right)^{m_A \gtrsim 2m_\phi} 10^{-3} \left(\frac{m_\phi}{10 \text{ MeV}} \right)^2 \frac{10 \text{ MeV}}{v}, \quad (5.25)$$

with the SM Higgs mass $m_h = 125 \text{ GeV}$ and the EW VEV $v_{\text{ew}} = 246 \text{ GeV}$. The analogous condition for an unchanged DS transition is automatically fulfilled for $v \ll v_{\text{ew}}$. For typical masses of $2 \text{ MeV} \lesssim m_\phi \lesssim 2m_\mu$, a lower bound on the mixing angle $\sin \theta$ then comes from the requirement to decay sufficiently early [240] and an upper bound is due to beam dump experiments at colliders [241]: $10^{-5} \lesssim \sin \theta \lesssim 10^{-4}$. Almost all points shown in fig. 5.2 therefore can obey the cosmological constraints and can have a separate EW and DS phase transition according to the condition eq. (5.25). For dark Higgs masses above the muon and pion threshold, the constraint on the lower bound relax significantly to $\sin \theta \gtrsim 10^{-9}$.

Dark flip-flop model

The only renormalisable interaction of the dark flip-flop model with the SM is the Higgs mixing, since no gauge boson is present in this model. Here, both scalar singlets can mix with the SM Higgs via $\lambda_{h\phi_i}|H|^2\phi_i$, but the general phenomenology remains very similar to the dark Abelian Higgs model discussed above. Both singlets can decay sufficiently quickly after the phase transition through the discussed mechanism into SM charged final states according to the mass thresholds passed. Additionally, this model comes with the Majorana fermion ψ . Typically, this is the heaviest DS state (cf. C.2) such that it is already strongly Boltzmann suppressed at temperatures $T \sim m_{\phi_i}$ and no additional constraints arise through it.

Conformal dark sector

In principle, the classically conformal model has the same interactions with the SM as the Abelian dark sector. In contrast to the other two models, the Higgs mixing term would always modify the dynamics of the phase transition in a significant way. The mass term $\lambda_{h\phi}v_{\text{ew}}^2\phi^2$ breaks the classical conformal symmetry that led to the slow running of the dark Higgs self-coupling and consequently to the strong phase transitions. A non-zero (negative) portal coupling would hence result in the phenomenology of the Abelian model. While the dark photon can decay efficiently via the kinetic mixing, the dark Higgs decay mediated via dark photons is loop suppressed and therefore difficult to realise for all masses of the relevant parameter points (cf. fig. C.3).

A possibility to circumvent these problems is to introduce effective, non-renormalisable couplings of the dark Higgs to e.g. electrons, as proposed in refs. [47] and [39]. This effective coupling is not too tightly constrained by supernova bounds [242, 243] and does not break the classically conformal symmetry. We will discuss these and additional possibilities for this conformal model in chapter 6, where we study the conformal Abelian model with an additional dark matter candidate in detail.

5.4. Confronting models with data

In the previous section, we have studied three mechanisms to generate a FOPT with a representative dark sector model each. The random scans over the model parameters showed that each model, in principle, exhibits parameter points that give a phase transition suitable to generate the required GW background to explain the PTA data. However, as we saw, the typical predictions of the models differed significantly. The Abelian and flip-flop models only predict a small fraction of the computed α and β values that lie in the preferred region. In contrast, large parts of the predicted values from the conformal model lie in the preferred region. For comparison, we combined the results of the previous section in the left panel of fig. 5.7.

Instead of randomly sampling over the parameter ranges, we can refine this analysis by systematically exploring the PTA likelihood describing the data. For this, we employ the nested

sampler **UltraNest** [177]. The exploration of the likelihood, especially in the flip-flop model, is numerically challenging for high dimensional input parameters, which is further complicated by the high numerical cost of a full evaluation of a phase transition with **TransitionListener** [157]. In light of these problems, we adapt the strategy to find parameter points that give a good fit in the Abelian and flip-flop models. In the former, we simply restrict the range $10^{-3} \leq \lambda \leq 1$ and for the latter we fix the two parameters $y = \gamma = 1$, reducing the problem to a four dimensional parameter space. Furthermore, due to the remaining numerical challenge in the flip-flop model, we use an initial **UltraNest** scan and use the 100 (unconverged) samples with the highest likelihood to initialise a dedicated MCMC sampler which further explores the regions around these points.

For all three models, we additionally restrict the results to points that have a successful phase transition. The resulting best-fit regions are then shown in the right panel of fig. 5.7 through their 1σ and 2σ contours. Note however, that due to the high numerical cost of the sampling in the flip-flop model, we terminated the sampling before full convergence. We will discuss the reasons behind these difficulties in more detail below, but we note here that running the sampler for longer time will refine the details the shape but does not affect the location of the best-fit point. Since we terminate the sampling before full convergence, we refrain from performing a Bayesian model comparison. Instead, we restrict the analysis to a frequentist model comparison based on the best-fit likelihoods. The location of these are indicated for each model in the $\alpha - \beta/H$ plane by the stars and given in tab. 5.2. They give very similar likelihoods ($\ln \mathcal{L}_{\text{PTA}} = (-103.21, -103.24, -103.28)$ for the Abelian, flip-flop and conformal model) indicating that each model can equally well describe the PTA data.

We can also observe that only the best-fit region of the conformal model shares an overlap with the region of the models generic prediction, while the other best-fit regions are displaced for the other two models. This implies a tuning of the underlying parameters for these models. To quantify this, we compute the second derivative of the likelihood in the direction of each model parameter, resulting in tab. 5.1. This confirms our statement from the discussion above: a change in $\ln \mathcal{L}$ in the conformal model requires a much larger change in g than the same change in any coupling in the other models. This quite significant tuning of the parameters found for the Abelian and flip-flop model also explain the numerical challenges we found in the sampling of the likelihood discussed above. We note here that, while $(-g^2 d^2 \ln \mathcal{L} / dg^2)^{-1/2}$ gives a measure of the relative amount of tuning around the best-fit points, it does not quantify the absolute tuning. A more careful analysis of the tuning would require to compute the derivative of the profiled likelihood, which follows a χ^2 distribution, instead of fixing the other parameters. Due to the numerical cost we however only perform this exercise for the conformal model and find that we can vary g by about 15% at the 2σ levels, indicating indeed only moderate tuning. It is also worth noting here, that in all models the dependence on the mass scale v is rather weak. This is due to the fact that a change in v simply shifts the GW signal in frequency.

This tuning in the parameters is not simply a relic of the chosen parameterisations of the potentials, but can be understood by the different mechanisms that generate the FOPTs. To see this, we inspect the shape of the bounce action and nucleation rates of the best-fit points (tab. 5.2), shown in fig. 5.8. The corresponding phase transition parameters are given in tab. 5.3. We can observe that the phase transitions proceed in different ways in the models. As shown in the left panel, in the conformal model (purple line), the action is generically flat, which makes it easy to achieve a small enough transition speed β/H at the nucleation threshold $S_3/T \simeq 200$ required for the PTA data. As discussed in sec. 5.3.1, the Abelian model (blue line) generically has a stronger dependence of the action on the temperature and therefore faster phase transitions (cf. fig. 5.3). The transition can be slowed down by a U-shape of the bounce action, which however requires to match the minimum precisely with

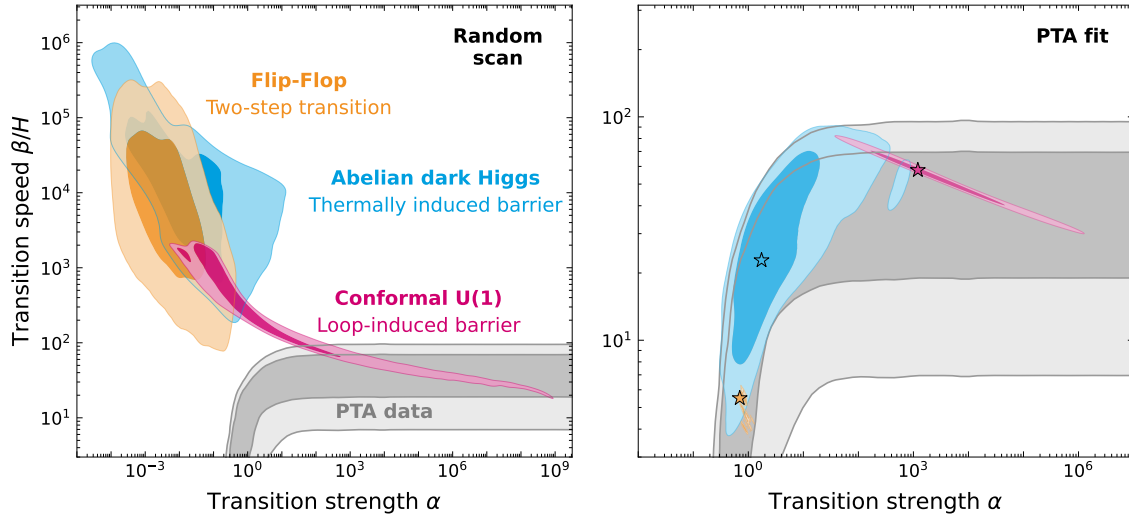


Figure 5.7.: *Left panel:* Generic predictions of the three example models in the $\alpha - \beta/H$ plane (coloured areas), combined from figs. 5.2, 5.5 and 5.6. The grey-shaded area shows the results for the model-independent fit to the PTA data for comparison, cf. figure 5.1. *Right panel:* Preferred regions for the models after sampling over the PTA likelihood. The stars indicating the respective best-fit points (cf. tables 5.2 and 5.3). Note that the contours in the right panel are only indicative for the Abelian Higgs and the flip-flop model.

the nucleation threshold $S_3/T \simeq 200$. This alignment induces the significant tuning. For the flip-flop, the situation is similar, however, since we find generally smaller α , the transition speed β/H has to compensate for this, leading to an even higher tuning of alignment of the slope at the nucleation threshold. Since these models show qualitatively different behaviour in the nucleation curves, we take this as an indication that these are representative of model classes that have these behaviours to fit the PTA data.

5.5. Discussion

In this section, we will now discuss the various assumptions that we made to arrive at the results presented in the previous section. We discuss these, starting with assumptions that we consider to have a small effect on the predictions of the preferred regions in α and β and then turn to potentially critical issues.

Conformal model		Abelian dark sector		
$-v^2 \frac{d^2}{dv^2} \ln \mathcal{L}$	$-g^2 \frac{d^2}{dg^2} \ln \mathcal{L}$	$-v^2 \frac{d^2}{dv^2} \ln \mathcal{L}$	$-\lambda^2 \frac{d^2}{d\lambda^2} \ln \mathcal{L}$	$-\tilde{g}^2 \frac{d^2}{d\tilde{g}^2} \ln \mathcal{L}$
7×10^1	5×10^3	1×10^2	5×10^5	4×10^8

Flip-flop					
$-v^2 \frac{d^2}{dv^2} \ln \mathcal{L}$	$-\lambda_0^2 \frac{d^2}{d\lambda_0^2} \ln \mathcal{L}$	$-\lambda_{12}^2 \frac{d^2}{d\lambda_{12}^2} \ln \mathcal{L}$	$-y^2 \frac{d^2}{dy^2} \ln \mathcal{L}$	$-\lambda_1^2 \frac{d^2}{d\lambda_1^2} \ln \mathcal{L}$	$-\gamma^2 \frac{d^2}{d\gamma^2} \ln \mathcal{L}$
9×10^2	3×10^6	2×10^7	2×10^7	5×10^7	2×10^8

Table 5.1.: Second derivative of the PTA likelihood $\ln \mathcal{L}$ with respect to the model parameters at the best-fit points marked with the stars in the right panel of fig. 5.7 (see tab. 5.2 and 5.3).

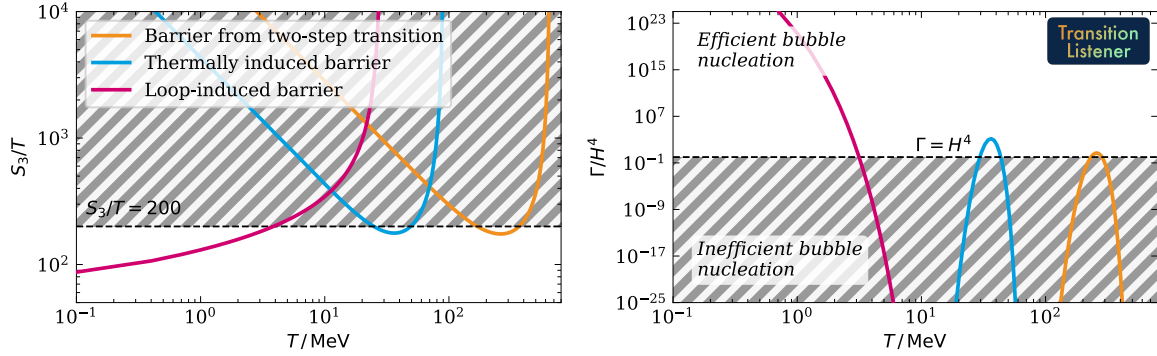


Figure 5.8.: Bounce actions S_3/T (left) and the transition rate Γ/H^4 (right) as functions of temperature for the benchmark points listed in tab. 5.2 and indicated as stars in fig. 5.7.

Model	Parameter	Value
Abelian Higgs $U(1)'$	$\tilde{g}$	2.7829
	λ	0.0406
	v/GeV	0.24
Conformal $U(1)'$	g	0.692
	v/GeV	0.14
Flip-flop	λ_0	0.02432
	λ_1	0.014524
	λ_{12}	0.023401
	v/GeV	0.927
	y	1.0
	γ	1.0

Table 5.2.: Benchmark parameter values for the three example models. We quote all significant digits obtained in the numerical analysis up to the degree of accuracy that is relevant for reproducing the PTA fit (cf. tab. 5.1).

Phase transition template

As indicated in fig. 5.1, the results for the GW signal from very slow transitions $\beta/H < 10$ become less reliable as these regimes are not yet well explored by numerical simulations. In this regime, the scaling of the GW amplitude with $(\beta/H)^{-1}$ ($(\beta/H)^{-2}$ for fast shock formation, cf. sec. 3.5.5) has not been confirmed by hydrodynamic simulations. Recent studies suggest instead that the amplitude and peak frequency have both a weaker dependence on the transition speed [189], which would shift the preferred region in fig. 5.1 towards lower values of β/H .

Additionally, the GW template that we implemented is based on simulations that only go up to transition strengths of $\alpha \lesssim 0.5$ [146]. Another approximation that we take is to evaluate the sound wave efficiency factor κ_{sw} at percolation, as commonly done [244]. This matters as κ_{sw} can change from nucleation to percolation and can underestimate the GW amplitude by orders of magnitude in extreme cases. This is typically only relevant for intermediate transition strengths, as weak transitions occur too fast for κ_{sw} to change significantly and strong transitions typically have $\kappa_{\text{sw}} \simeq 1$ at nucleation as well as at percolation. Here, a more careful treatment would require to take the time dependence of the energy budget into account as seen in simulations [146]. In our results, only the flip-flop model shows intermediate strengths in the favoured region which, could shift the parameters.

Benchmark point	α	β/H	RH	T_{nuc} MeV	T_{p} MeV	T_{reh} MeV	$\ln \mathcal{L}_{\text{PTArcade}}$
Abelian dark Higgs	1.74	22.8	0.19	43.6	34.7	46.0	−103.21
Conformal $U(1)'$	821	57.9	0.08	3.16	2.58	14.5	−103.28
Flip-flop	0.70	5.5	0.80	285	173	192	−103.42

Table 5.3.: Phase transition parameters for the three benchmark points given in table 5.2. In the last column we show the log-likelihood values for the NANOGrav 15 yr data obtained using PTArcade.

Phase transition mechanisms

We focused our analysis on three conceptually different mechanisms to realise a first order phase transition. These mechanisms are not the only possibilities, as for example quantum – instead of thermal – tunneling can also realise slow phase transitions, as the nucleation rate is not temperature dependent in this case. Examples for this include a first-order QCD phase transition [245], which can fit the PTA data. Another possibility is not to rely on the standard nucleation rate in a homogeneous background, but to consider bubble nucleations induced by the presence of topological defects, such as domain walls or cosmic strings. These can enhance the false vacuum decay rate and determine the bubble separation by their distance [246–249]. This could be relevant for the flip-flop model, where the first cross-over transition could create domain walls, which we have assumed to vanish in our analysis. These could enhance the decay rate of the false vacuum in the second step.

Homogenisation before BBN

Recently, it has been shown that spatial inhomogeneities of 25% of the baryon-to-photon ratio around $T \approx 3 \text{ MeV}$ at length scales larger than the horizon [223] can survive until BBN and alter the light element formations to an observable degree. The phase transitions we considered all occur at $T \approx 10 - 200 \text{ MeV}$ and thus could potentially be subject to these constraints. However, the analysis in ref. [223] did not take the bulk fluid motion created by the expanding bubbles into account which could speed up the homogenisation process compared to only baryon diffusion. Due to these uncertainties, we do not include this as a constraint, but note that it could affect the strong and late transitions found in the conformal model. Here, further work would be needed to study the inhomogeneities after a FOPT to estimate the impact on the nucleosynthesis prediction.

We summarise, that while the assumptions and caveats discussed above could impact our analysis, we do not expect them to significantly alter the main conclusions. Still, future work on the modelling of FOPT, especially for slow transitions, is required to fully exploit the GW background measured by the PTA collaborations to probe dynamics in the early universe.

5.6. Conclusions

In this chapter, we have studied the possibility that the GW background at nanohertz frequencies found by the PTA measurements could be sourced by a dark sector phase transition at MeV temperature scales. This study is based on the 15 yr NANOGrav dataset [3], which we first studied in a model-independent analysis by inferring the requirements on the transition strength α , speed β/H and reheating temperature T_{reh} . Here, we updated and confirmed the results based on earlier data releases [49], that the PTA data require generally a rather strong and slow transition. As this model independent study does not account for the correlation between the phase transition parameters that arise from the underlying particle physics

models, we further studied three representative models that obtain a FOPT in different ways. These included a thermally induced barrier, realised in a dark Abelian Higgs model, a two-step (flip-flop) transition in a model with two scalar singlets and a loop-induced barrier from a classically conformal Abelian dark sector. We found that, while all three model classes can produce a phase transition that fits the PTA data, only the conformal model can do so without the necessity for significant parameter tuning. We traced this back to the different mechanisms by which the phase transition proceeds, which are shown in fig. 5.8.

The PTA data requires a rather slow transition ($20 \lesssim \beta/H \lesssim 100$), that is realised differently by the models. To achieve this in the Abelian model, the nucleation rate has to peak at the right temperature and be sufficiently flat around percolation in order not to proceed too quickly. This can only be achieved by a significant tuning in the model parameters (cf. fig. 5.3). In the case of the two-step transition, we found even slower transition speeds were needed $\beta/H \lesssim 10$, as the model generally predicts weaker transitions. This required an even larger amount of tuning on the model parameters, as typically a second field direction rather enhances than decreases the vacuum decay rate. In contrast to the other models, the conformal model naturally leads to slow transitions, which comes from the weak dependence of the potential barrier on the temperature. This translates into a flat nucleation rate around percolation and subsequently results in generically strong supercooling.

We further discussed the viability of these phase transitions at MeV temperatures in the light of BBN constraints. While we found that the GW signal itself does not affect bounds from ΔN_{eff} , difficulties can arise from the requirement that the DS decays before neutrino decoupling. Generally, these constraints can be avoided by coupling the DS to the SM so that they thermalise after the phase transition and decay into SM particles. The required lifetimes $\tau \lesssim 1$ s can be achieved by Higgs mixing or kinetic mixing of the dark photon with the SM photon. In the conformal scenario this, however, might require the introduction of additional states in the DS, as the Higgs mixing would spoil the conformality of the model. Furthermore, we discussed possible refinements and potential caveats in our analysis, but concluded that they would not affect our main results. Therefore, we consider the different mechanisms to achieve a FOPT with the model classes presented here as generic possibilities to explain the PTA data.

With the third data release of the IPTA in the near future [250], it will become increasingly important to refine the modelling of the predicted GW signal from FOPT, especially in the strong supercooling regime. More precise data will further constrain the spectral shape of the observed signal, therefore an accurate description of the GW signal from the different sources is crucial to determine its origin. Should future data not rule out a FOPT origin, by observing anisotropies characteristic to supermassive black hole mergers [251, 252], it will shrink the viable regions in the generic $\alpha - \beta/H - T_{\text{reh}}$ parameter space, which could help to further distinguish between model classes.

Sub-GeV dark matter and the PTA signal

This chapter is based on the publication [39]. My contribution to this work were computing the first-order phase transition and gravitational wave signal for this model, understanding the PTA constraints and implementing `TransitionListener` as a backend of `GAMBIT`, as well as contributing to the interpretation of the results.

6.1. Introduction

In the previous chapter, we have studied at length the general requirements on a DS phase transition to explain the recent observation of a stochastic GW background at nanohertz (nHz) frequencies observed by the PTA collaborations. In particular, we have seen that the signal requires a sub-GeV mass scale of the DS symmetry breaking to match the frequency of the PTA data. At the same time, this mass range has gained an increased interest in the context of the observed DM abundance, as direct detection experiments have put tighter and tighter constraints on heavier dark matter [253, 254]. In this sub-GeV mass range, DM can avoid these strong constraints and can be produced as a thermal relic from the freeze-out process in the early universe.

This has led to rapid progress in the search program for sub-GeV DM through beam-dump experiments and scattering detectors [255–257]. These DM candidates have a wide variety of complementary cosmological and astrophysical constraints. These range from BBN and CMB constraints through modifications of the expansion history or energy injection by DM annihilations and decays [219, 258, 259], to cosmic ray constraints [260] and the evolution of DM halos [261, 262]. The viability of sub-GeV DM despite these constraints has been demonstrated by a recent study [263] that performed a global fit using the `GAMBIT` global fitting framework [52]. The study identified viable parameter space for thermally produced scalar and fermionic sub-GeV DM, that interact with the SM via a new $U(1)'$ gauge boson (dark photon), which kinetically mixes with the SM photon. However, the study did not investigate the mechanism of the mass generation of the DS states.

In this chapter, we will connect the study of the phase transition in a DS that can explain the PTA data from the previous chapter to the idea that the sub-GeV DM mass is generated

through the same symmetry breaking that also leads to the GW signal. For this, we consider the DS to contain a dark Higgs boson that obtains a VEV and spontaneously breaks the $U(1)'$ symmetry through a FOPT and generates the DS masses. The study of the different model classes in the previous chapter motivates to additionally assume a near conformal symmetry, where the mass scale is generated through radiative corrections [112, 264, 265], which leads to a strong phase transition that can naturally explain the large amplitude of the PTA signal. Although classically conformal DS models have been studied in the literature [47, 48, 224, 227–229, 266–270] and shown to be able to generate the strong and slow phase transitions necessary for the PTA data, typically these studies assumed that the DS states decay such that there is no DM candidate left. For notable exceptions, see refs. [268] and [269].

Compared to the conformal DS studied in chapter 5, which consisted only of a dark Higgs and a dark photon, a minimal extension to add a stable DM candidate is to introduce a fermion. This increases the free parameters to only four: the VEV v , gauge coupling g , Yukawa coupling y and the kinetic mixing parameter κ . The former two are tightly constrained by the requirement to fit the PTA data, the third sets relic abundance through the DM mass and the last one acts as a portal to the SM. A priori, it is unclear if this rather minimal model can satisfy all the constraints and additionally explain both the PTA data and also the observed DM relic abundance.

The simplest possible mechanism to produce the DM in such a model, i.e. DM annihilating into dark Higgs bosons, was studied in ref. [38] which showed that this implies a DS mass scale around the EW scale and a GW signal in the millihertz frequency range. In the sub-GeV mass range, this scenario would underproduce the DM by orders of magnitude. Therefore, a mechanism to suppress the DM annihilations is required. The two possibilities that we consider here are the forbidden dark matter regime, i.e. a kinematic threshold [270] and a secluded DS with a non-negligible chemical potential [271].

In this chapter, we will study in detail the phenomenology of the dark sector for these two scenarios and show that it can fit both the PTA data as well as the observed DM relic abundance. The chapter is structured as follows. In sec. 6.2 we introduce the near conformal DS model, its effective potential, and the interactions with the SM. The modelling of the GW signal and the constraints coming from the PTA data are discussed in sec. 6.3. In sec. 6.4 we discuss the computation of the relic density through the freeze-out mechanism and review relevant cosmological, astrophysical, and accelerator constraints on the model in sec. 6.5. The results of global fits for both scenarios are presented in sec. 6.6 and discussed in sec. 6.7. Finally, we conclude in sec. 6.8.

6.2. Conformal sub-GeV dark matter

In the previous chapter, we have discussed at length the general requirements for a dark sector phase transition to explain the PTA data. Here, we will examine the most promising model in more detail and additionally consider the possibility that it gives a dark matter candidate with the correct relic abundance today. The model is similar to the conformal model from the previous chapter (cf. sec. 5.3.3), with the addition of a dark matter candidate. The Lagrangian of this classically conformal $U(1)'$ model reads

$$\mathcal{L} = |D_\mu \Phi|^2 - \frac{1}{4} F'_{\mu\nu} F'^{\mu\nu} + \bar{\chi}_1 i \not{D} \chi_1 + \bar{\chi}_2 i \not{D} \chi_2 - \left(\frac{y_1}{2} \Phi \bar{\chi}_1^c \chi_1 + \frac{y_2}{2} \Phi^* \bar{\chi}_2^c \chi_2 + \text{h.c.} \right) - V_0(\Phi), \quad (6.1)$$

which consists of a complex scalar Φ (dark Higgs), two left-handed fermions $\chi_{1,2}$ (dark matter) and the gauge boson A'_μ (dark photon). The covariant derivative reads $D_\mu = \partial_\mu + igQA'_\mu$, where we set the $U(1)'$ charges to $Q_\Phi = 1$, $Q_{\chi_1} = -1/2$ and $Q_{\chi_2} = 1/2$ such that the model

is anomaly free. For simplicity, we assume here that the fermions are degenerate in their Yukawa coupling to the dark Higgs. Such a degeneracy would, for example, result from an exchange symmetry $\chi_1 \leftrightarrow \chi_2^c$. As in the previous chapter, the tree-level potential of the scalar is

$$V_0(\Phi) = \lambda (\Phi^* \Phi)^2, \quad (6.2)$$

which satisfies both the classical conformal and $U(1)'$ symmetry. Analogous to the previous chapter, the renormalised 1-loop zero-temperature potential reads (cf. sec. 5.3.3)

$$V_{1\text{-loop}}(\phi_b, T=0) = \sum_a \pm \frac{n_a}{64\pi^2} \frac{m_a^4(v)}{v^4} \phi_b^4 \left[\log \left(\frac{\phi_b^2}{v^2} \right) - \frac{1}{2} \right], \quad (6.3)$$

which follows from adopting the same renormalisation conditions. The addition of the fermion fields however slightly modifies the relation for the self-coupling λ ,

$$\lambda = 11 \sum_a \pm \frac{n_a}{48\pi^2} \frac{m_a^4(v)}{v^4} = \frac{11}{48\pi^2} (10\lambda^2 + 3g^4 - y^4), \quad (6.4)$$

as now also the Yukawa coupling contributes. Note that for large y the potential becomes unstable and unbounded from below, which puts the bound on the Yukawa coupling $y < 10\lambda^2 + 3g^4$. Through the radiative symmetry, breaking the DS states obtain the background field dependent masses terms

$$m_\phi^2(\phi_b) = 3\lambda\phi_b^2, \quad m_\varphi^2(\phi_b) = \lambda\phi_b^2, \quad m_{A'}^2(\phi_b) = g^2\phi_b^2, \quad m_\chi(\phi_b) = \frac{y\phi_b}{\sqrt{2}}. \quad (6.5)$$

At finite temperature, the particles additionally obtain the Debye masses

$$\Pi_\phi = \left(\frac{\lambda}{3} + \frac{y^2}{12} + \frac{g^2}{4} \right) T^2, \quad \Pi_\varphi = \left(\frac{\lambda}{3} + \frac{y^2}{12} + \frac{g^2}{4} \right) T^2 \quad \text{and} \quad \Pi_{A'_L} = \frac{5}{12} g^2 T^2, \quad (6.6)$$

which enter the daisy term of the effective potential.

In fig. 6.1 we show the dark Higgs mass m_ϕ and the ratio of the DM and dark Higgs mass m_χ/m_ϕ in the left and right panels respectively in the $g - y$ plane with a fixed VEV of $v = 100 \text{ MeV}$. The white region with $g \lesssim 0.55$ marks the parameter space where the phase transition does not start (or complete) in the lifetime of the universe. Here, the potential barrier persists for too long, such that the background field stays trapped in the false vacuum. Most notably, the mass of the dark Higgs mainly depends on the gauge coupling g , such that the ratio m_χ/m_ϕ becomes largely independent of g and mainly varies with y . Additionally, the dark photon is typically the heaviest state in the relevant parameter space.

As discussed in the previous chapter (cf. sec. 5.3.3) the logarithmic varying of the zero temperature potential eq. (6.3) with the background field value, leads to a potential barrier that lasts up to low temperatures and therefore to generically strong and slow transitions. This can be inspected more closely by looking at the effective potential, including the thermal contributions in fig. 6.2. The conformal symmetry produces a potential that is quite flat around the origin, allowing a potential barrier to persist up until small temperatures, leading to delayed (supercooled) transitions and eventually large GW signals.

6.2.1. Interactions

After the breaking of the $U(1)'$ symmetry, the following interactions between the DS states arise

$$\mathcal{L}_{\text{int}} \supset -\lambda v \phi^3 - \frac{\lambda}{4} \phi^4 + g^2 v A'_\mu A'^\mu \phi + \frac{g^2}{2} \phi^2 A'_\mu A'^\mu + \sum_i \frac{g}{2} Q_i \bar{\chi}'_i \gamma^\mu \gamma^5 \chi'_i A'_\mu - \frac{y}{2\sqrt{2}} \phi \bar{\chi}'_i \chi'_i, \quad (6.7)$$

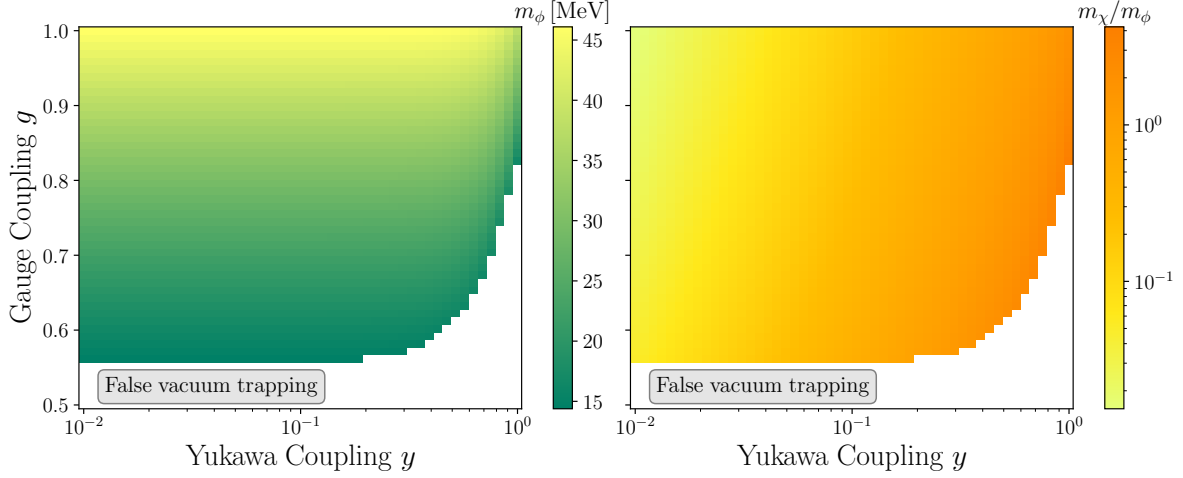


Figure 6.1.: Dark Higgs mass m_ϕ and DM mass ratio m_χ/m_ϕ in dependence of the Yukawa y and gauge coupling g . The VEV is fixed here to $v = 100$ MeV.

with the two Majorana fermions $\chi'_{1,2} = \chi_{1,2} + \chi_{1,2}^c$. Since these two left-handed fermions are mass-degenerate, we can combine them into a single Dirac fermion [272]

$$\chi = \frac{1}{\sqrt{2}} (\chi'_1 + i\chi'_2) , \quad (6.8)$$

such that the mass and interaction with the dark Higgs simplify to $\mathcal{L} \supset -m_\chi \bar{\chi}\chi - y/\sqrt{2}\phi \bar{\chi}\chi$. Due to the opposite charges of the fermions $Q_{\chi_i} = \pm 1/2$, the dark photon interactions cannot, in general, be simplified in that way because the Majorana fermions couple with opposite sign to A' . However, as the sign of the charges does not enter any process we consider in the following study, we can also simplify the DM-dark photon interaction with the effective term $\mathcal{L} \supset g/2 \bar{\chi}\gamma^\mu \gamma^5 \chi A'_\mu$. The opposite signs of the charges would only enter processes involving both χ_1 and χ_2 , which we do not consider here.

For the dynamics of the phase transition, a coupling to the SM is not required. However, as discussed in the previous chapter, the energy released in the phase transition close to BBN is tightly constrained. In order not to modify the observed cosmology, the majority of dark sector energy density has to be transferred to the SM sector before neutrino decoupling. We therefore require a portal that enables decays or annihilations of the dark sector states. The two renormalisable possibilities that were discussed in chapter 5, were the Higgs portal and the gauge boson mixing. The first would however spoil the conformal symmetry, since after the EW phase transition it would induce the mass term $\lambda_{h\phi} v_{EW} |\Phi|^2$. Therefore, we adopt the alternative of kinetic mixing through coupling the dark photon to the SM photon

$$\mathcal{L} \supset \frac{\kappa}{2} F'_{\mu\nu} F^{\mu\nu} , \quad (6.9)$$

with $F_{\mu\nu}$ denoting the SM photon field strength tensor. For the expected mass scale of the dark sector $v_\phi < 1$ GeV, the dark photon will be light compared to the Z boson, which can hence be neglected and we obtain the effective coupling of A'_μ to the SM fermions

$$\mathcal{L}_{\text{portal}} = -\kappa e A'_\mu \sum_f q_f \bar{f} \gamma^\mu f , \quad (6.10)$$

where we sum over all the SM fermions with non-vanishing electric charges q_f . For the parameter range $10^{-7} < \kappa < 10^{-3}$, the decay of dark photons into electron-positron pairs becomes efficient above the MeV scale, as well as scattering off dark sector states on charged

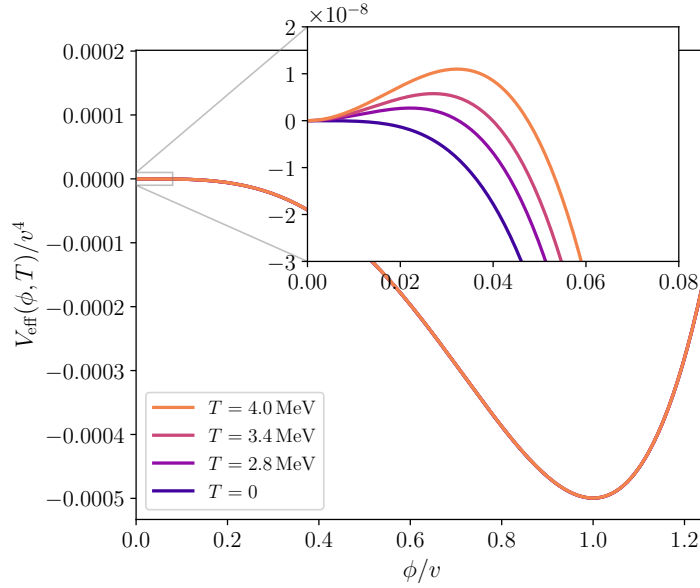


Figure 6.2.: Effective potential around the percolation temperature ($T_{\text{perc}} = 2.8 \text{ MeV}$) of benchmark point *A* from tab. 6.1 with $v = 173$. The zoom-in shows the potential barrier that persists until very small temperatures.

SM particles in the plasma. This admits the assumption that the dark sector shares a common temperature with the SM and the phase transition hence reheats both sectors simultaneously, as opposed to the discussion in ref. [49]. The fermion however, constitutes a stable dark matter candidate, which can annihilate into SM particles via the dark photon portal or, if kinematically allowed, into DS states. We will study the resulting relic abundance in more detail in sec. 6.4.

The dark Higgs can decay via a dark photon-loop into SM leptons. For heavy dark photons $m_{A'} \gg m_\phi$ and $m_\phi \gg m_f$ the decay width is given by [273]

$$\Gamma_{\phi \rightarrow f \bar{f}} = \frac{27e^4 \kappa^4 g^2 m_\phi}{128\pi^5} \frac{m_f^2}{m_{A'}^2}. \quad (6.11)$$

Below the muon threshold, only the decay into electrons is possible and we obtain the approximate lifetime

$$\tau_\phi \approx 2500 \text{ s} \left(\frac{\kappa}{10^{-4}} \right)^4 \left(\frac{g}{0.75} \right)^2 \frac{m_\phi}{30 \text{ MeV}} \left(\frac{100 \text{ MeV}}{m_{A'}} \right)^2. \quad (6.12)$$

Due to the loop suppression of the decay, the lifetime of the dark Higgs is hence large compared to the Hubble time before BBN. We find that the kinetic mixing alone is not sufficient to fully deplete the dark sector energy density between the phase transition $T_{\text{reh}} = \mathcal{O}(10) \text{ MeV}$ and BBN.

There are several possibilities to enhance the decay of the dark Higgs into SM particles. One would be the effective coupling to photons, which is, however, excluded in the mass range of interest by experimental data and supernova constraints [274, 275]. Instead, we will here consider the effective coupling of the dark Higgs to electrons for which supernova constraints are weaker [242, 243]. An example to generate such an effective coupling could arise by introducing new heavy vector-like leptons that, after integrating them out, give the effective interaction

$$\mathcal{L}_{\text{int}} \supset \frac{1}{\Lambda^2} (\phi^* \phi) \bar{l}_L e_R H + \text{h.c.}, \quad (6.13)$$

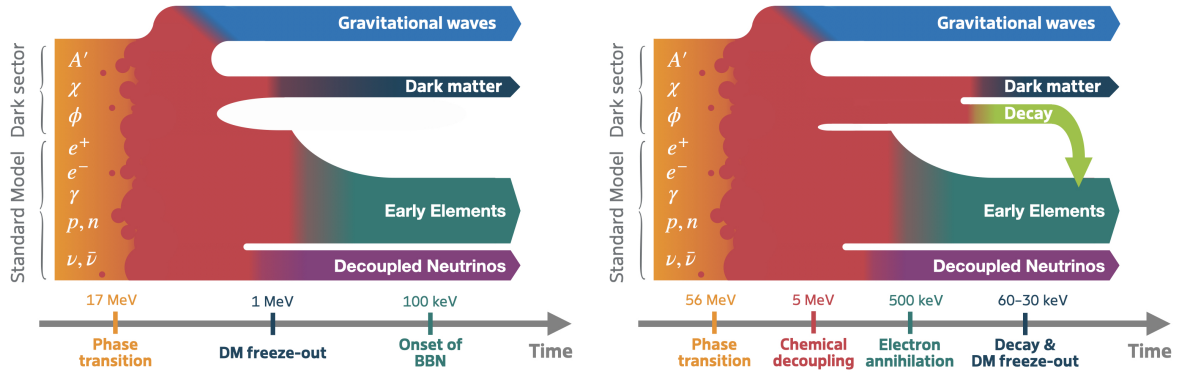


Figure 6.3.: *Left panel:* Cosmological history of the coupled dark sector scenario corresponding to point A in tab. 6.1. *Right panel:* Cosmological history of the secluded dark sector scenario corresponding to point B in tab. 6.1. The qualitative difference is in the dark Higgs, which is always in thermal equilibrium in the coupled scenario, while it decouples together with the DM in the secluded scenario and decays during or after BBN. This illustration was kindly provided by C. Tasillo.

Parameter	g	y	δ	κ	v	$m_{A'}$	m_ϕ	m_χ	T_p	T_{reh}	α	$(\beta/H)_{RH}$
Unit	-	-	-	-	MeV	MeV	MeV	MeV	MeV	MeV	-	-
Point A	0.677	0.224	-0.322	2.29×10^{-6}	173	117	36.3	27.4	2.28	16.8	4.7×10^3	50.9
Point B	0.601	0.234	6.48×10^{-3}	2.7×10^{-4}	692	416	114	115	1.21	55.9	9.48×10^6	27.1

Table 6.1.: Model parameters, masses and phase transition parameters for two benchmark points. The point A corresponds to the best-fit point of the coupled dark sector of the global fit discussed in sec. 6.6.1. Point B corresponds to the best-fit point of the secluded dark sector global fit after imposing an additional condition on the lifetime of the dark Higgs as discussed in sec. 6.6.2.

which reduces to the effective interaction $y_{\text{eff}}\phi\bar{e}e$ with $y_{\text{eff}} = v_h v/(\Lambda^2)$ after the EW and $U(1)'$ symmetry breaking. For details on a possible UV model that realises this coupling, see appendix A of ref. [39].

With this, we have two different scenarios that we can study. The first is the case of a *coupled dark sector*. Here, we assume a value of the effective dark Higgs coupling to the electrons large enough such that the dark Higgs bosons decay efficiently, but small enough not to impact the phase transition. The second is the case of a *secluded dark sector* where only the decay through the dark photon loop is allowed. In the latter case, we have to carefully examine constraints from BBN on the dark Higgs, as a non-negligible population could remain until keV temperatures in some part of the parameter space.

To understand the cosmological history around the phase transition, it is illustrative to focus on a benchmark point for each scenario. These points are summarised in tab. 6.1, where point A corresponds to the coupled scenario and point B to the secluded dark sector. A sketch of the two scenarios is given in fig. 6.3. In the coupled dark sector (left panel), the dark matter candidate χ freezes out after the phase transition and slightly before neutrino decoupling. Since the dark Higgs is heavier and we assumed efficient coupling, it decays even earlier, avoiding bounds from BBN. The right panel shows the scenario for the secluded dark sector. Due to loop-suppressed decay of the dark Higgs, the whole dark sector freezes out after the phase transition and the dark Higgs decays during and after BBN. This leads to tight constraints on the model parameters as we will see in sec. 6.5.

6.3. The PTA data

In the following section, we will discuss our modelling of the stochastic GW background. Here we include both an astrophysical contribution from the inspiralling of supermassive BHB and a contribution from the DS FOPT

$$h^2\Omega_{\text{gw}}(f) = h^2\Omega_{\text{gw}}^{\text{BH}}(f) + h^2\Omega_{\text{gw}}^{\text{PT}}(f). \quad (6.14)$$

In the following, we will examine how the requirements on the GW signal to fit the PTA data constrain the model parameters.

6.3.1. Modelling of the GW signal

We proceed with the modelling of the astrophysical and cosmological source of the GW background in the same way as in the previous chapter (cf. sec. 5.2). However, this time, we explicitly include the astrophysical signal as a broken power law

$$h^2\Omega_{\text{gw}}^{\text{BH}}(f) = \frac{2\pi^2}{3H_{100}^2} A^2 \left(\frac{f}{1\text{yr}^{-1}} \right)^{5-\gamma} \text{yr}^{-2}. \quad (6.15)$$

Here, we have $H_{100} = H_0/h = 100 \text{ km s}^{-1} \text{ Mpc}^{-1}$ and the present day Hubble rate is $H_0 = 67.8 \text{ km s}^{-1} \text{ Mpc}^{-1}$. As recommended by the NANOGrav collaboration [71], we use the Gaussian likelihood for the amplitude A and spectral index γ

$$\mu_{A,\gamma} = \begin{pmatrix} -15.615 \\ 4.707 \end{pmatrix} \quad \text{and} \quad \text{cov}_{A,\gamma} = \begin{pmatrix} 0.279 & -0.003 \\ -0.003 & 0.124 \end{pmatrix}. \quad (6.16)$$

Since the DS model contains the massive gauge bosons A' that couple strongly ($g \gtrsim 0.55$) to the scalar, we expect even for strong transitions that the FOPT occurs through bubbles that expand with a relativistic, but terminal velocity $v_w \simeq 1$, such that the GW signal will be sourced by sound waves after the bubble collisions. Therefore, we expect the signal from the FOPT to follow the double broken power law as discussed in sec. 3.5.5.

We can check the assumption of a sound wave dominated signal by studying the bubble expansion velocity more carefully. As the transition radiation of the massive gauge bosons creates additional pressure on the bubble wall that grows with the bubble wall Lorentz factor $\gamma = 1/\sqrt{1-v_w^2}$, they prevent a run-away behaviour [130, 137]. We check this explicitly by computing the bubble wall Lorentz factor γ_{eq} (cf. eq. (3.166)), for which the pressure from transition radiation becomes larger than the driving pressure. By comparing this to the would-be Lorentz factor at percolation if transition radiation was neglected, γ_* we obtain the efficiency factor for the energy released that goes into the bubble wall κ_{col} (see sec. 3.5.3). In the left panel of fig. 6.4, we show κ_{col} and see that only a tiny fraction of the energy released in the transition goes into the acceleration of the bubble walls, i.e. they very quickly reach a terminal velocity.

For bubbles that expand as deflagrations and hybrids, it has been shown that the assumption of LTE gives a good approximation of the bubble wall velocity [181]. Using this approximation, we compute the wall velocity using the code provided by ref. [176] and show the result in the $y-g$ plane for $v = 100 \text{ MeV}$ in fig. 6.4. The LTE approximation predicts a large bubble wall velocity $v_w \gtrsim 0.9$ for all parameter points. In the regions around the benchmark points (tab. 6.1), shown as the red pentagon and yellow star, the LTE approximation predicts a wall velocity of $v_w \simeq 1$, as the bubbles expand as detonations. However, it has been shown that the LTE approximation overestimates the wall velocity for detonations, as it predicts the pressure to be a monotonically decreasing function of v_w in this case [176]. We therefore

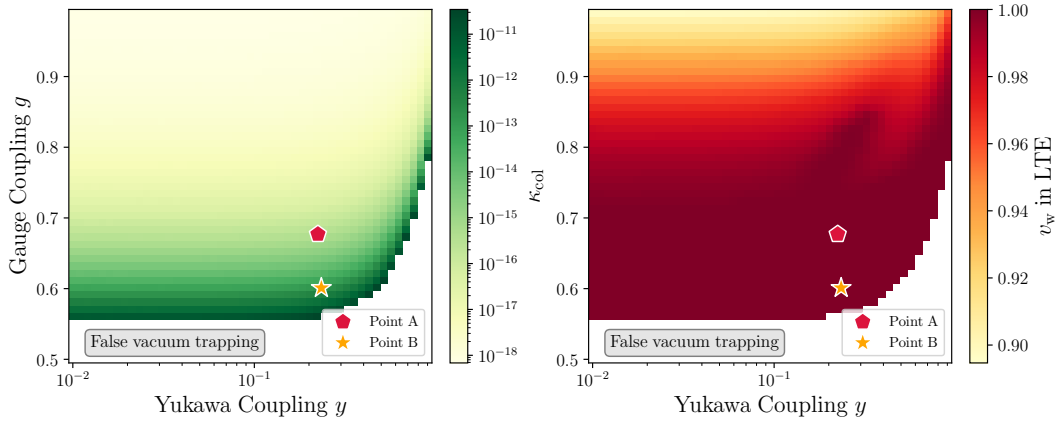


Figure 6.4.: *Left:* Efficiency factor for bubble collisions κ_{col} showing that the energy in the bubble walls can be neglected. *Right:* Bubble wall velocity computed in LTE at the nucleation temperature. The couplings of the benchmark points *A* and *B* from tab. 6.1 are shown as the red pentagon and yellow star respectively. Here the VEV is fixed to $v = 100$ MeV.

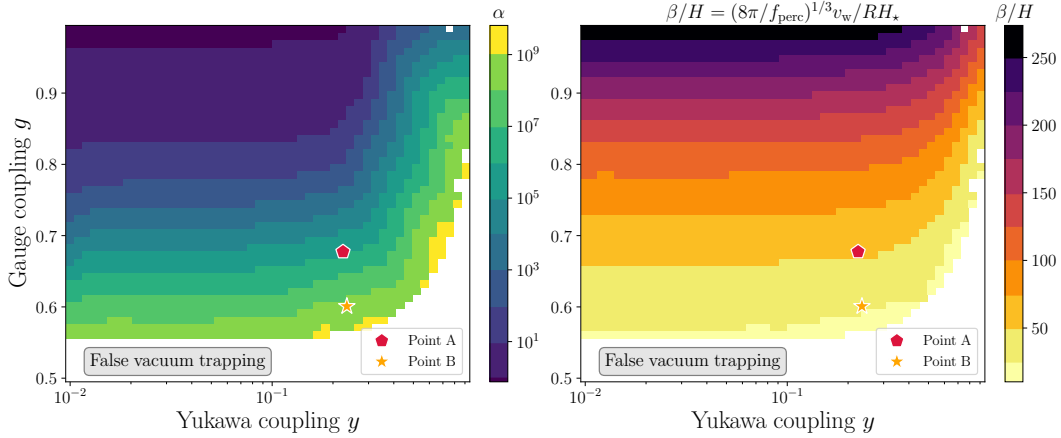


Figure 6.5.: Transition strength α and transition speed $(\beta/H)_{RH}$ in the $g - y$ plane. The couplings of the benchmark points *A* and *B* from tab. 6.1 are shown as the red pentagon and yellow star respectively. Here the VEV is fixed to $v = 100$ MeV.

employ the code `WallGo` [159] that determines the wall velocity including out-of-equilibrium effects. By implementing the model, we verify that around the benchmark points, the computation including out-of-equilibrium effects only results in sub-percent level deviations. In summary, we can hence treat the bubble expansion as relativistic, but not ultra-relativistic, such that the sound wave contribution is indeed the dominant contribution.

To get an intuition for the predicted phase transition, we show the dependence of the transition strength α and speed $(\beta/H)_{RH}$ on the couplings g and y in fig. 6.5. We fixed $v = 100$ MeV, as the resulting α and $(\beta/H)_{RH}$ values are (neglecting a dependence of g_{eff}) almost independent and only the peak frequency $f_{\text{peak}} \propto v$ is set by on the choice of the VEV. In large regions of the parameter space, the model predicts strong phase transitions that are correlated with large bubble separations (i.e. slow transitions), as already shown in the previous chapter. For these strong transitions ($\alpha \gg 1$), the kinetic energy fraction saturates to $K \simeq 1$, so the GW amplitude is primarily determined by the transition speed $(\beta/H)_{RH}$. We show the values of the couplings of the benchmark points from tab. 6.1 as the red pentagon and yellow star in the figure.

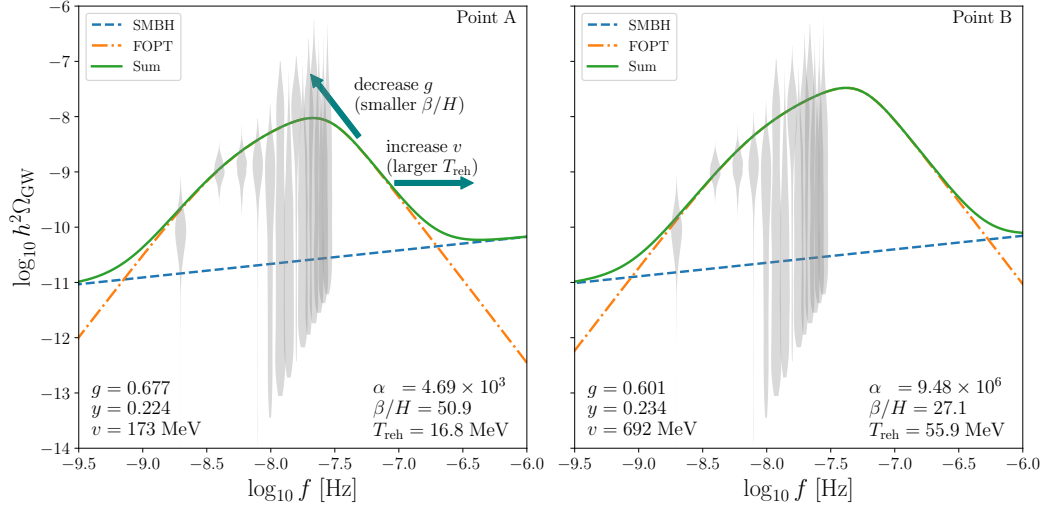


Figure 6.6.: Combined gravitational wave spectra from FOPT and BHBs for the benchmark points given in tab. 6.1. The NANOGrav 15 yr data is shown the grey violins. The BHB signal has the amplitude and slope $(\log_{10} A, \gamma) = (-15.67, 4.755)$ and $(-15.66, 4.756)$ for point A (left) and B (right) respectively.

6.3.2. Comparing the predicted GW signal with PTA data

Before we examine the constraints on the model parameters through the PTA data, let us first inspect the GW spectra of the benchmark points given in tab. 6.1. The left panel of fig. 6.6 corresponds to the coupled dark sector (point A) where a good fit to the PTA data can be achieved by a strong and slow transition with $\alpha = 4.69 \times 10^3$ and $(\beta/H)_{RH} = 50.9$ with a reheating temperature $T_{\text{reh}} = 16.8 \text{ MeV}$. The right panel corresponds to the secluded dark sector (point B), which requires an even stronger and slower transition with $\alpha = 9.48 \times 10^6$ and $(\beta/H)_{RH} = 27.1$ for a good fit. This comes with a slightly smaller gauge coupling g compared to the coupled scenario and a larger reheating temperature $T_{\text{reh}} = 55.9 \text{ MeV}$ that shifts the signal to higher frequencies, which is compensated by the larger amplitude. The reason behind the larger reheating temperature will be discussed in sec. 6.6.2. For both scenarios the combined FOPT and BHB signal gives significantly better fit to the PTA data than the best-fit of only a BHB signal with $\Delta \ln \mathcal{L}_{\text{PTA}} = 6.8$ and $\Delta \ln \mathcal{L}_{\text{PTA}} = 6.6$ for the coupled and secluded dark sector respectively.

In the next step, we examine the general constraints that the fit of the GW signal to the PTA data puts on the model parameters. In fig. 6.5, we have seen that the dependence of the phase transition parameters on the Yukawa coupling is mild for $y \lesssim 0.3$. Therefore, we fix $y = 0.01$ and scan over the gauge coupling and VEV, computing the signal at every point in the plane (without the BHB contribution). The result is shown in fig. 6.7 in terms of the amplitude of the signal at $f = 10 \text{ nHz}$, which is close to the centre of the log-spaced Fourier spectrum of the PTA data. The grey hatching corresponds to region disfavoured on the 2σ level by the likelihood. We can observe that the PTA data requires a certain amplitude of the signal at this frequency, such that the rising slope of the FOPT spectrum fits the PTA data. This puts a lower limit on the VEV, as the peak of the signal has to sit at frequencies larger than $f_{\text{peak}} \gtrsim 10^{-8} \text{ Hz}$, translating into $v \gtrsim 50 \text{ MeV}$. Larger values of the VEV shift the signal to higher frequencies, which can be compensated with larger amplitudes, i.e. smaller g . The preferred region hence decreases in g with increasing v . Below this preferred region (smaller g), the amplitude of the FOPT signal becomes too large and overshoots the PTA data, while at larger g the amplitude of the FOPT signal is too small and here an additional contribution

from the BHBs would be needed to explain the data. For $v \gtrsim 700$ MeV, the peak frequency finally becomes too large to be compensated with an increase of the peak amplitude.

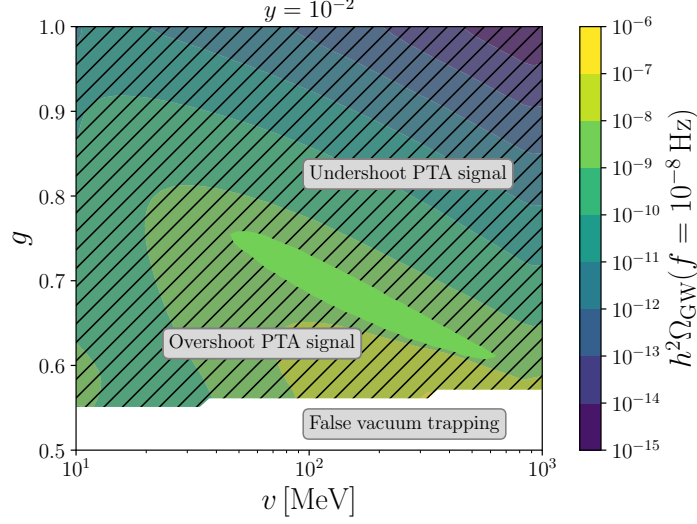


Figure 6.7.: Dependence of the GW amplitude signal from the DS phase transition at $f = 10^{-8}$ Hz on the gauge coupling g and VEV v . For concreteness the Yukawa coupling is fixed to $y = 10^{-2}$. The unshaded region shows the 2σ region favoured by the PTA likelihood, computed with PTArcade [103].

6.4. Relic density calculation

The relic abundance of the DM particle χ is in general set by two types of processes. One that keeps the DM in chemical equilibrium with the DS and one that connects the DS with the SM. The first type includes the annihilation (and production) of DM into dark Higgs particles $\bar{\chi}\chi \leftrightarrow \phi\phi$. We will see that the dark photon is heavy in the relevant parameter region $m_{A'} \gg m_\chi, m_\phi$ such that its contribution to the inter-DS processes is suppressed. In contrast, the second type of process relies on off-shell dark photons to mediate DM conversion to SM fermions ($\bar{\chi}\chi \leftrightarrow e^+e^-$) and to enable (inverse) dark Higgs decays ($\phi \leftrightarrow e^+e^-$). The efficiency of these processes is determined by the kinetic mixing parameter κ . In contrast to the above processes, another type, scatterings off DS states on SM fermions, will always be efficient in the considered ranges of κ , if the electrons are relativistic and abundant. Therefore, we assume that the DS shares a common temperature with the SM.

The DM relic abundance is then set by the number changing processes $\bar{\chi}\chi \leftrightarrow e^+e^-$ and $\bar{\chi}\chi \leftrightarrow \phi\phi$. Since the electrons and positrons are always in thermal equilibrium with the photons in the relevant temperature range, the freeze-out of the former process can be computed using the standard methods discussed in sec. 2.3.4. This however, does not necessarily hold for the latter process. In the scenario that the dark Higgs bosons can only decay via dark photon loops into the SM, the DS can depart from chemical equilibrium with the SM. These two scenarios were introduced as the *coupled dark sector* and the *secluded dark sector* in sec. 6.2.1. For the relic density calculations in the following we will use DarkSUSY [276] interfaced to GAMBIT via the DarkBit [277] interface.

6.4.1. Coupled dark sector

In the coupled dark sector scenario, we assume that the dark Higgs can efficiently annihilate into electrons, such that we can assume a vanishing chemical potential throughout the DM freeze-out. The process that sets the relic density is here $\bar{\chi}\chi \leftrightarrow \phi\phi$. For $m_\chi > m_\phi$, these

annihilations are very efficient, since this implies a large Yukawa coupling $y \gtrsim 0.3$ (cf. fig. 6.1). This would result in a strong depletion and under-abundance of the DM. Therefore, it is necessary for the DM particle to be the lightest state in the DS $m_\chi < m_\phi$ such that the annihilations are kinematically suppressed by the mass difference during the freeze-out [270].

6.4.2. Secluded dark sector

We can show the secluded dark sector evolution (see right panel of fig. 6.3) in terms of the underlying particle process in fig. 6.8. At high temperatures, shortly after the phase transition, the dark sector is in thermal equilibrium with the SM, as number changing processes between the two sectors and within the DS are efficient. However, once the DM annihilation into electrons becomes inefficient, the dark sector leaves chemical equilibrium with the SM and the combined number of dark Higgs bosons, DM particles and DM antiparticles stays constant. This can be expressed in terms of the yield $Y_i = n_i/s$ as

$$Y_{\bar{\chi}} + Y_{\chi} + Y_{\phi} = 2Y_{\chi} + Y_{\phi} = \text{const}, \quad (6.17)$$

where the second equality follows from $n_{\bar{\chi}} = n_{\chi}$. Since the dark photon is heavy $m_{A'} \gg m_\chi, m_\phi$, it quickly decays and becomes Boltzmann suppressed after the phase transition, such that we do not need to account for it here. We determine this constant at the dark sector decoupling temperature T_f^{SM} , where the process $\bar{\chi}\chi \leftrightarrow e^+e^-$ freezes out. As long as the dark sector remains in thermal equilibrium with itself, the yield of dark Higgs bosons and DM are related through detailed balance

$$Y_{\chi}^2 \langle \sigma v \rangle_{\chi\bar{\chi} \rightarrow \phi\phi} = Y_{\phi}^2 \langle \sigma v \rangle_{\phi\phi \rightarrow \chi\bar{\chi}}, \quad (6.18)$$

with $\langle \sigma v \rangle$ denoting the thermally averaged cross sections. Using eqs. (6.17) and (6.18), the evolution of the yield of DM and the dark Higgs bosons can then be determined, see app. D.1 for details. Now, with the thermally averaged cross sections, the freeze-out temperature T_f^{ϕ} of the conversion $\bar{\chi}\chi \leftrightarrow \phi\phi$ (bottom panel of fig. 6.8) sets the relic abundance of the DM. The remaining dark Higgs bosons eventually decay to electron-positron pairs which, depending on the lifetime, adds additional constraints from BBN and CMB as we discuss in sec. 6.5.

In both the coupled and secluded dark sector scenarios, we compute the relic abundance in the two ways discussed and compare it to the Planck measurement of $h^2\Omega_{\text{DM}} = 0.12 \pm 0.001$ [8]. We emphasise however, that the theory uncertainty is significantly larger than the measurement uncertainty. In the coupled scenario, this comes from neglecting effects of early kinetic decoupling and in the secluded sector, we approximate the freeze-out of the $\bar{\chi}\chi \leftrightarrow \phi\phi$ as instantaneous. To account for these uncertainties, we include a factor of two uncertainty in the Gaussian likelihood for the relic density prediction

$$\log_2 \left(\frac{\Omega_{\text{DM}} h^2}{0.12} \right) = 0 \pm 1. \quad (6.19)$$

We will see however, that the relic density depends exponentially on the model parameters in the studied ranges, such that the factor of two only translates into a small shift in the model parameters.

6.5. Constraints

So far we have discussed the phenomenology of the DS in terms of the GW signal that is constrained by the PTA data (sec. 6.3) and the DM freeze-out, which is constrained by the observed DM abundance today (sec. 6.4). The sub-GeV dark sector particles however also have to obey constraints from searches at colliders, as well as astrophysical and cosmological constraints. In this section, we give an overview of these constraints.

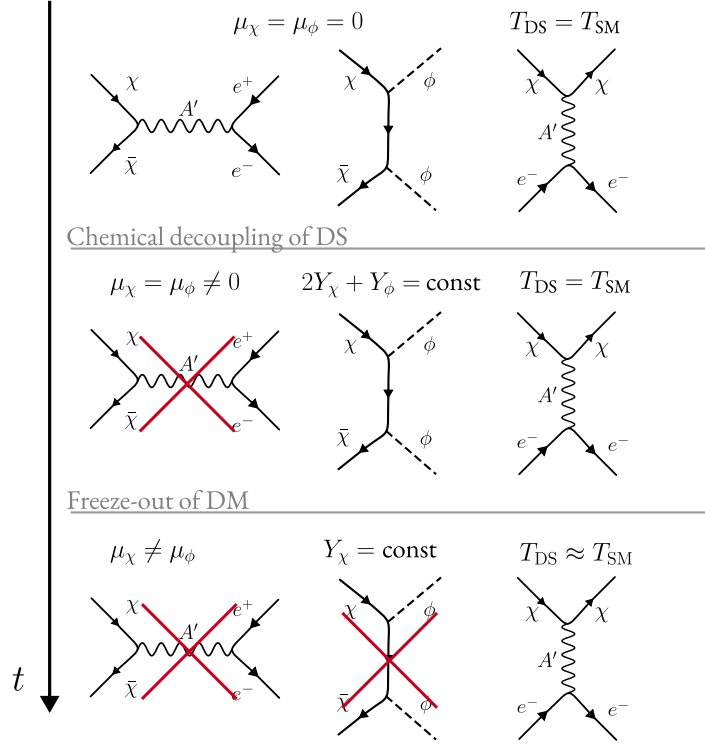


Figure 6.8.: Dominant processes for the thermalisation and subsequent decoupling of SM electrons, the DM particle χ and the dark Higgs boson ϕ in the *secluded dark sector* scenario. The three rows correspond to equilibrium between DS and SM, chemical decoupling of the DS and the DM freeze-out. The crossed-out processes become inefficient at the respective times.

6.5.1. Cosmological constraints

As we saw in sec. 6.3, the nanohertz frequencies of the PTA data restricts the mass scale of the DS particles in the range of $\mathcal{O}(10 - 100)$ MeV, such that non-negligible abundances at $\mathcal{O}(100 \text{ keV})$ temperatures can affect BBN and change the primordial element abundances. If the particles are coupled efficiently to the SM, their number densities will be Boltzmann suppressed, avoiding this problem, but they can still affect the cosmic expansion through their extra energy density at neutrino decoupling. Effectively, this translates into a lower bound on the mass of the lightest dark sector state (the DM candidate χ) $m_\chi \gtrsim 10 \text{ MeV}$. The public code `AlterBBN` [278] implements this effect of extra energy density on the primordial element abundances and is interfaced to the `GAMBIT` module `CosmoBit` [279].

In the secluded scenario, we however expect a non-negligible abundance of the dark sector states to remain and decay during or after BBN. These out-of-equilibrium decays and annihilations can change the standard cosmological history in more complex ways. These late decays inject energy into the plasma and raise the photon temperature. This decreases the relative neutrino temperature and therefore also decreases N_{eff} and at the same time decreases the baryon-to-photon ratio. To account for the effects on N_{eff} , we use `AlterBBN` to compute the changes and compare it to the Planck likelihood $N_{\text{eff}} = 2.99 \pm 0.17$, which combines TT, TE, EE + lowE + lensing + BAO measurements [8]. The effect on the baryon-to-photon ratio is most tightly constrained by the value measured at CMB, which requires a different procedure. Assuming a fixed value at CMB $\eta_{\text{CMB}} = 6.117 \cdot 10^{-10}$, the Boltzmann equation for the dark Higgs energy density and the Friedmann equation is solved backwards to BBN times, yielding the value η_{BBN} that is required to accommodate the entropy injection through

the dark Higgs decays. This value of η_{BBN} , is then used in **AlterBBN** to compute the effect on the primordial abundances. For details and the implementation in **GAMBIT** see ref. [274].

For lifetimes of $\tau_\phi > 10^4$ s, instead stronger constraints come from the photodisintegration of light nuclei [219], as high-energy photons dissociate nuclei instead of forming low-energy electromagnetic cascades. This is implemented in the code **ACROPOLIS** [220], which takes the predicted abundances of **AlterBBN** and calculates the further evolution. Even longer lifetimes are heavily constrained by CMB measurements [280], but we find lifetimes in the preferred parameter ranges to be limited to $\tau_\phi \ll 10^7$ s, such that these constraints are not relevant.

6.5.2. Direct and indirect detection constraints

The annihilation of the DM particles χ into SM fermions or dark Higgs bosons both proceed via p -wave and therefore are strongly suppressed in the non-relativistic limit. Constraints from CMB and astrophysical systems like the bullet cluster that would give strong constraints on s -wave annihilations [263], are therefore not relevant.

In principle, direct detection experiments could probe the model via scatterings of dark matter particles off SM fermions via the effective interaction

$$\mathcal{L}_{\text{eff}} = \frac{1}{\Lambda^2} \bar{\chi} \gamma^\mu \gamma^5 \chi \bar{f} \gamma_\mu f, \quad (6.20)$$

by the exchange of dark photons. The resulting cross section is momentum-suppressed and together with the low sensitivity of detecting scatterings for sub-GeV DM particles gives no relevant constraints from direct detection experiments as well for this model.

6.5.3. Missing energy searches

The cosmological consistency of the scenario relies on a relatively fast decay of the dark sector states, as we have seen in sec. 6.5.1. This requires the kinetic mixing κ to be relatively large and opens up the possibility of the dark photons being produced at colliders and constrained through missing energy searches. After a dark photon has been produced, the larger inter-dark-sector coupling lets it predominantly decay into dark sector states, which would show up as missing energy in colliders. We include constraints on the dark photons from LSND [281, 282], MiniBooNE [283], NA64 [64] and BaBar [284] as implemented in ref. [263]. For further details, see ref. [39]

6.5.4. Dark matter self-interactions

The self-interaction of dark matter is most stringently constrained by observations of the Bullet Cluster, which consists of a smaller subcluster passing through a larger main cluster. Ejections of DM particles through self-interactions from the subcluster lead to a mass loss of the subcluster, which is constrained by observations of the mass-to-light ratio. The self-interaction cross sections in the non-relativistic limit are given by the velocity independent expressions

$$\sigma_{\chi\chi \rightarrow \chi\chi} = \frac{y^2}{256\pi v^2} \left(3 - 4 \frac{m_\chi^2}{m_\phi^2} \right)^2, \quad (6.21)$$

$$\sigma_{\chi\bar{\chi} \rightarrow \chi\bar{\chi}} = \frac{y^2}{128\pi v^2} \left(7 - 4 \frac{m_\chi^2}{m_\phi^2} + 16 \frac{m_\chi^4}{m_\phi^4} \right). \quad (6.22)$$

Using these cross sections, the scattering and ejection of DM particles from the subcluster can be computed. This results in a mass loss fraction of the subcluster that can be used to constrain the cross sections [285–287]. For the details on this, we refer to ref. [263].

6.6. Results

We now turn to exploring the two phenomenologically distinct cases with the global fitting framework **GAMBIT** [52]. This tool contains different modules that implement collider constraints (**ColliderBit**), the cosmological constraints by interfacing **AlterBBN** and **ACROPOLIS** (**CosmoBit**), and we extended it by adding an interface to **TransitionListener** and **PTArcade** to obtain the likelihood for the PTA data.

We refer to the first scenario that we explore as the *coupled dark sector*, where we assume efficient coupling of the dark Higgs, such that the DS remains in chemical equilibrium during the freeze-out of the DM. The second scenario we refer to as the *secluded dark sector*, as we do not assume additional couplings to the SM beyond the kinetic mixing of the dark photon. This will result in the dark sector to leave chemical equilibrium with the SM before the DM freeze-out and leads to additional constraints as dark Higgs bosons decay during and after BBN. As we will see, this results in preferences for different regions in parameter space.

Let us now briefly discuss the model parameters and their ranges. As we have seen in sec. 6.3.2, the gauge coupling g is mainly responsible for the strength of the phase transition. A priori, it could take any value up to the perturbativity bound $g < \sqrt{4\pi}$, but as we saw in fig. 6.7, only a narrow range gives a strong first order phase transition. Therefore, we restrict it to $0.3 \leq g \leq 1$. In a similar manner, we restrict the VEV to values in the range $10 \text{ MeV} \leq v \leq 1 \text{ GeV}$, where the frequency of the GW signal lies in the nanohertz region. This also translates into an upper bound on the dark Higgs mass $m_\phi < 200 \text{ MeV}$ such that decays into muons and pions do not play a role.

The DM mass, controlled by the parameter y , is strongly constrained by the relic density from the freeze-out process. In the coupled scenario, we restrict $0.15 \leq y \leq 0.45$, corresponding to the regime of forbidden annihilations $0.5 \lesssim m_\chi/m_\phi \lesssim 1$. In the secluded scenario, we find $m_\chi \approx m_\phi$ so that it is more convenient to introduce the mass splitting parameter

$$\delta = \frac{m_\chi - m_\phi}{m_\chi}, \quad (6.23)$$

that we vary between $10^{-3} \leq \delta \leq 0.1$. The last parameter of the model is the kinetic mixing of the dark and SM photon. In the sub-GeV range, values of $\kappa > 10^{-3}$ are excluded by dark photon searches, which we choose as an upper bound. For a lower bound, we set $\kappa > 10^{-7}$, as even lower values have no impact on phenomenology. As the secluded dark sector relies only on the kinetic mixing to deplete the DS, this coupling will be generally larger and we can restrict it to $10^{-5} < \kappa < 10^{-3}$.

We explore the global likelihood constructed for our constraints by **GAMBIT** in these parameter spaces for the two scenarios using the sampler **Diver** [288] with a population size of 38000 and the convergence threshold 10^{-5} .

6.6.1. Coupled dark sector scenario

We start the discussion of the results with a general overview of the parameters. We saw that the gauge coupling g was mainly responsible for the strength and speed of the phase transition, while the VEV v set the frequency of the signal. The dependence on the Yukawa coupling y was only mild, as we concluded in sec. 6.3.1. Therefore, the fit to the PTA data determines the combination of g and v , while the Yukawa coupling determines the DM relic abundance through the freeze-out of the process $\chi\bar{\chi} \leftrightarrow \phi\phi$. For the coupled scenario, the kinetic mixing κ is irrelevant as it does not enter the effective potential nor determine the interactions between DS and SM which is instead given by the effective interactions of the dark Higgs.

The allowed parameter regions are shown in fig. 6.9 for the coupled scenario in terms of the profiled likelihood ratio with respect to the best-fit point marked with the star (point A in tab. 6.1). The top row shows the $g - v$ plane, which is mostly constrained through the PTA data. As already seen in fig. 6.6, the gauge coupling determines the amplitude of the signal through the degree of supercooling and mean bubble size at collision, while the overall frequency is set by the VEV. The allowed region here corresponds to a signal where the rising slope of the signal fits the PTA data ($h^2\Omega_{\text{gw}} \simeq 10^{-8}$ at $f \simeq 10^{-8}$). Overall, larger amplitudes with decreasing g are compensated by shifting the signal to larger frequencies with larger v . This leads to the viable region of $g \simeq 0.57 - 0.75$ and $v \simeq 60 - 900$ MeV. The right top panel shows the same parameter plane, but with the shading indicating the transition speed $(\beta/H)_{RH}$ instead. Additionally, we show the contour of fitting the FOPT signal alone to the PTA data with the black contour, which follows the overall shape of the allowed region. Since we include a BHB component in the fit, the results here allow for slightly lower values of g , where the BHB signal can compensate. The lower bound on g comes from the requirement to not overshoot the PTA signal, which is not modified by the additional BHB contribution. The typical values of the transition speed range from $(\beta/H)_{RH} \simeq 15 - 45$ corresponding to large bubble sizes and significant supercooling. This can be seen more clearly from the percolation temperature of the best-fit point $T_{\text{perc}} \sim 2$ MeV, which is about two orders of magnitude lower than the VEV.

The combination of g and v determines the mass of the dark photon $m_A = gv$, which is hence as well restricted by the PTA data to $m_{A'} \simeq 50 - 600$ MeV. The same holds for the dark Higgs since, for $y^4 \ll g^4$, the mass is mainly determined by g (cf. eq. (6.4)) through $m_\phi \approx 0.46gm_{A'}$. This gives the range $m_\phi \simeq 20 - 170$ MeV.

The lower left panel of fig. 6.9 shows the allowed parameter region for the DM mass determined through the Yukawa coupling $m_\chi = yv/\sqrt{2}$. For Yukawa couplings $y \gtrsim 0.65g^2$, the DM would be heavier than the dark Higgs mass and together with the large coupling would deplete the dark matter too efficiently through the process $\chi\bar{\chi} \rightarrow \phi\phi$, to leave the observed relic abundance behind. This gives the requirement of $m_\chi < m_\phi$ where the annihilation is kinematically suppressed at low temperatures. This gives an approximate dependence of the relic abundance on the Boltzmann suppression factor $\exp(\Delta m/T_f)$ with the mass difference $\Delta m = m_\phi - m_\chi$ and the freeze-out temperature T_f . We find a ratio of $m_\chi/m_\phi \simeq 0.7 - 0.9$ required to give the right abundance, as can be seen in the lower left panel of fig. 6.9. Larger DM masses give a relic abundance which is too small, while smaller masses lead to too much DM. As the dark Higgs mass depends on the gauge coupling, as discussed above, this requirement on the mass ratio gives the tight positive correlation between g and y shown in the lower right panel.

With the viable parameter space found, we can discuss the thermal history of the coupled scenario with the example of the best-fit point. The phase transition is supercooled until bubbles nucleate and percolate at $T_{\text{perc}} = 2.28$ MeV, which reheats the plasma of the combined dark and SM sectors back to $T_{\text{reh}} = 16.8$ MeV. After the phase transition, the dark sector is already non-relativistic with masses of $m_A = 117$ MeV, $m_\phi = 36$ MeV and $m_\chi = 27$ MeV, such that it is quickly depleted by dark Higgs bosons decaying into electron-positron pairs. The dark matter freezes out around neutrino decoupling $T_f = 1.2$ MeV. At this point the other, heavier DS states are already strongly suppressed such that they do not affect the subsequent cosmological evolution. We can quantify this by the value found of $N_{\text{eff}} = 3.023$ that only slightly deviates from the standard value.

In the favoured region, we found the mass ratio $m_\chi/m_\phi \gtrsim 0.7$ to be required to set the correct relic abundance through the process $\chi\bar{\chi} \leftrightarrow \phi\phi$. For smaller mass ratios the relic abundance could in principle also be reached via an off-shell dark photon mediated annihilation $\chi\bar{\chi} \rightarrow A'^* \rightarrow e^+e^-$. For the best-fit point this could be achieved for $\kappa \sim 2 \cdot 10^{-3}$ which is ruled out

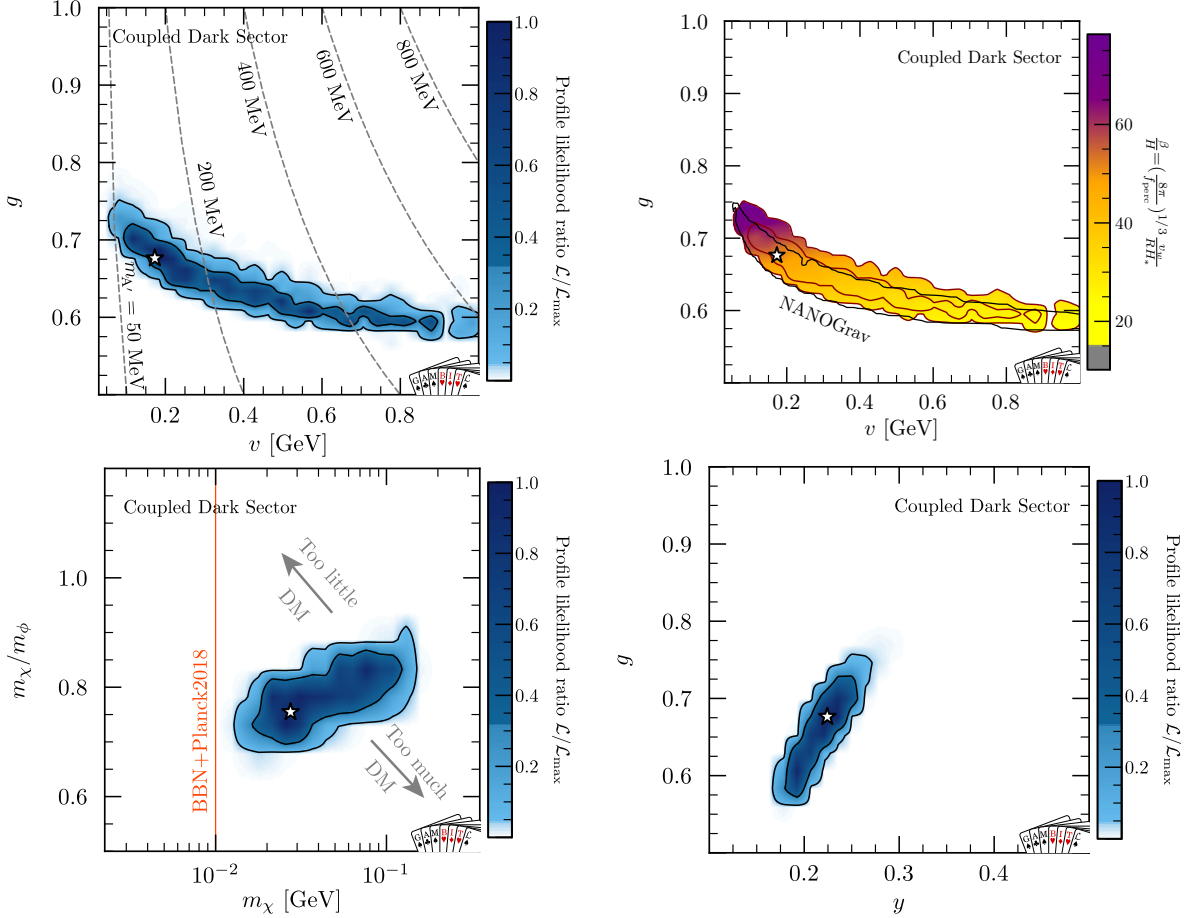


Figure 6.9.: Parameter regions determined through a global-fit analysis in terms of the profile likelihood (blue shading) for the coupled dark sector scenario. The dashed lines in the top-left panel show the lines of constant dark photon mass $m_{A'} = gv$. Instead of the profile likelihood, we show the phase transition speed $(\beta/H)_{RH}$ in the colour shading. The overlaid black lines show the preferred parameter region by the PTA data for a FOPT-only GW signal, cf. fig. 6.7.

by the null result of NA64 which poses an upper bound of $\kappa \sim 2 \cdot 10^{-4}$ for $m_{A'} \approx 120$ MeV. Therefore, no parameter space opens up due to this scenario and the kinetic mixing κ remains unconstrained.

6.6.2. Secluded dark sector scenario

Let us now continue with the results of the secluded dark sector. As opposed to the coupled scenario discussed above, now the kinetic mixing parameter will play a crucial role in depleting the energy density of the DS in order to avoid cosmological bounds. As we will see, the bounds on κ by NA64 shift the dark photon to higher masses and therefore also the VEV. Since the kinetic mixing has no influence on the GW signal, overall results in the $g - v$ plane remain the same as can be seen in the upper left panel of fig. 6.10. The best-fit point however has shifted to larger dark photon masses. This is due to the NA64 bounds shown in the $\kappa - m_{A'}$ plane in the upper right panel. For masses $m_{A'} \lesssim 200$ MeV, the upper bounds on κ become increasingly strict. For the best-fit region with $m_{A'} \simeq 200 - 600$ MeV, the mixing parameter can take values up to $\kappa \approx 4 \cdot 10^{-4}$. This shift of the VEV required by the collider bounds leads to larger masses of the dark Higgs and DM as well, as can be seen in the lower left panel, which are now around 20 – 200 MeV.

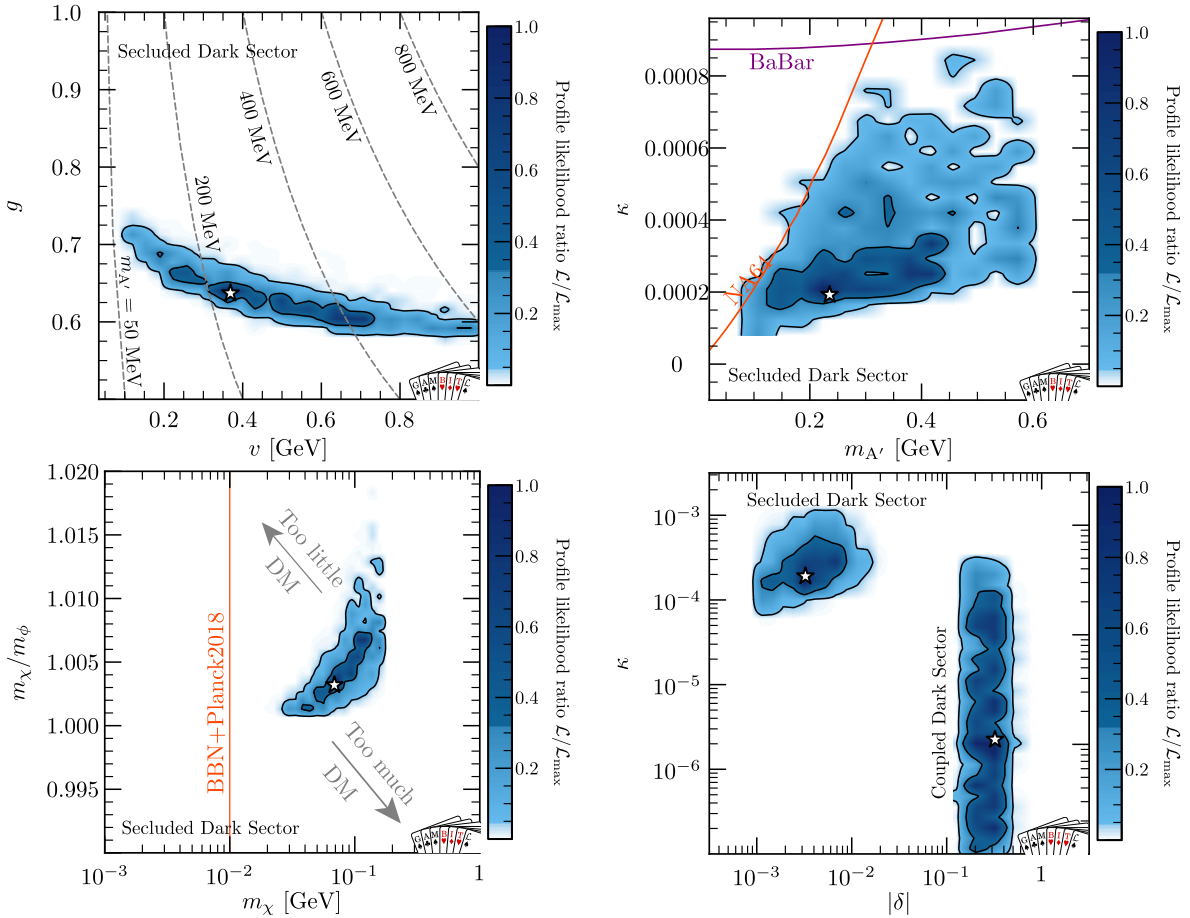


Figure 6.10.: Allowed parameter regions in terms of the profile likelihood (blue shading) determined through a global-fit analysis for the secluded scenario. In the top-left panel we show the lines of constant dark photon mass $m_{A'} = gv$ as the dashed lines. We explicitly show relevant experimental constraints beyond those from the PTA GW signal.

As explained in sec. 6.4.2, the relic density now requires a small mass splitting between the DM and dark Higgs, with a slightly larger DM mass. This leads to the allowed region in the $\kappa - |\delta|$ plane shown in the lower right panel with $10^{-3} \lesssim \delta \lesssim 10^{-2}$. For larger values of the mass splitting δ , the DM would efficiently annihilate into dark Higgs and result in a too small relic abundance. For smaller or negative mass splittings, the dark Higgs would instead deplete into DM particles, leaving behind too much DM relic density.

Additionally, we also show the result of the coupled scenario in the lower right panel to highlight the main differences between the two scenarios. The coupled scenario has an almost unconstrained value of κ , while the relative mass difference is $-0.1 \lesssim \delta \lesssim -0.4$. This makes it easier for the model to explain both dark matter as well as the PTA data at the expense of requiring additional couplings of the dark Higgs. In the secluded scenario these values are much more tightly constrained. The kinetic mixing κ is as large as possible and just below the exclusion limits, while the relative mass difference is tightly tuned to obtain the observed relic abundance. The latter scenario therefore has the advantage that it will become testable in collider experiments. With tighter bounds on κ , also the tuning in δ will increase in order to produce the right abundance of DM.

We can take a closer look at the dark Higgs bosons in the context of their impact on standard cosmology in fig. 6.11. Besides the dark Higgs lifetime τ_{ϕ} , also the abundance of dark Higgs bosons plays a role. We parameterise it here in terms of the relative abundance

$f_\phi = \tilde{\Omega}_\phi/\Omega_{\text{DM}}$, where $\tilde{\Omega}_\phi$ is the would-be abundance of dark Higgs bosons for $\tau_\phi \rightarrow \infty$. In the non-relativistic limit, the chemical decoupling of the DS is set through the parameter combination $\kappa^2 g^2 m_\chi^2 / (m_{A'}^2 - 4m_\chi^2)^2$ (see app. D.1 for the cross section), and since the dark Higgs is the lightest state, it dominates the dark sector abundance. This results in the upper left panel of fig. 6.11. An earlier decoupling through a smaller value of the parameter combination leads indeed to a larger dark Higgs abundance f_ϕ . Instead, the lifetime of the dark Higgs predominantly depends on the kinetic mixing parameter through $\tau_\phi \propto \kappa^{-4}$ (cf. eq. 6.12), as shown in the upper right panel of the figure. As κ is not precisely determined by the constraints and enters with the fourth power, this leads to the range of lifetimes between $10\text{ s} \lesssim \tau_\phi \lesssim 10^4\text{ s}$, so that the dark Higgs decays during or even after BBN. The lower bound on τ_ϕ comes from the upper bound on κ from the collider constraints seen already in fig. 6.10.

The upper bound on the lifetime can be understood by the lower row of fig. 6.11. Here we show the constraints on the dark Higgs abundance and lifetime from primordial element abundances and CMB measurements. For the dark Higgs abundances that we obtain here, the constraints on the dark Higgs lifetime only become relevant for $\tau_\phi \gtrsim 10^4\text{ s}$. For smaller lifetimes, e.g. $\tau_\phi = 100\text{ s}$, larger abundances of $f_\phi \sim 10^4$ would be allowed, while the other constraints on the parameters restrict $f_\phi < 500$. This changes once constraints from photodisintegration become relevant; for lifetimes of $\tau_\phi \gtrsim 10^4\text{ s}$ this already includes abundances with $f_\phi \sim 10$. This constraint from BBN hence imposes an upper bound on $\tau_\phi \lesssim 10^4\text{ s}$ which translates into the lower bound on the kinetic mixing $\kappa > 10^{-4}$.

Now let us briefly discuss the cosmological history of the benchmark point corresponding to this scenario, shown in the right panel of fig. 6.3. The phase transition occurs at the percolation temperature $T_{\text{perc}} = 1.9\text{ MeV}$ and due to the large supercooling ($\alpha = 9.48 \times 10^6$) reheats the combined SM and DS plasma to $T_{\text{reh}} = 55.9\text{ MeV}$. The dark sector states already start here to become non-relativistic with the masses $m_{A'} = 416\text{ MeV}$, $m_\phi = 114\text{ MeV}$ and $m_\chi = 115\text{ MeV}$. Around temperatures of 5.3 MeV , the DS decouples chemically from the SM, while the dark Higgs and DM particles stay in equilibrium until $T_f^\phi \approx 30\text{ keV}$. The decay of the dark Higgs at this point however already becomes relevant for $T_{\text{decay}} \approx 60\text{ keV}$. Therefore, the benchmark point is in conflict with the assumption of $T_f^\phi > T_{\text{decay}}$ that is needed for the consistency of our DM relic abundance computation. A more careful treatment would here require to solve the coupled Boltzmann equations, which would come with an increased numerical cost. This is further illustrated by the lower right panel of fig. 6.11, where the shading (red to green) shows the largest ratio $T_f^\phi/T_{\text{decay}}$ for each point in the $\tau_\phi - f_\phi$ plane. Here, green points ($T_f^\phi > T_{\text{decay}}$) satisfy the assumption of the relic density calculation while the red points ($T_f^\phi < T_{\text{decay}}$) do not. We can see that a region with $\tau_\phi \gtrsim 10^3\text{ s}$ exists where the computation is valid. This implies that there indeed exists viable parameter space where all requirements are satisfied simultaneously, without affecting the qualitative picture presented in fig. 6.10.

Here, it is also worth noting that the energy density in the dark Higgs is completely negligible at their decay. For an extreme point with $f_\phi = 1000$ and $\tau_\phi = 10^3$, the energy density in the dark Higgs bosons only amounts to 10^{-2} of the radiation energy density. Therefore, the entropy injected by the decaying dark Higgs bosons is negligible and we do not need to account for dilution of the GW signal or the DM abundance.

6.7. Discussion

In our global-fit analysis, we found parameter points for both the coupled as well as for the secluded dark sector scenario that can account for the PTA signal and the relic DM abundance

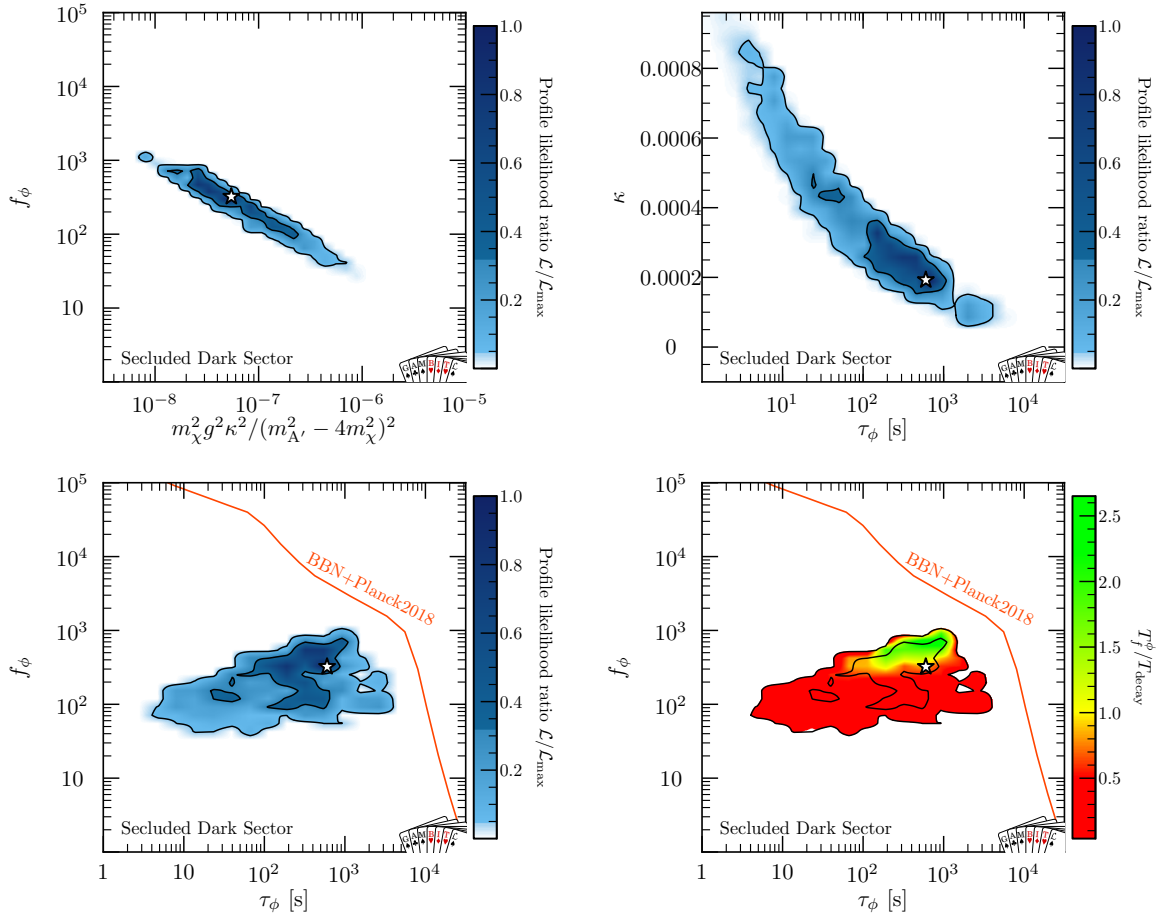


Figure 6.11.: Allowed parameter regions for the secluded dark sector for the dark Higgs boson lifetime τ_ϕ and would-be abundance $f_\phi = \tilde{\Omega}_\phi/\Omega_{\text{DM}}$ in terms of the profile likelihood (blue shading). In the lower right panel, we show instead the largest ratio of the decoupling temperature and dark Higgs decay temperature each point of the $\tau_\phi - f_\phi$ plane (red to green shading). The exclusion limit in the lower row is taken from ref. [217]

while complying with the relevant cosmological and laboratory constraints. Here, we want to discuss the prospects of testing the viable parameter regions with upcoming experiments and future GW observations.

The combination of the individual PTA data sets in the upcoming release of the IPTA is expected to reach a significance of more than 5σ of the Hellings and Downs correlation curve and to establish a discovery of the GW background at nanohertz frequencies [289]. The combined and future datasets of the individual PTA collaborations will also shed more light on the origin of the signal. If the data reveals anisotropies or individual sources in the sky [100, 290], such a finding would favour the astrophysical origin of the signal. On the other hand, improved constraints on the spectral shape of the GW background could provide more hints towards the origin of the signal. With the current data we saw that the peak frequency and amplitude of the FOPT signal can vary significantly, such that we expect the model to also provide a good fit to future measurements, provided that future measurements of an extended frequency range follow the raise in the frequency spectrum. Deviations from a simple rising spectrum would enable to pinpoint a peak frequency of the GW spectrum or disfavour the FOPT explanation if does not match the double broken power law of the FOPT prediction [86].

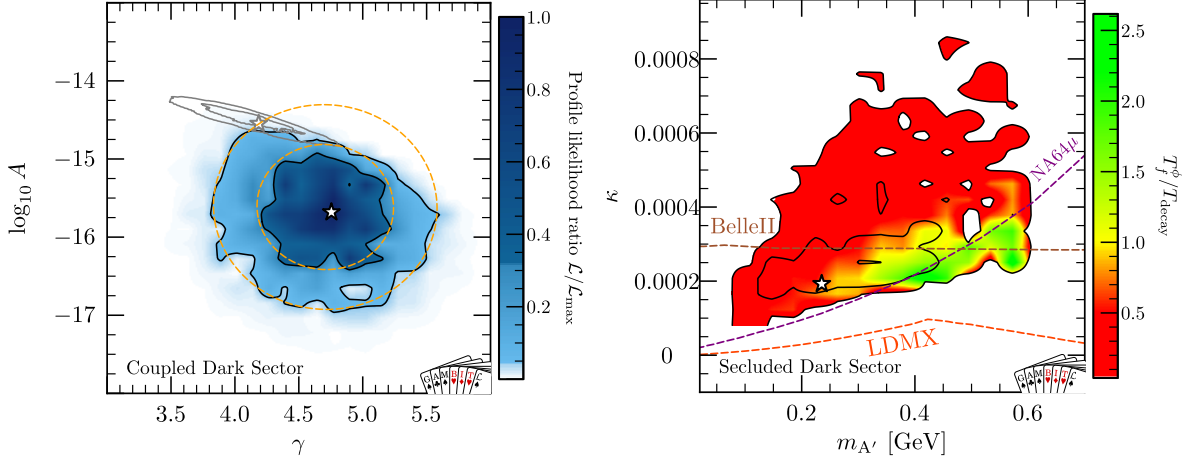


Figure 6.12.: *Left panel:* Allowed parameter regions of the amplitude A and spectral index γ of the BHB GW signal. The yellow ellipses indicate the Gaussian likelihoods inferred from astrophysical modelling and simulations (see eq. (6.16)), while the grey ellipses show the preferred region for a BHB only explanation of the PTA data. The blue shaded region shows the preferred parameters for the combined analysis of a BHB and FOPT contribution to the GW background. *Right panel:* Projected sensitivities in the $m_{A'} - \kappa$ plane of planned and proposed experiments that search for invisible dark photon decays. The shading shows the ratio $T_f^\phi/T_{\text{decay}}$ and indicates regions with ratios $T_f^\phi/T_{\text{decay}} < 1$ where the relic density computation may be unreliable.

To interpret the PTA data, it is also essential to improve the understanding of the astrophysical source of supermassive BHBs. In our analysis, we have modelled the BHB contribution as a simple power law with a likelihood for the amplitude A and spectral index γ based on simulations and modelling of observed BHB populations. This modelling gives a signal that only allows for an explanation of a fraction of the GW signal. This likelihood of the parameters (eq. (6.16)) is shown in the left panel of fig. 6.12 as yellow ellipses. When fitting the PTA data with only a BHB contribution (grey ellipses), we observe a significant shift in the parameters, showing the underlying tension. Upon including the FOPT contribution, this tension is resolved and only a part of the parameter space that would give a too large combined amplitude of the signal is disfavoured. An explanation of the PTA data with only a BHB contribution is therefore disfavoured with the current modelling of BHB. Recent N-body simulations of populations BHB mergers [43] also suggest that new physics or different black hole to host galaxy mass ratios are needed to explain the large amplitude from BHB alone.

Besides the GW phenomenology, the dark sector model also provides the target of dark photons to search for at Belle II [291] and fixed-target experiments, such as NA64 with a muon beam [235] or the planned experiment LDMX [292, 293]. As shown in the right panel of fig. 6.12, these experiments will significantly improve the bounds on the kinetic mixing κ in the sub-GeV mass range for dark photons and LDMX has the potential to fully probe the allowed range of κ in the secluded dark sector scenario.

Furthermore, new CMB data from e.g. CMB-S4 [294] would tighten the constraints on ΔN_{eff} and changes in the neutrino temperature and the baryon-to-photon ratio. This would place an upper bound on the GW amplitude and also further constrain the DM annihilations and dark Higgs decays. A further confirmation of the SM value of N_{eff} could however be accommodated for by increasing the VEV and with it the DS masses.

On the side of the modelling of the GW signal from the FOPT, our simple 1-loop daisy resummed approach of the computation of the effective potential is subject to sizeable uncer-

tainties due to arbitrary renormalisation scale and gauge choices, that has been shown to lead to orders of magnitude uncertainties in the resulting GW amplitude and frequency [114, 190]. The development of effective field theory methods for calculation that rigorously treat the resummation of the infrared divergences and allow the computation of higher order corrections has been shown to significantly reduce the uncertainties of the resulting GW spectrum [192, 295–297]. Nevertheless, we note here that we expect the more rigorous treatment of the effective potential may slightly shift the regions of preferred parameter space, but not to qualitatively impact the conclusions, as shown in ref. [190].

We additionally expect further advances in the description of the hydrodynamics of phase transitions with strong supercooling from improved numerical simulations, better understanding of turbulence [146, 298] and improved understanding of the dynamics of strong supercooling [136, 299, 300]. Even without more data, this could lead to shifts in the preferred parameter space. Moreover, an improved treatment of the relic density calculation, through a proper treatment of the coupled Boltzmann equations, effects of kinetic decoupling [301, 302] and number changing processes [303–305], could help to further narrow down the preferred parameter space of this model.

6.8. Conclusion

In this chapter, we have studied the possible connection of the stochastic GW background measured by the PTA collaborations and the puzzle of the origin of dark matter. A first-order phase transition in a dark sector in the early universe offers a mechanism to explain both observations. We demonstrated that a rather simple model, consisting of a dark Higgs boson, a dark photon and a fermionic dark matter candidate, can give a FOPT that is strong enough to fit the PTA data and at the same time give rise to the mass of the DM candidate, which subsequently freezes out and gives the observed abundance of DM today as a thermal relic.

To match the observed GW signal at nanohertz frequencies with peak amplitudes of $h^2\Omega_{\text{gw}} \sim \mathcal{O}(10^{-8})$, the phase transition has to occur around MeV temperatures and be supercooled, which places the mass scale of the DS particles around $\mathcal{O}(100 \text{ MeV})$. Such a strong phase transition shortly before neutrino decoupling and BBN can result in a significant amount of energy in the DS, that could impact the standard cosmological evolution if it is not efficiently transferred to the SM. We therefore have studied two scenarios of how this DS energy density is depleted, the *coupled dark sector* and the *secluded dark sector*. In the first scenario, we assumed additional efficient interactions of the dark Higgs with electrons, which let it decay quickly before BBN. In the second scenario, the only portal between the DS and the SM is the kinetic mixing between dark and SM photon, which is strongly constrained by laboratory experiments and makes it impossible to completely deplete the dark Higgs abundance before BBN. This gives rise to late decays during and after BBN, leading to additional constraints from cosmological observables, such as N_{eff} and the primordial abundance of light elements.

To include these cosmological and complementary laboratory constraints, we performed global fits for both scenarios and identified viable parameter regions that can both fit the PTA data and reproduce the DM relic density. In the coupled scenario, we find that the relic density requirement dominantly constrains the DM mass, while the PTA data mainly constrains the VEV and gauge coupling. In contrast, the kinetic mixing parameter remains unconstrained, as the sufficiently fast depletion of the DS before BBN is ensured through the assumed effective interaction between dark Higgs bosons and electrons. The secluded scenario however relies only on the kinetic mixing of the photons to deplete the dark sector and hence requires as large values of it as possible. Since the kinetic mixing of dark photons with SM photons is also subject to laboratory searches, this parameter is strongly constrained, which makes the scenario testable with future experiments such as LDMX or Belle II. In light of these

constraints, the dark Higgs mass has to be somewhat larger than in the coupled scenario to ensure lifetimes $\tau_\phi < 10^4$ s that allow the dark Higgs bosons to deplete before they can alter the light element abundances through photodisintegration of nuclei by decaying electromagnetically. The required larger mass scale shifts the GW signal to larger peak frequencies and therefore also larger amplitudes to maintain a good fit to the PTA data.

The upcoming third data release of the IPTA is expected to better resolve the spectral shape of the GW background and shed more light on the origin of this signal. It is therefore important to disentangle and understand the possible contributions from astrophysics through inspiralling supermassive BHBs and cosmological sources, such as first-order phase transitions that we studied in this work.

Over the past decade, the field of gravitational wave astronomy has evolved from the detection of the first GW by LIGO in 2015 to evidence found for a stochastic background of GW at nanohertz frequencies in 2023, marking the beginning of an era of gravitational wave cosmology. Direct observations of the early cosmos, using optical and radio telescopes, are restricted to the cosmic microwave background, since at earlier times the universe was opaque to electromagnetic radiation. In contrast, gravitational waves travel freely through even the earliest times and carry a wealth of information about the processes that created them to us today. This signal, should it not come entirely from astrophysical sources, could be sourced by processes in the early universe at times from milli- to microseconds after the end of inflation. Understanding the processes in the early universe which could have created a GW signal that we would see today as a stochastic background is crucial to the interpretation of current and upcoming data. In this thesis, we have contributed to the efforts by studying the phenomenon of first-order phase transitions in dark sectors in the early universe.

In chapter 4, we have presented the numerical tool `TransitionListener` that allows to systematically explore dark sector models with respect to their first-order phase transition properties. It implements the analysis pipeline from a fundamental particle physics model, encoded in the effective potential to the computation of the phase transition parameters and the evaluation of the GW spectra. In this framework, we model the influence of two different coexisting phases during a first-order phase transition on the cosmic expansion. This allows to take into account the back-reaction of the phase transition on the Hubble rate, which refined the computation of the reheating temperature after the phase transition. The main innovations of the code are efficient numerical algorithms that we developed to compute the evolution of the true-vacuum fraction in these transitions. This permits to directly extract the nucleation, percolation and reheating temperature, as well as the relevant length scale of the transition. A comparison of these more consistent calculations of the phase transition parameters with common simplifications has shown that these refinements are crucial in the regime most relevant for future observations: the regime of slow and strong transitions.

We employed `TransitionListener` in chapter 5 to systematically study the requirements on a dark sector phase transition that could explain the large amplitude seen in the pulsar timing array data measured at nanohertz frequencies. First, we performed a model-independent analysis of the 15 yr PTA data to infer the preferred regions of the parameter space of the

phase transition strength α , speed β/H and reheating temperature T_{reh} . Thereby, we updated earlier results based on previous data releases and confirmed that the interpretation of the data in terms of a phase transition at MeV temperatures requires that it is both strong and slow. While on the model-independent level, the explanation of the PTA observations in terms of a first-order phase transition is viable, we further studied the question of how generic such a signal is, once the correlation between the phase transition parameters arising from the underlying particle physics models is taken into account. In the remainder of the chapter, we studied three representative models that exhibit a first-order phase transition realised through different mechanisms. These are a thermally induced potential barrier realised in an Abelian dark Higgs model, a two-step transition with a zero-temperature potential barrier in a model composed of two scalar singlets and a near conformal Abelian model with a loop-induced potential barrier. All three model classes were found to generate phase transitions strong and slow enough to explain the PTA data, but only the conformal model could do so without requiring significant tuning of the model parameters. The reason for this is the weak temperature dependence of the potential barrier that automatically leads to strong supercooling and hence strong transitions. Such a strong dark sector phase transition at MeV temperatures can leave a sizeable amount of energy in the dark sector that could alter the cosmic history. Generally, the constraints from BBN and CMB observations can be avoided by allowing the dark sector states to decay into SM particles before BBN. We discussed several ways of how these decays could be realised in each model and concluded that for all three models viable possibilities exist.

In chapter 6, we connected the phase transition to the open question of the so far undetected dark matter. We studied the hypothesis that the PTA data could be explained by a dark sector phase transition that also produces the observed relic abundance of dark matter today. Since the PTA signal at nanohertz frequencies requires a phase transition in a dark sector with a mass scale around $\mathcal{O}(100 \text{ MeV})$, this leads to a sub-GeV dark matter candidate. Concretely, we have studied a classically conformal dark sector with a dark Higgs, a dark photon and a fermionic dark matter candidate charged under a $U(1)'$ symmetry. Here, we considered two ways in which the energy density could be depleted after the phase transition, the *coupled* and *secluded dark sector*. In the former, we assumed an efficient decay of the dark Higgs to electrons through an effective coupling arising through higher-dimensional operators. In the latter, we only assumed kinetic mixing between the dark and SM photons to transfer the energy density. Due to bounds on the kinetic mixing from dark photon searches at missing-energy experiments, in this scenario, the dark Higgs bosons do not fully deplete before BBN, leading to additional cosmological constraints. To determine whether the two scenarios can explain the PTA data, the observed DM relic abundance, while simultaneously avoiding current constraints from cosmology, astrophysics and laboratory experiments, we performed a global fit using the fitting framework **GAMBIT**.

In both scenarios, we found viable parameter space that was mainly constrained by the PTA data and the relic density requirement. Additionally, in the secluded dark sector scenario, we obtained a narrow best-fit region for the kinetic mixing $\kappa \simeq (1 - 4) \cdot 10^{-4}$. The parameter needs to be as large as possible to efficiently deplete the dark sector before BBN, while dark photon searches at colliders give a tight upper bound in the preferred dark photon mass range $m_{A'} \simeq 200 - 700 \text{ MeV}$. We found that improved bounds on κ through future searches for dark photons at collider experiments, such as Belle II and NA64 μ , will probe large parts of parameter space, while the proposed experiment LDMX even provides the possibility to fully exclude the secluded scenario. As the kinetic mixing parameter is largely unconstrained in the coupled dark sector scenario, here it will be instead more relevant for future work to study the origin and implications of the assumed coupling of the dark Higgs to electrons.

The observation of a gravitational wave background at nanohertz frequencies has just marked the beginning of the field of gravitational wave cosmology. With future data releases of the IPTA and individual PTA collaborations, we expect to improve our understanding of the origin and nature of this stochastic signal. In this work, we took a step to disentangle the possible origins between cosmological and astrophysical sources. Upcoming and planned experiments that probe larger frequencies, such as LISA and the ET will extend our reach to even earlier times, where the extreme temperatures of the primordial plasma probe particle physics at energies that we could never hope to recreate in laboratory experiments.

Appendix of chapters 2 and 3

A.1. Details on the PTA likelihood

Here we will briefly give an overview of the computation of the PTA likelihood as implemented in the tool `PTArcade` [103] that we employed, by follow along ref. [76].

The data measured by the PTA collaborations is the time-of-arrival (TOA) of the pulsar signals. Here, we write this data as a vector $\vec{t}_{\text{obs}}$ containing the N_{TOA} measurements. By comparing the measurements to the TOAs predicted by the timing models $\vec{t}_{\text{pred}}$ (cf. eq. (2.95), the timing residuals $\vec{\delta t}$ can be written as

$$\vec{\delta t} \equiv \vec{t}_{\text{obs}} - \vec{t}_{\text{pred}} = \vec{n} + \mathbf{F}\vec{a} + \mathbf{M}\vec{e}. \quad (\text{A.1})$$

Here, the first term $\vec{n} = (n_1, \dots, n_{N_{\text{TOA}}})^T$ is the vector of white noise left for the number N_{TOA} of TOA observed, after accounting for all the systematic effects on the TOA. These are assumed to be random variables with zero mean, and the covariance matrix $\mathbf{N}$ of these parameters is set to the value found in the individual pulsar noise studies.

The second term describes the time-correlated stochastic processes. This accounts for the GW signal, as well as pulsar intrinsic long-timescale noise processes, so-called *red noise*. These processes can be modelled as a Fourier series

$$f(t) = \sum_{k=1}^{N_f} a_k \sin\left(\frac{2\pi kt}{T_{\text{obs}}}\right) + \sum_{k=1}^{N_f} b_k \cos\left(\frac{2\pi kt}{T_{\text{obs}}}\right). \quad (\text{A.2})$$

Since only long-timescale, i.e. low-frequency, processes are of interest, the series is cut at N_f terms. The default values are here for the red noise $N_{f,\text{red}} = 30$ and GW background $N_{f,\text{GW}} = 14$. The time correlated contribution to the timing residuals is therefore given by $\vec{t}_{\text{red}} = \mathbf{F}\vec{a}$, where $\vec{a} = (a_1, b_1, \dots, a_n, b_n)^T$ and design matrix $\mathbf{F}$ contains the sine and cosine functions evaluated at the observed TOAs $\vec{t}_{\text{obs}}$.

The coefficients are then modelled as zero-mean random variables with the covariance matrix $\phi = \langle \vec{a} \vec{a}^T \rangle$ given by

$$[\phi]_{(ak)(bj)} = \varphi_{ak} \delta_{kj} \delta_{ab} + \Gamma_{ab} \Phi_j \delta_{kj}, \quad (\text{A.3})$$

where a and b are the indices of the different pulsar, while k and j are the indices of the Fourier modes. The first term describes here the pulsar intrinsic red noise that is modelled for the individual pulsars by a simple power-law

$$\varphi_a(f) = \frac{A_a^2}{12\pi^2 T_{\text{obs}}} \left(\frac{f}{\text{yr}^{-1}} \right)^{-\gamma_a} \text{yr}^3 \quad (\text{A.4})$$

with amplitude A_a and spectral index γ_a . From this, the coefficients $\varphi_{ak} = \varphi_a(k/T_{\text{obs}})$ are extracted. The second term in the covariance matrix models the GW background. Is given by the Hellings and Downs correlation Γ_{ab} (cf. eq. 2.110) and the amplitude of the GW background parameterised as

$$h^2 \Omega_{\text{gw}}(f, \vec{\theta}) = \frac{8\pi^4 f^5 T_{\text{obs}}}{H_0^2/h^2} \Phi(f, \vec{\theta}). \quad (\text{A.5})$$

which is evaluated at the Fourier bins $\Phi_k = \Phi(k/T_{\text{obs}}, \vec{\theta})$. Here, $\vec{\theta}$ denotes the parameters that describe the GW background.

The last term in the timing residuals models deviations in the estimates of the timing model parameters $\vec{\beta}$ that was constructed by direct pulsar observations. By assuming that the difference between the initial estimate of the parameters $\vec{\beta}_0$, that model the arrival times of the individual pulsars, are small, the predicted TOAs can be written as

$$\vec{t}_{\text{pred}}(\vec{\beta}) = \vec{t}_{\text{pred}}(\vec{\beta}_0) + \left(\sum_i \frac{\partial \vec{t}_{\text{pred}}}{\partial \beta_i} \Big|_{\vec{\beta}_0} (\beta_j - \beta_{j,0}) \right). \quad (\text{A.6})$$

With this, the predicted TOAs become $\vec{t}_{\text{pred}}(\vec{\beta}) = \vec{t}_{\text{pred}}(\vec{\beta}_0) + \mathbf{M}\vec{\epsilon}$, where $\mathbf{M}$ is the matrix of the partial derivatives of the TOAs for each timing model parameter and $\vec{\epsilon} = \vec{\beta} - \vec{\beta}_0$ is the small deviation from the initial estimates.

We continue by grouping together the long-timescale processes and linear deviations in the pulsar modelling into $\vec{b} = (\vec{\epsilon} \vec{a})^T$ and $\mathbf{T} = [\mathbf{M} \ \mathbf{F}]$. This allows to write the PTA likelihood as

$$p(\vec{\delta t} | \vec{b}, \vec{\theta}) = \frac{\exp \left(-\frac{1}{2} (\vec{\delta t} - \mathbf{T}\vec{b})^T \mathbf{N}^{-1} (\vec{\delta t} - \mathbf{T}\vec{b}) \right)}{\sqrt{\det(2\pi \mathbf{N})}} \times \frac{\exp \left(-\frac{1}{2} \vec{b}^T \mathbf{B}^{-1} \vec{b} \right)}{\sqrt{\det(2\pi \mathbf{B})}} \quad (\text{A.7})$$

where the first term is the likelihood for the white noise, while the second term accounts for the long-timescale processes. Here, matrix $\mathbf{B} = \text{diag}(\infty, \Phi)$ contains the diagonal matrix of infinities ∞ , which corresponds to flat priors of $\vec{\epsilon}$ (and become zero upon inverting $\mathbf{B}$).

In the end, we are only interested in the likelihood of the GW parameters, $\vec{\theta}$, so we can analytically marginalise over the parameters $\vec{b}$ and obtain the PTA likelihood

$$p_{\text{PTA}}(\vec{\delta t} | \vec{\theta}) = \int d\vec{b} p(\vec{\delta t} | \vec{b}, \vec{\theta}) = \frac{1}{\det(2\pi \mathbf{C})} \exp \left(-\frac{1}{2} \vec{\delta t}^T \mathbf{C}^{-1} \vec{\delta t} \right), \quad (\text{A.8})$$

with $\mathbf{C} = \mathbf{N} + \mathbf{T} \mathbf{B} \mathbf{T}^T$.

Fitting a model to the timing data always involves inverting the matrix $\mathbf{C}$, which can be numerically too slow for inference. A way to speed this up is given by neglecting the correlation between the amplitudes at the different frequencies, i.e. performing a fit to the *free spectrum* [230]. The free spectrum describes the posterior distribution $p(\Phi_i | \vec{\delta t})$ of the GW amplitude Φ_i at each frequency bin. These posterior distributions are usually represented

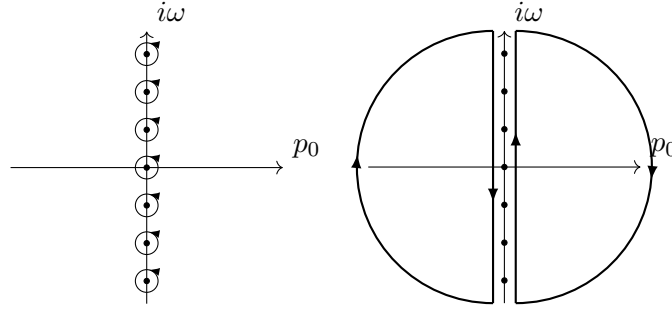


Figure A.1.: The contour lines relating the residua of the hyperbolic function cosh (dots) to an integration along the imaginary axis.

as a violin plot, as seen in the left panel of fig. 2.8. This factorises the likelihood into the product over the Fourier bins

$$p_{\text{PTA}}(\vec{\theta}) = \prod_{k=1}^{N_{f,\text{GW}}} \frac{p(\Phi_k|\vec{\delta t})}{p(\Phi_k)} \bigg|_{\phi_k=\Phi(k/T_{\text{obs}},\vec{\theta})}. \quad (\text{A.9})$$

where $p(\Phi_k)$ is the prior probability for the GW amplitude of the model. The evaluation of this likelihood is typically orders of magnitude faster than evaluating eq. (A.8), which is why we use this likelihood in the analysis in chapters 5 and 6. We do this by utilising the code `ceffyl` [230] via the interface wrapper provided by `PTArcade` [103].

A.2. Matsubara sums

Here, we briefly review the methods to evaluate the Matsubara sums that show up e.g. in the hard thermal masses at finite temperature.

The change from zero- to finite-temperature can be summarised in the replacement rule for integrals over expressions containing fields

$$\int \frac{d^4 p}{(2\pi)^4} f(p) \rightarrow T \sum_{n=-\infty}^{\infty} \int \frac{d^3 p}{(2\pi)^3} f(\omega_n, \mathbf{p}). \quad (\text{A.10})$$

The evaluation of the infinite sum over the Matsubara frequencies can be performed by using the pole structure of the hyperbolic sine and cosine functions, see e.g. [105, p. 41]. These two functions

$$\frac{1}{2} \coth\left(\frac{z}{2T}\right) = \frac{1}{2} + \frac{1}{e^{z/T} - 1}, \quad (\text{A.11})$$

$$\frac{1}{2} \sinh\left(\frac{z}{2T}\right) = \frac{1}{2} - \frac{1}{e^{z/T} + 1}. \quad (\text{A.12})$$

have poles at $z = i\omega_n$ for bosonic frequencies $\omega_n = 2\pi nT$, and for the fermionic frequencies $\omega_n = (2n + 1)\pi T$, respectively. This can be used to rewrite the infinite sum as an adequate contour integral over these hyperbolic functions.

The sum over the Matsubara frequencies is equivalent to an integration over the contour lines around every pole along the imaginary axis, as shown on the left of fig. A.1.

We can deform this contour into two closed half-circles along the imaginary axis, as shown on the right. With this, the Matsubara sum reduces to integrations over the p_0 component along the imaginary axis

$$2\pi iT \sum_{n=-\infty}^{\infty} f(p_0 = i\omega_n) = \int_{-i\infty+\epsilon}^{i\infty+\epsilon} dp_0 (f(p_0) + f(-p_0)) \left(\frac{1}{2} \pm \frac{1}{e^{z/T} \mp 1} \right), \quad (\text{A.13})$$

where the negative sign of the argument of the second term comes from the orientation of the contour integral. This equality holds as long as $f(p_0)$ has no poles along the imaginary axis.

A.3. Thermal masses

In the calculation of the hard thermal masses, the following common sum-integrals appear. Using the method discussed in the previous section, they can be evaluated in the high-temperature limit $T \gg m$ as

$$T \oint \frac{d^3k}{(2\pi)^3} \frac{1}{\omega_n^2 + k^2} = \begin{cases} \frac{T^2}{12} & \text{bosons} \\ -\frac{T^2}{24} & \text{fermions} \end{cases} \quad (\text{A.14})$$

$$T \oint \frac{d^3k}{(2\pi)^3} \frac{\omega_n}{\omega_n^2 + k^2} = \begin{cases} -\frac{T^2}{24} & \text{bosons} \\ \frac{T^2}{48} & \text{fermions} \end{cases} \quad (\text{A.15})$$

$$T \oint \frac{d^3k}{(2\pi)^3} \frac{k^2}{\omega_n^2 + k^2} = \begin{cases} \frac{T^2}{8} & \text{bosons} \\ -\frac{T^2}{16} & \text{fermions} \end{cases} \quad (\text{A.16})$$

Here, the zero-temperature, UV-divergent part of each integral has been neglected, since it will be cancelled by the counterterms introduced to renormalise the CW potential.

Let us use these results to compute the typical contributions to the thermal masses of scalars and gauge bosons.

Scalars:

The contribution from a self-interaction term $\lambda\phi^4$ to the thermal mass is

$$\text{---}\bullet\text{---} \bigcirc \text{---} = \frac{1}{2} T \oint \frac{d^3k}{(2\pi)^3} \left(\frac{\lambda}{\omega_n^2 + k^2} \right) \supset \lambda \frac{T^2}{24}. \quad (\text{A.17})$$

The coupling to Dirac fermions $y\chi\bar{\chi}\phi/\sqrt{2}$ gives rise to the contribution

$$\text{---}\bullet\text{---} \bigcirc \text{---} = -\frac{y^2}{2} T \oint \frac{d^3k}{(2\pi)^3} \left(\frac{\text{tr} [k\!\!\!/]}{(\omega_n^2 + k^2)^2} \right) \supset 4y^2 \frac{T^2}{48}. \quad (\text{A.18})$$

Finally, the interaction with gauge bosons amounts to the contribution

$$\text{---}\bullet\text{---} \text{---} \text{---} = \frac{2ig^2}{2} T \oint \frac{d^3k}{(2\pi)^3} \text{tr} [\Pi_{\mu\nu}] = 3g^2 T \oint \frac{d^3k}{(2\pi)^3} \frac{1}{(\omega_n^2 + k^2)} \supset 3g^2 \frac{T^2}{12} \quad (\text{A.19})$$

Here, we used that the photon propagator in the Landau gauge contracted reduces to $\Pi_\mu^\mu = -3i/(\omega_n^2 + k^2)$.

Gauge bosons

Gauge bosons can receive a thermal mass from the interactions with scalars and fermions. Starting with a $g^2\phi^2 A_\mu^2$ term, the contribution is

$$\begin{aligned} \text{---}\bullet\text{---} \bigcirc \text{---} &= g^2 T \oint \frac{d^4k}{(2\pi)^4} \left(\frac{-g_{\mu\nu}}{\omega_n^2 + k^2} \right) \\ &\supset \begin{cases} \frac{g^2}{6} T^2 & (\text{longitudinal}), \\ 0 & (\text{transversal}). \end{cases} \end{aligned} \quad (\text{A.20})$$

In the case of a term $g^2\phi(\partial_\mu\phi)A^\mu$, the contribution becomes

$$\begin{aligned}
 \text{---}\text{wavy}\text{---}\bullet\text{---}\text{dashed circle}\text{---}\bullet\text{---}\text{wavy}\text{---} &= -g^2T \oint \frac{d^3k}{(2\pi)^3} \left(\frac{2k_\mu}{\omega_n^2 + k^2} \frac{2k_\nu}{\omega_n^2 + k^2} \right) \\
 &\supset \begin{cases} 2(\frac{g^2}{6} + \frac{g^2}{6})T^2 & (\text{longitudinal}), \\ 0 & (\text{transversal}). \end{cases}
 \end{aligned} \tag{A.21}$$

Finally, the contribution from fermions is given by

$$\begin{aligned}
 \text{---}\text{wavy}\text{---}\bullet\text{---}\text{solid circle}\text{---}\bullet\text{---}\text{wavy}\text{---} &= -g^2T \oint \frac{d^3k}{(2\pi)^3} \left(\frac{\text{tr}[\gamma_\mu \not{k} \gamma_\nu \not{k}]}{(\omega_n^2 + k^2)^2} \right) \\
 &\supset \begin{cases} 4g^2 \frac{T^2}{12} & (\text{longitudinal}), \\ 0 & (\text{transversal}). \end{cases}
 \end{aligned} \tag{A.22}$$

B.1. Abelian dark Higgs example model

Here, we review the phase transition properties of the Abelian dark Higgs model that we use to demonstrate the calculations in TL (chapter 4) and study in the context the PTA data (chapter 5). It is composed of a complex scalar field Φ charged under a new $U(1)'$ symmetry and a new gauge boson A'_μ . The model can be summarised with the Lagrangian

$$\mathcal{L} = |D_\mu \Phi|^2 - \frac{1}{4} A'_{\mu\nu} A'^{\mu\nu} - V_0(\Phi). \quad (\text{B.1})$$

Here, the covariant derivative is $D_\mu = \partial_\mu + igA'_\mu$ and the field strength tensor of the gauge boson is given by $A'_{\mu\nu} = \partial_\mu A'_\nu - \partial_\nu A'_\mu$. After symmetry breaking $\Phi = (\phi_b + \phi + i\varphi)/\sqrt{2}$ the tree-level potential of the background field becomes

$$V_0(\phi) = -\frac{\mu^2}{2}\phi^2 + \frac{\lambda}{4}\phi^4, \quad (\text{B.2})$$

with the VEV given by the minimum at $v = \sqrt{\mu^2/\lambda}$. The spectrum in the broken phase consists of a scalar ϕ , a Goldstone boson φ , and a gauge boson with transverse A'_T and longitudinal A'_L polarisations. The field-dependent masses of these states are

$$\begin{aligned} m_\phi^2 &= -\mu^2 + 3\lambda\phi^2 + \Pi_\phi, & m_{A'_T}^2 &= g^2\phi^2, \\ m_\varphi^2 &= -\mu^2 + \lambda\phi^2 + \Pi_\phi, & m_{A'_L}^2 &= m_{A'}^2 + \Pi_{A'_L}, \end{aligned} \quad (\text{B.3})$$

with the thermal masses

$$\Pi_\phi = \left(\frac{\lambda}{3} + \frac{g^2}{4}\right) T^2, \quad \Pi_{A'_L} = \frac{g^2}{3} T^2. \quad (\text{B.4})$$

The UV divergences of the 1-loop corrections require to introduce counterterms give a contribution to the effective potential with the same form as the tree-level potential in eq. (B.2),

$$V_{\text{ct}} = -\frac{\delta\mu^2}{2}\phi^2 + \frac{\delta\lambda}{4}\phi^4. \quad (\text{B.5})$$

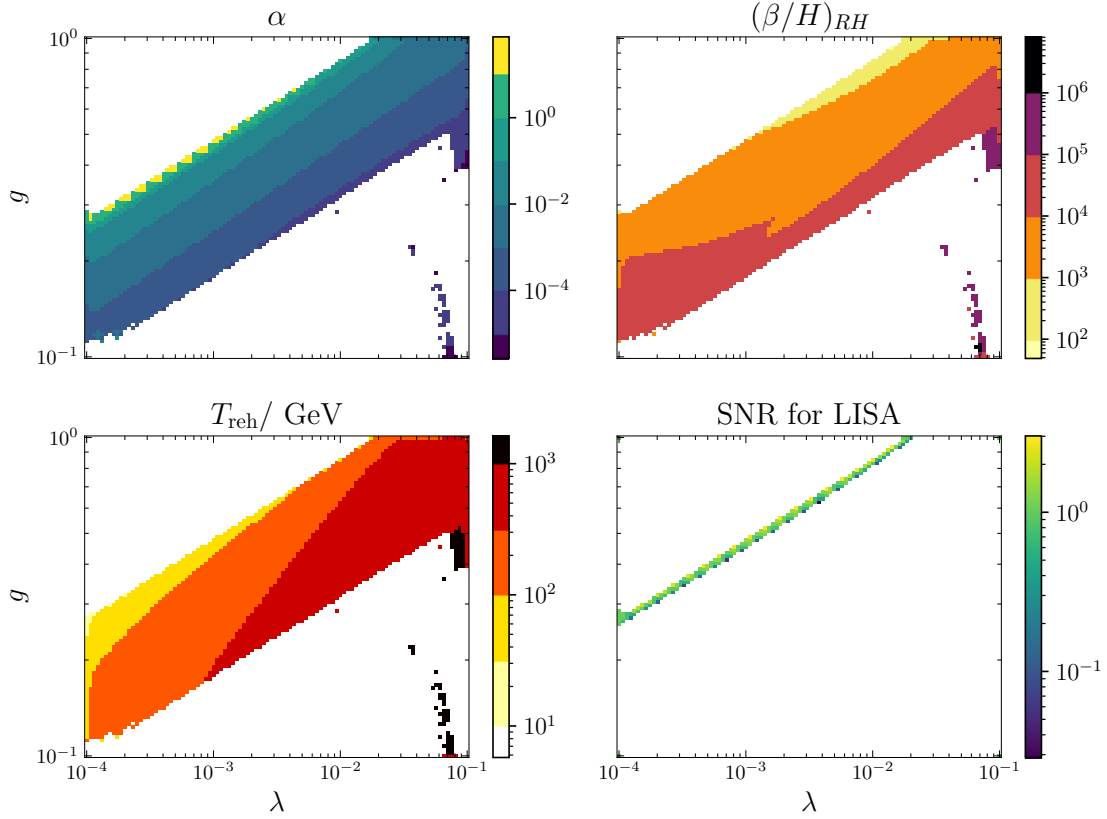


Figure B.1.: Overview of the phase transition parameters of the example $U(1)'$ model in the $\lambda - g$ plane, while the VEV is fixed to $v = 1$ TeV.

The values of the counterterms are fixed by the renormalisation conditions, which we implemented to fix the mass of the scalar and the vev to the tree-level values

$$\delta\mu^2 = \left(\frac{3}{2\phi} \frac{dV_{\text{cw}}}{d\phi} - \frac{1}{2} \frac{d^2V_{\text{cw}}}{d\phi^2} \right) \Big|_{\phi=v} \quad \text{and} \quad \delta\lambda = \left(\frac{1}{2\phi^3} \frac{dV_{\text{cw}}}{d\phi} - \frac{1}{2\phi^2} \frac{d^2V_{\text{cw}}}{d\phi^2} \right) \Big|_{\phi=v}. \quad (\text{B.6})$$

This simple model only has three parameters, the self-interaction λ , the gauge coupling g and the VEV v . In terms of the phase transition, the first two determine the strength and transition speed, while the VEV only shifts the energy scale of the transition, i.e. the transition temperature.

To obtain an overview, we therefore show the phase transition parameters $\alpha, \beta/H$ and T_{reh} , as well as the SNR for LISA in the $\lambda - g$ plane in fig. B.1. The colour shaded band show the regions with a FOPT. Below the band, the transition is a cross-over, while above the band, the transition does not complete and stays trapped in the false-vacuum. As we can see in the upper left panel, for a fixed self-interaction, increasing the gauge coupling leads the model from a weak phase transition $\alpha \sim 10^{-4}$ to an increasingly strong transition $\alpha \sim 10^2$ and more supercooling. We find this behaviour is due to the increase of the thermal potential barrier with an increasing value of g . This trend is followed by the reheating temperature shown in the lower left panel. With increasing supercooling along an increasing gauge coupling, the temperature after the phase transition decreases, as the transition is delayed and the expansion of the universe decreases the temperature before the phase transition occurs. The transition speed is shown in the upper right panel and anti-correlates with the transition strength. For small gauge couplings, the transition is fast and slows down with increasing

gauge coupling. Finally in the lower right panel we show the resulting SNR for the planned LISA experiment. Only a small band in the $\lambda - g$ plane with the most supercooled transitions would be observable.

B.2. CP-conserving Two-Higgs Doublet model

The CP-conserving Two-Higgs Doublet model (2HDM) [28, 186] encompasses two Higgs doublets $\Phi_a = (\phi_a^+, \phi_a^0)^T$ with $a = 1, 2$ that are charged under $SU(2)_L \times U(1)_Y$. If we assume a softly broken $\mathbb{Z}_2$ symmetry $(\Phi_1, \Phi_2) \rightarrow (-\Phi_1, \Phi_2)$, the tree-level potential of the model is given by

$$V_0(\Phi_1, \Phi_2) = m_{11}^2 |\Phi_1|^2 + m_{22}^2 |\Phi_2|^2 - (m_{12}^2 \Phi_1^\dagger \Phi_2 + \text{h.c.}) + \frac{\lambda_1}{2} |\Phi_1|^4 + \frac{\lambda_2}{2} |\Phi_2|^4 + \lambda_3 |\Phi_1|^2 |\Phi_2|^2 + \lambda_4 (\Phi_1^\dagger \Phi_2)(\Phi_2^\dagger \Phi_1) + \frac{\lambda_5}{2} ((\Phi_1^\dagger \Phi_2)^2 + \text{h.c.}). \quad (\text{B.7})$$

Here, the CP-even components of the two Higgs doublets ϕ_a^0 can be decomposed as

$$\Phi_a = \begin{pmatrix} \phi_a^+ \\ \phi_a^0 \end{pmatrix} = \begin{pmatrix} \phi_a^+ \\ \frac{1}{\sqrt{2}} (\phi_a + \varphi_a + i\psi_a) \end{pmatrix}. \quad (\text{B.8})$$

The fields ϕ_a denote here the static background fields. Their combined expectation value gives the electroweak vacuum $\langle \phi_1 \rangle^2 + \langle \phi_2 \rangle^2 = v_1^2 + v_2^2 = v_{\text{EW}}^2$ at zero temperature. For simplicity, we restrict our implementation to CP-even neutral background fields and set possible intermediate charge- and CP-breaking minima to zero $\langle \phi_a^+ \rangle = \langle \psi_a \rangle = 0$. Under these restrictions the two-dimensional tree-level potential of the background fields becomes

$$V_0(\phi_1, \phi_2) = \frac{1}{2} m_{11}^2 \phi_1^2 + \frac{1}{2} m_{22}^2 \phi_2^2 - m_{12}^2 \phi_1 \phi_2 + \frac{\lambda_1}{8} \phi_1^4 + \frac{\lambda_2}{8} \phi_2^4 + \frac{\lambda_{345}}{4} \phi_1^2 \phi_2^2, \quad (\text{B.9})$$

with $\lambda_{345} = \lambda_3 + \lambda_4 + \lambda_5$. The mass matrices of the CP-even (φ_a), CP-odd (ψ_a) and charged scalar (ϕ_a^+) read

$$\mathcal{M}_{\text{even}}^2 = \begin{pmatrix} m_{11}^2 + \frac{3}{2} \lambda_1 \phi_1^2 + \frac{1}{2} \lambda_{345} \phi_2^2 + \Pi_1 & -m_{12}^2 + \lambda_{345} \phi_1 \phi_2 \\ -m_{12}^2 + \lambda_{345} \phi_1 \phi_2 & m_{22}^2 + \frac{3}{2} \lambda_2 \phi_2^2 + \frac{1}{2} \lambda_{345} \phi_1^2 + \Pi_2 \end{pmatrix}, \quad (\text{B.10})$$

$$\mathcal{M}_{\text{odd}}^2 = \begin{pmatrix} m_{11}^2 + \frac{1}{2} \lambda_1 \phi_1^2 + \frac{1}{2} \lambda_{34-5} \phi_2^2 + \Pi_1 & -m_{12}^2 + \lambda_5 \phi_1 \phi_2 \\ -m_{12}^2 + \lambda_5 \phi_1 \phi_2 & m_{22}^2 + \frac{1}{2} \lambda_2 \phi_2^2 + \frac{1}{2} \lambda_{34-5} \phi_1^2 + \Pi_2 \end{pmatrix}, \quad (\text{B.11})$$

$$\mathcal{M}_{\text{ch}}^2 = \begin{pmatrix} m_{11}^2 + \frac{1}{2} \lambda_1 \phi_1^2 + \frac{1}{2} \lambda_3 \phi_2^2 + \Pi_1 & -m_{12}^2 + \frac{1}{2} \lambda_{45} \phi_1 \phi_2 \\ -m_{12}^2 + \frac{1}{2} \lambda_{45} \phi_1 \phi_2 & m_{22}^2 + \frac{1}{2} \lambda_2 \phi_2^2 + \frac{1}{2} \lambda_3 \phi_1^2 + \Pi_2 \end{pmatrix}, \quad (\text{B.12})$$

with $\lambda_{34-5} = \lambda_3 + \lambda_4 - \lambda_5$, $\lambda_{45} = \lambda_4 + \lambda_5$. The diagonal entries of the mass matrices receive a contribution from the hard thermal masses

$$\Pi_1 = (12\lambda_1 + 8\lambda_3 + 4\lambda_4 + 3(3g_2^2 + g_1^2)) \frac{T^2}{48} + \Pi_{\text{ferm},1}, \quad (\text{B.13})$$

$$\Pi_2 = (12\lambda_2 + 8\lambda_3 + 4\lambda_4 + 3(3g_2^2 + g_1^2) + 12y_t^2) \frac{T^2}{48} + \Pi_{\text{ferm},2}. \quad (\text{B.14})$$

Depending on whether the down-type quarks couple to the first or second Higgs doublet, either Π_1 or Π_2 receive a contribution from the bottom quark

$$\Pi_{\text{ferm},i} = \begin{cases} 12y_b^2 \frac{T^2}{48} & \text{if Yukawa type} = i, \\ 0 & \text{else.} \end{cases} \quad (\text{B.15})$$

In order to obtain the mass eigenstates after symmetry breaking, the mass matrices can be diagonalised. This gives the light and heavy Higgs bosons h and H , the pseudo scalar A , the neutral and charged Goldstones G^0 , $G^\pm$ and the charged scalars $H^\pm$. These are related to the gauge eigenstates via

$$\begin{pmatrix} G^\pm \\ H^\pm \end{pmatrix} = R(\beta) \begin{pmatrix} \phi_1^\pm \\ \phi_2^\pm \end{pmatrix}, \quad \begin{pmatrix} G^0 \\ A \end{pmatrix} = R(\beta) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \begin{pmatrix} H \\ h \end{pmatrix} = R(\alpha) \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \quad (\text{B.16})$$

The rotation matrices R are of the form

$$R(\beta) = \begin{pmatrix} \cos \beta & \sin \beta \\ -\sin \beta & \cos \beta \end{pmatrix}, \quad (\text{B.17})$$

where the angle β is fixed by the VEV ratio $\tan \beta = v_2/v_1$. Therefore, the model parameters are the quartic couplings λ_i for $i = 1, \dots, 5$, the soft-breaking mass m_{12}^2 , $\tan \beta$ and the Yukawa type. Furthermore, CP-conservation requires all these parameters to be real. The mass spectrum of the gauge bosons is

$$m_{W_T}^2 = \frac{g_2^2}{4}(\phi_1^2 + \phi_2^2), \quad m_{W_L}^2 = \frac{g_2^2}{4}(\phi_1^2 + \phi_2^2) + \Pi_{W_L}. \quad (\text{B.18})$$

$$m_{B_T}^2 = \frac{g_1^2 + g_2^2}{4}(\phi_1^2 + \phi_2^2), \quad m_{B_L}^2 = \frac{g_1^2 + g_2^2}{4}(\phi_1^2 + \phi_2^2) + \Pi_{B_L}, \quad (\text{B.19})$$

where the longitudinal components receive the thermal masses $\Pi_{W_L} = 2g_2^2 T^2$ and $\Pi_{B_L} = 2g_1^2 T^2$. From the fermions, we only include the most important contributions to the potential from the top, bottom and tau. Their field-dependent masses are

$$m_t^2 = y_t^2 \phi_i^2, \quad m_b^2 = y_b^2 \phi_i^2, \quad m_\tau^2 = y_\tau^2 \phi_i^2, \quad (\text{B.20})$$

where the Higgs doublet they couple to depends on the Yukawa type.

For the determination of the counterterms we follow the same on-shell scheme prescription as BSMPT [167]. The counterterm potential is

$$\begin{aligned} V_{\text{ct}} = & \delta m_{11}^2 \Phi_1^\dagger \Phi_1 + \delta m_{22}^2 \Phi_2^\dagger \Phi_2 - \delta m_{12}^2 (\Phi_1^\dagger \Phi_2 + \Phi_2^\dagger \Phi_1) \\ & + \frac{\delta \lambda_1}{2} (\Phi_1^\dagger \Phi_1)^2 + \frac{\delta \lambda_2}{2} (\Phi_2^\dagger \Phi_2)^2 + \delta \lambda_3 (\Phi_1^\dagger \Phi_1) (\Phi_2^\dagger \Phi_2) \\ & + \frac{\delta \lambda_5}{2} \left[(\Phi_1^\dagger \Phi_2)^2 + (\Phi_2^\dagger \Phi_1)^2 \right]. \end{aligned} \quad (\text{B.21})$$

The vector of counterterms reads

$$\delta = (\delta m_{11}^2, \delta m_{22}^2, \delta m_{12}^2, \delta \lambda_1, \delta \lambda_2, \delta \lambda_3, \delta \lambda_5)^T, \quad (\text{B.22})$$

with $\delta \lambda_4 = 0$ fixed by the chosen renormalisation prescription.

The renormalisation conditions are chosen to fix the masses and mixing angles to the tree-level values:

$$\begin{aligned} \partial_i (V_{\text{CW}} + V_{\text{ct}})|_v &= 0, \quad i \in \{4, 6\}, \\ \partial_i \partial_j (V_{\text{CW}} + V_{\text{ct}})|_v &= 0, \quad (i, j) \in \{(4, 4), (6, 6), (4, 6), (5, 5), (0, 0)\}. \end{aligned} \quad (\text{B.23})$$

where, $i, j = 0, \dots, 7$ denote the indices of the fields in the vector

$$(\text{Re } \phi_1^+, \text{Im } \phi_1^+, \text{Re } \phi_2^+, \text{Im } \phi_2^+, \phi_1, \psi_1, \phi_2, \psi_2)^T. \quad (\text{B.24})$$

B.3. Analytical relation between transition speed and bubble size

Here, we provide details on the analytic relation between R_{sep} and β at percolation, as first presented in ref. [178]. To start, we approximate the nucleation rate as an exponential function around the percolation time t_{perc} and neglecting the cosmic expansion. With these simplifications we obtain (cf. eq. (4.36))

$$\Gamma(t) \approx \Gamma_{\text{perc}} e^{-\beta(t-t_{\text{perc}})} \quad \text{and} \quad P_{\text{f}}(t) \approx \exp\left(-\frac{8\pi v_{\text{w}}^3}{\beta^4} \Gamma_{\text{perc}} e^{-\beta(t-t_{\text{perc}})}\right). \quad (\text{B.25})$$

If we neglect the cosmic expansion in the bubble number density as well, we obtain

$$\begin{aligned} n(t) &\approx \int_{-\infty}^t dt' \Gamma(t') P_{\text{f}}(t') = -\frac{\beta^3}{8\pi v_{\text{w}}^3} \int_{-\infty}^{t_{\text{perc}}} dt \frac{d}{dt} \left(\exp\left(-\frac{8\pi v_{\text{w}}^3}{\beta^4} \Gamma_{\text{perc}} e^{-\beta(t-t_{\text{perc}})}\right) \right) \\ &= \frac{\beta^3}{8\pi v_{\text{w}}^3} \left(1 - \exp\left(-\frac{8\pi v_{\text{w}}^3}{\beta^4} \Gamma_{\text{perc}}\right) \right) = \frac{\beta^3}{8\pi v_{\text{w}}^3} (1 - P_{\text{f}}(t_{\text{perc}})). \end{aligned} \quad (\text{B.26})$$

Hence, the mean bubble separation at percolation can be related to the transition speed through

$$R_{\text{sep}}(t_{\text{perc}}) = \frac{1}{n(t_{\text{perc}})^{1/3}} \approx \left(\frac{8\pi}{f_{\text{perc}}} \right)^{1/3} \frac{v_{\text{w}}}{\beta}. \quad (\text{B.27})$$

The factor $f_{\text{perc}} = 1 - P_{\text{f}}(t_{\text{perc}}) \approx 0.29$ accounts for the non-vanishing true-vacuum fraction.

C.1. Details on the parameter distributions

Here we give more details on the distribution of the model parameters that result from the fit of the PTA data. Starting with the Abelian dark Higgs model, we show the parameter space and mass spectrum of the **UltraNest** (blue) and random scan (grey) in fig. C.1. The fit to the PTA data most strongly constrains the parameter $\tilde{g} = g\lambda^{-1/4}$, which determines the height of the potential barrier relative to the potential depth and thus the strength and speed of the transition. The requirement for a sufficiently strong transition translates here into the peak around $\tilde{g} \simeq 2.5 - 3$. Smaller values of $\tilde{g}$ give transitions that are too weak and fast to reach the necessary amplitude in the GW signal. Conversely λ is less constrained and ranges from 10^{-3} to 1, as many combinations of g and λ can give the required value of $\tilde{g}$. The VEV of the model is the least constrained parameter, spanning values between $2 \cdot 10^1 \text{ MeV} \lesssim v \lesssim 10^3 \text{ MeV}$. The primary effect of v is to set the temperature scale of the transition and thus the reheating temperature that determines the peak frequency of the signal. For the observed signal around the nanohertz frequencies, this only requires a mild tuning. The lower bound comes here from the requirement that the peak of the signal does not fall below $f_{\text{peak}} \sim 10^{-8}$ where the higher frequency bins would not be fitted well anymore, cf. fig. 5.1. The required couplings and VEV lead to mass ranges of the dark Higgs and dark photon of $m_\phi \simeq 2 - 10^3 \text{ MeV}$ and $m_{A'} \simeq 10 - 10^3 \text{ MeV}$ respectively.

Next, we show the results for the flip-flop model with the two-step phase transition in fig. C.2. Note that we fixed the parameters $y = \gamma = 1$ to reduce the numerical challenge of fitting the PTA data. Similar to the Abelian model, the VEV v is least constrained. Compared to that, the couplings λ_1 and λ_{12} , set the relative height of the zero-temperature potential barrier, are strongly tuned as can be seen in their narrow posterior distribution. The coupling λ_0 , that determines the overall shape of the two-dimensional potential instead is less constrained. We attribute the peaks in its posterior distribution to the incomplete sampling that we discussed in the main text.

Finally, in fig. C.3, we show the results for the conformal model. Here we find that the preferred value of the VEV lies in the range $80 \text{ MeV} \lesssim v \lesssim 400 \text{ MeV}$. In contrast to that, the gauge coupling is more tightly constrained to $0.6 \lesssim g \lesssim 0.7$, in agreement with the results in chapter 6. This leads to a typical mass of the dark Higgs around tens of MeV and masses of the dark photon around 100 MeV.

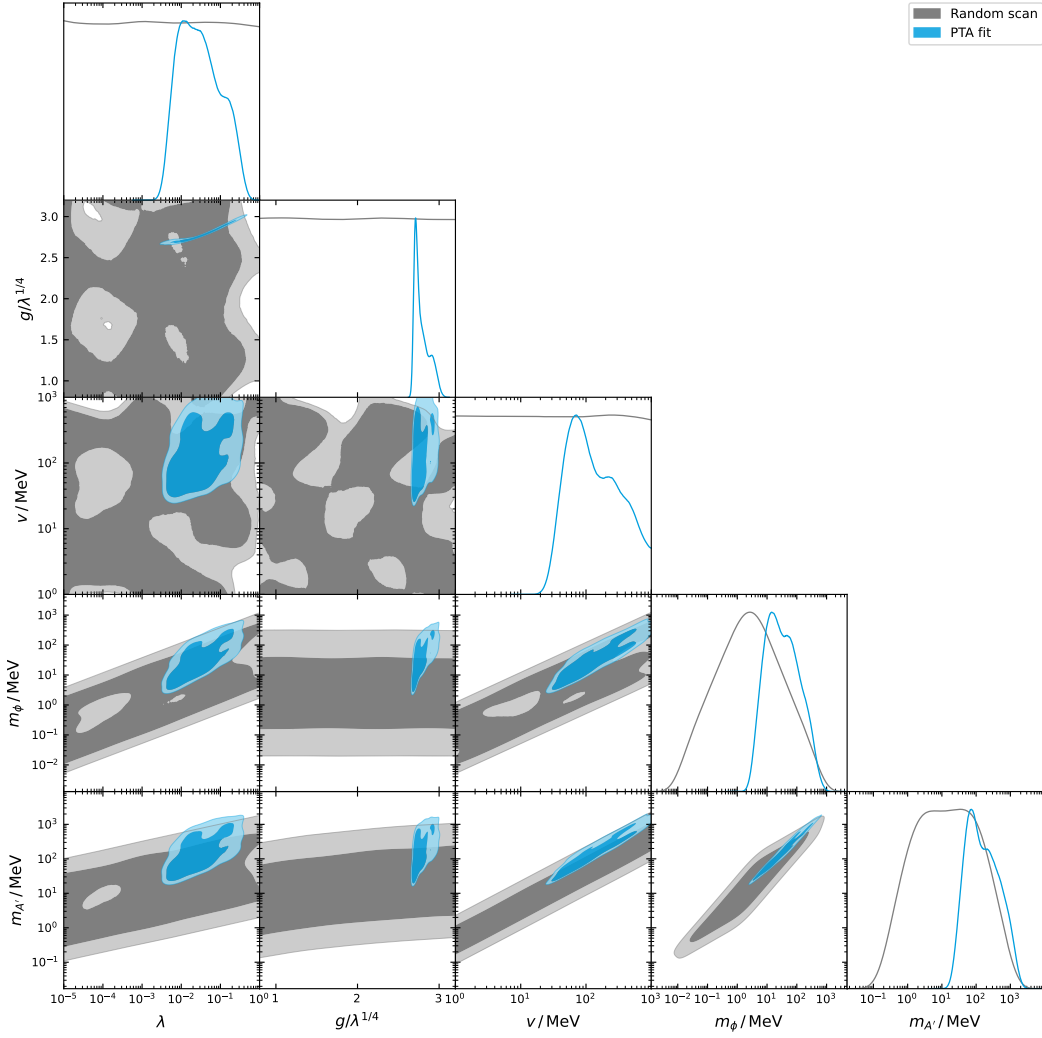


Figure C.1.: Preferred regions of the Abelian dark Higgs model (blue) after sampling over the PTA likelihood shown as a triangle plot. The random samples are shown in grey.

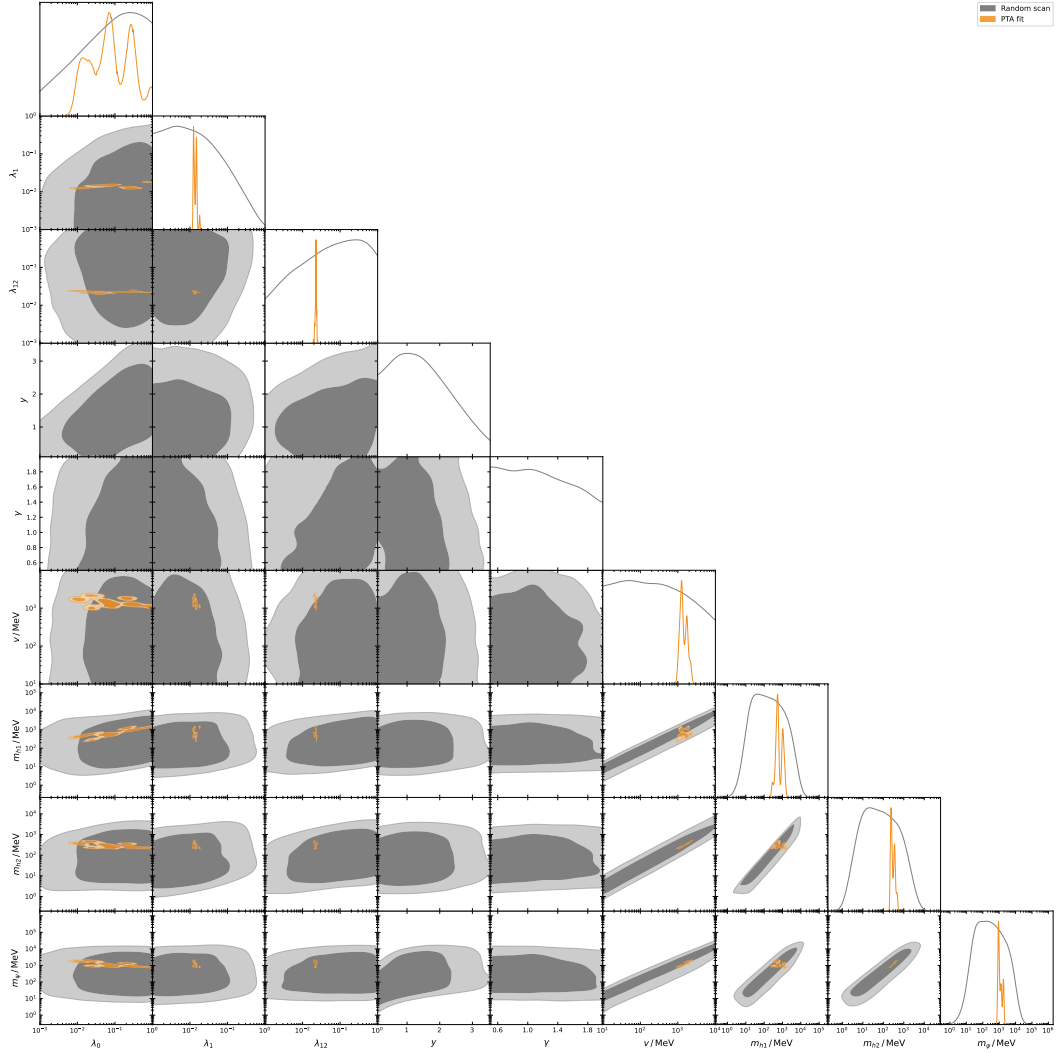


Figure C.2.: Preferred regions of the flip-flop model (yellow) after sampling over the PTA likelihood shown as a triangle plot. The random samples are shown in grey. Note that the couplings y and γ have been fixed to unity for the PTA fit (indicated by missing posterior distributions in the respective panels). The posteriors in the λ_0 direction are rather poorly sampled due to numerical challenges in achieving a sufficiently slow phase transition.

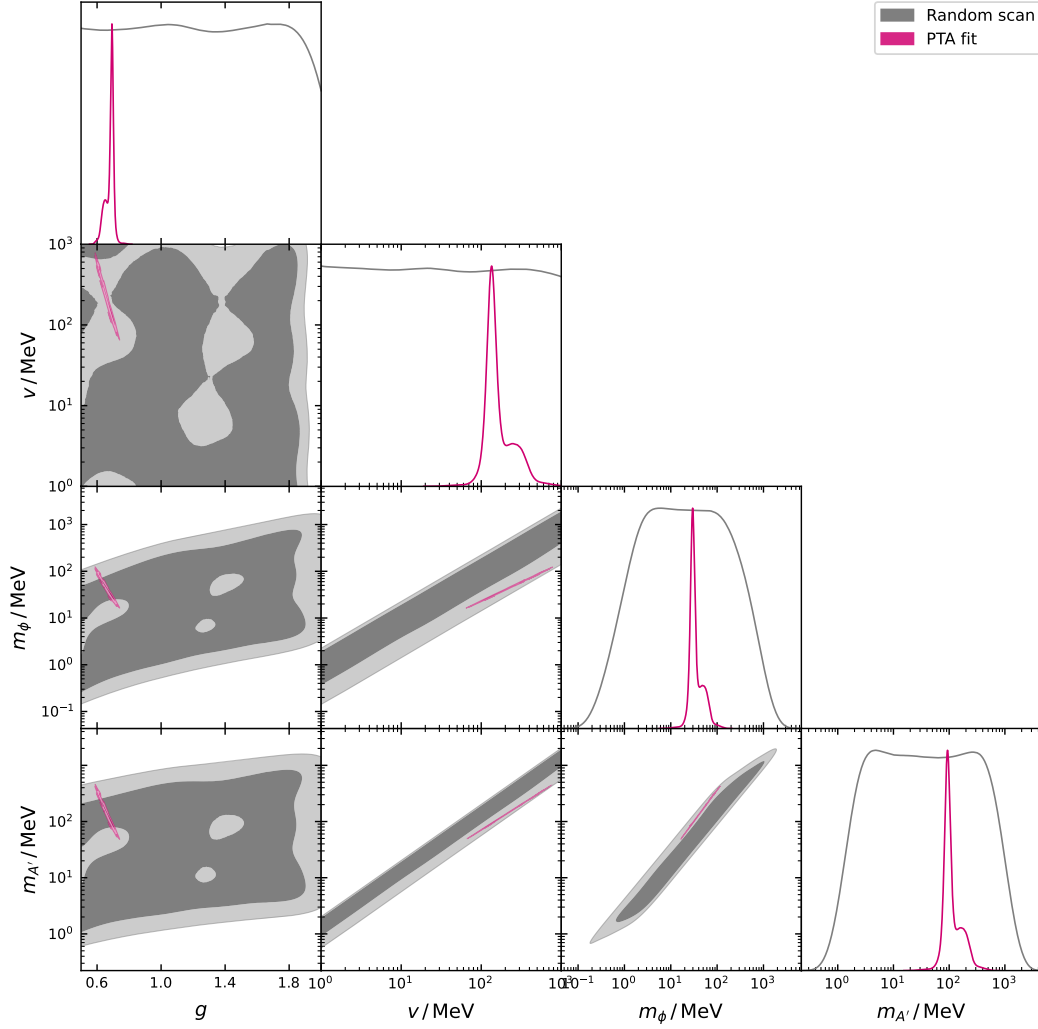


Figure C.3.: Preferred regions of the conformal model (purple) after sampling over the PTA likelihood shown as a triangle plot. The random samples are shown in grey.

D.1. Details on the freeze-out computation a secluded dark sector

Here, we provide details on the computation of the DM relic density for a secluded dark sector. In this scenario, the inter-DS interactions $\bar{\chi}\chi \leftrightarrow \phi\phi$ are more efficient than the annihilation and production processes $\bar{\chi}\chi \leftrightarrow e^+e^-$ that maintain chemical equilibrium between the DS and the SM. That means, the latter process freezes out first at T_f^{SM} leading the DS to develop a non-negligible chemical potential at the freeze-out of the former process T_f^ϕ .

To compute the relic density in this scenario, we proceed in two steps. First we determine the decoupling temperature of the DS T_f^{SM} , where ϕ and χ are in chemical equilibrium. Then we determine how the subsequent interactions $\bar{\chi}\chi \leftrightarrow \phi\phi$ change the relic density until DM freeze-out.

For the first step, we employ the standard routines of **DarkSUSY** [276] to determine T_f^{SM} together with the would-be DM relic abundance $\tilde{\Omega}_\chi h^2$ that we would obtain by ignoring the $\bar{\chi}\chi \leftrightarrow \phi\phi$ processes. Up until the decoupling, the DS states are still in chemical equilibrium and can be described by Maxwell-Boltzmann distributions. Therefore, the ratio of their abundances at T_f^{SM} can be written as

$$\frac{Y_\chi}{Y_\phi} = \frac{Y_\chi^{\text{eq}}}{Y_\phi^{\text{eq}}} = 2(1 - \delta)^{-3/2} e^{-\delta x}, \quad (\text{D.1})$$

with $\delta = 1 - m_\phi/m_\chi$ and $x = m_\chi/T$. The factor 2 accounts for the 2 spin degrees of freedom of the DM compared to the one of the dark Higgs. For the second step, we assume that the freeze-out of dark matter occurs before the dark Higgs bosons decay. This implies that the total DS yield stays constant

$$Y_{\bar{\chi}} + Y_\chi + Y_\phi = 2Y_\chi + Y_\phi = \text{const.} \quad (\text{D.2})$$

Before the DM freezes out, the inter-DS conversion processes are efficient, such that detailed balance implies

$$Y_\chi^2 \langle \sigma v \rangle_{\bar{\chi}\chi \rightarrow \phi\phi} = Y_\phi^2 \langle \sigma v \rangle_{\phi\phi \rightarrow \bar{\chi}\chi}. \quad (\text{D.3})$$

We can evaluate these two conditions at both T_f^{SM} and T_f^ϕ to find $\Omega_\chi h^2$. By using $\Omega_\chi h^2 / \tilde{\Omega}_\chi h^2 = Y_\chi(T_f^\phi) / Y_\chi(T_f^{\text{SM}})$ and eq. (D.1), we can then estimate the relic density as

$$\Omega_\chi h^2 \simeq \tilde{\Omega}_\chi h^2 \times \frac{1 + \frac{1}{2} \frac{g_\phi}{g_\chi} (1 + \delta)^{3/2} e^{\delta x_f^{\text{SM}}}}{1 + \frac{1}{2} \sqrt{\bar{r}(x_f^\phi)}}, \quad (\text{D.4})$$

with

$$\bar{r} = \frac{\langle \sigma v \rangle_{\bar{\chi}\chi \rightarrow \phi\phi}}{\langle \sigma v \rangle_{\phi\phi \rightarrow \bar{\chi}\chi}}. \quad (\text{D.5})$$

The DM relic abundance is then given by $\Omega_{\text{DM}} h^2 = 2\Omega_\chi h^2$.

To evaluate eq. (D.4), we note that the ratio of the cross sections is simply

$$\frac{(\sigma v)_{\chi\chi \rightarrow \phi\phi}}{(\sigma v)_{\phi\phi \rightarrow \chi\chi}} = \frac{1}{2} \frac{1}{4} \frac{\sqrt{s - 4m_\phi^2}}{\sqrt{s - 4m_\chi^2}}. \quad (\text{D.6})$$

Here, the factor $1/2$ comes from ϕ being self-conjugate and the factor $1/4$ comes from the different spin degrees of freedom. By employing the expression for the thermally averaged cross sections for Maxwell-Boltzmann distributions [306], we can write $\bar{r}$ as

$$\bar{r} \equiv \frac{\langle \sigma v \rangle_{\chi\chi \rightarrow \phi\phi}}{\langle \sigma v \rangle_{\phi\phi \rightarrow \chi\chi}} = \frac{m_\chi K_2^2(m_\phi/T)}{m_\phi K_2^2(m_\chi/T)} \frac{\int d\tilde{s} (\sigma v)_{\chi\chi \rightarrow \phi\phi} \sqrt{\tilde{s} - 1} (2\tilde{s} - 1) K_1\left(\frac{2\sqrt{\tilde{s}} m_\chi}{T}\right)}{\int d\tilde{s}_\phi (\sigma v)_{\phi\phi \rightarrow \chi\chi} \sqrt{\tilde{s}_\phi - 1} (2\tilde{s}_\phi - 1) K_1\left(\frac{2\sqrt{\tilde{s}_\phi} m_\phi}{T}\right)} \quad (\text{D.7})$$

$$\simeq \frac{(1 - \delta)^3 K_2^2[x(1 - \delta)]}{8K_2^2[x]} \frac{\int d\tilde{s} \sqrt{\tilde{s} - 1} (2\tilde{s} - 1) K_1[2\sqrt{\tilde{s}}]}{\int d\tilde{s} \sqrt{\tilde{s} - 1} (2\tilde{s}(1 - \delta)^{-2} - 1) K_1[2\sqrt{\tilde{s}}]}. \quad (\text{D.8})$$

Here, we defined $\tilde{s} = s/(4m_\chi^2)$, $\tilde{s}_\phi = s/(4m_\phi^2) = \tilde{s}(1 - \delta)^{-2}$ with the integration domains restricted to $\max(1, (1 - \delta)^2) \leq \tilde{s} < \infty$. In the second line, we used $\sigma v \approx \text{const}$, which holds for s-wave. We evaluate eq. (D.8) at the freeze-out condition $n_\chi^2 \langle \sigma v \rangle_{\chi\chi \rightarrow \phi\phi} = n_\phi^2 \langle \sigma v \rangle_{\phi\phi \rightarrow \chi\chi} \sim n_\chi H$, which in practice amounts to numerically solving the condition

$$Y_\chi(x_f^{\text{SM}}) \frac{1 + \frac{1}{2} \frac{g_\phi}{g_\chi} (1 - \delta)^{3/2} e^{\delta x_f^{\text{SM}}}}{1 + \frac{1}{2} \sqrt{\bar{r}(x_f^\phi)}} \langle \sigma v \rangle_{\chi\chi \rightarrow \phi\phi}(x_f^\phi) = H(x_f^\phi) / s(x_f^\phi). \quad (\text{D.9})$$

Finally, we show the resulting DM relic density in fig. D.1 as a function of the mass splitting δ for the benchmark point of the secluded dark sector (tab. 6.1). For the region where the DM annihilation is kinematically suppressed $m_\chi < m_\phi$ ($\delta < 0$), the relic density $\Omega_\chi h^2$ is hardly affected by the presence of the dark Higgs bosons, as most of the energy density already at the decoupling of the DS from the SM already resides in the DM (cf. eq. (D.1)). This changes rapidly at the switch to positive mass splittings $\delta > 0$, where the DM can annihilate efficiently into the dark Higgs bosons after the SM freeze-out, while now the inverse process is kinematically suppressed. The result is an exponential suppression of the DM relic density. Generally, we see that the DM freeze-out occurs late compared to the SM decoupling $x_f^\phi \gg x_f^{\text{SM}} \sim 12$ for the benchmark points. At the equal mass threshold $\delta = 0$, the process $\bar{\chi}\chi \leftrightarrow \phi\phi$ remains very efficient up until large values of $x_f^\phi \sim 10^4$. This a posteriori justifies the separation of the relic density computation into two distinct steps.

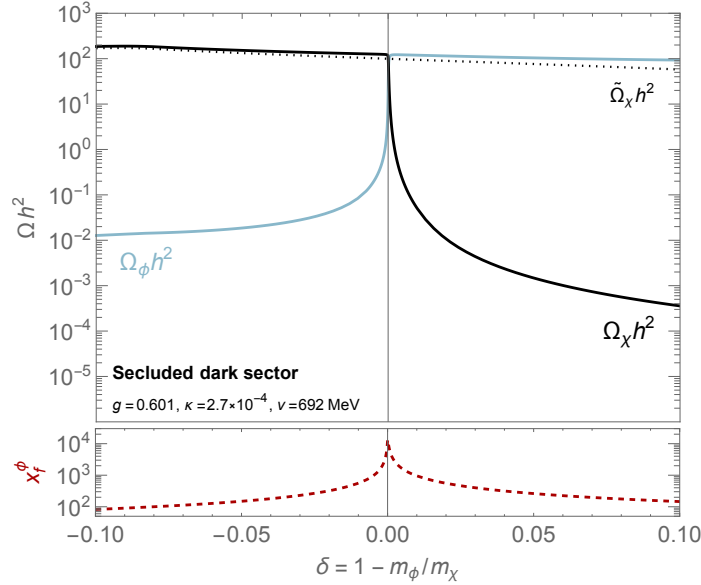


Figure D.1.: *Top panel:* DM relic abundance (black line) as a function of the mass splitting δ for the benchmark point of the secluded dark sector scenario (point B in tab. 6.1). Neglecting dark Higgs decays, the would-be abundance $\Omega_\phi h^2$ is shown as the blue line. The black dotted line shows the would-be abundance of the DM if the process $\bar{\chi}\chi \leftrightarrow \phi\phi$ were to be neglected. *Bottom panel:* Value of $x = m_\chi/T$ at the freeze-out of the process $\bar{\chi}\chi \leftrightarrow \phi\phi$.

We note here that a crucial assumption in this computation is that the dark Higgs bosons and the DM remain in kinetic equilibrium and that the dark Higgs bosons only decay after the DM freeze-out. We can estimate that χ will decouple from the SM once the electrons become Boltzmann suppressed, i.e. around $T \sim m_e$. This happens only shortly before the freeze-out of DM at $T_f^\phi \simeq 50 - 200 \text{ keV}$ in the best-fit region. The assumption that the dark Higgs bosons share a common temperature with the DM is typically fulfilled for $m_\phi \lesssim m_\chi$, but starts to deviate for the “forbidden” regime $m_\phi \gtrsim m_\chi$ [270]. Here, the effect would be an underestimation of the DM relic density by a factor of a few in our approach [301, 302]. To include these effects, one would have to numerically solve the full coupled Boltzmann equations at the phase-space level. However we expect the resulting shift in the couplings to be only small, as the relic density depends exponentially on the DM annihilation rate. We therefore neglect this effect in our analysis.

We address the second assumption – that the dark Higgs bosons only decay after the DM freeze-out – in the colour scale of the bottom right panel of fig. 6.11. There, we can see that some part of the parameter space do not fulfil the requirement $T_f^\phi < T_{\text{decay}}$ (red), however a significant part of the parameter space does not face this problem (green). This unproblematic region is shown in fig. D.2, where we removed all points that do not fulfil $T_f^\phi > T_{\text{decay}}$. The effect of this cut on the parameter space is a shift towards larger VEV v and mass splitting δ and an apparent restriction on the kinetic mixing $\kappa \lesssim 10^{-4}$. Comparing this to the dark Higgs lifetime eq. (6.12), we see that this is the region of larger lifetimes, i.e. smaller T_{decay} .

For completeness, we list here the two cross sections that enter the relic density calculation above.

$$(\sigma v)_{\chi\bar{\chi} \rightarrow e^+e^-} = \frac{g^2 \kappa^2 e^2 (s - 4m_\chi^2)(2m_e^2 + s)}{24\pi s((m_{A'}^2 - s)^2 + \Gamma_{A'}^2 m_{A'}^2)} \frac{s}{2(s - 2m_\chi^2)} \sqrt{1 - \frac{4m_e^2}{s}}. \quad (\text{D.10})$$

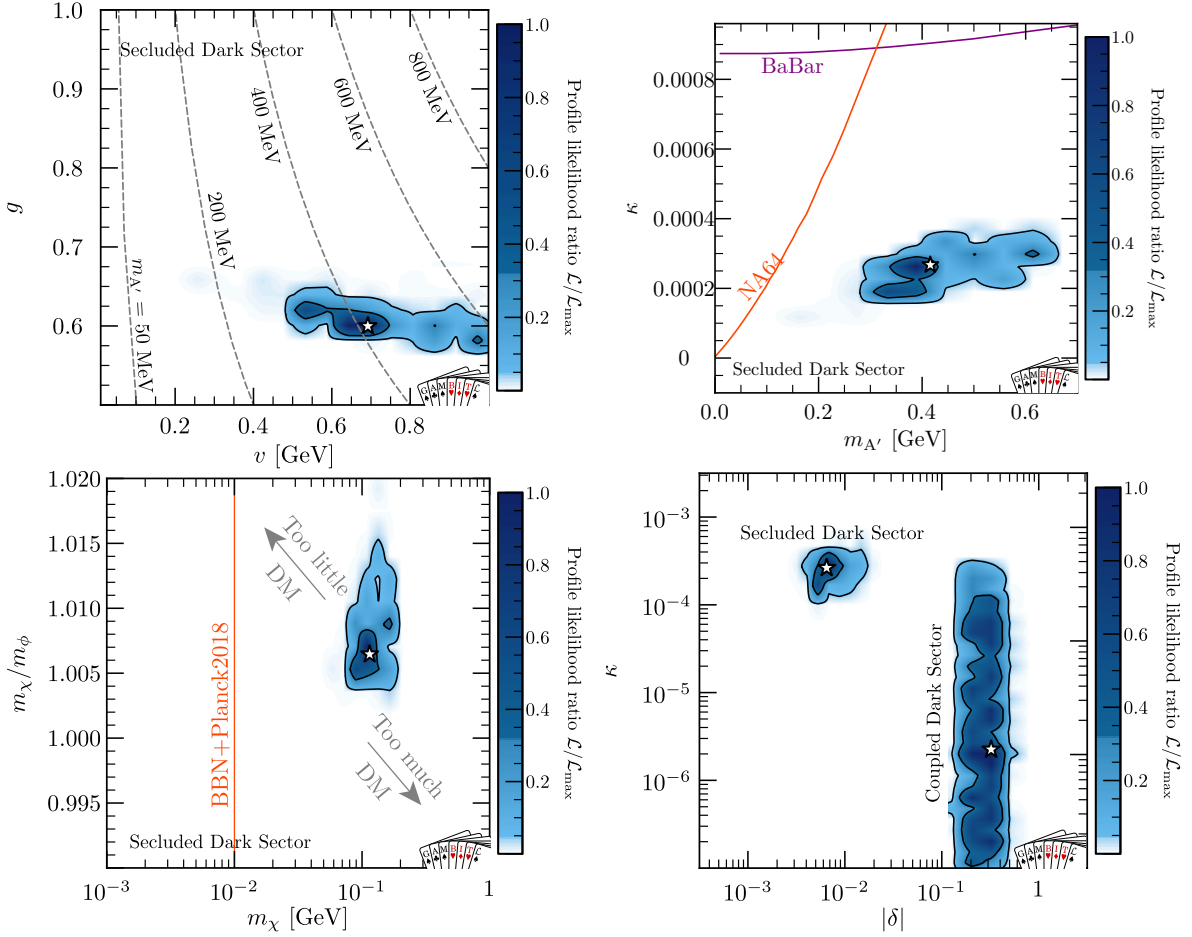


Figure D.2.: Allowed parameter region determined through a global-fit for the secluded dark sector in terms of the profile likelihood (blue shading). Compared to fig. 6.10 only points with $T_f^\phi > T_{\text{decay}}$, i.e. for which the dark Higgs bosons decay only after DM decoupling are shown.

$$\begin{aligned}
 (\sigma v)_{\chi\bar{\chi} \rightarrow \phi\phi} &= \frac{y^2}{32\pi s v^2} \frac{s}{2(s - 2m_\chi^2)} \sqrt{1 - \frac{4m_\phi^2}{s}} \\
 &\times \left[\frac{2m_\phi^4 (s - 4m_\chi^2)}{(m_\phi^2 - s)^2} + \frac{8m_\chi^2 m_\phi^2}{m_\phi^2 - s} + \frac{m_\chi^2 (m_\phi^2 - 4m_\chi^2)^2}{m_\chi^2 (4m_\phi^2 - s) - m_\phi^4} - 2m_\chi^2 \right. \\
 &+ \left(-\frac{2m_\chi^2 (16m_\chi^2 (m_\phi^2 - s) + 4sm_\phi^2 + 32m_\chi^4 - 6m_\phi^4 - s^2)}{\sqrt{s - 4m_\chi^2} \sqrt{s - 4m_\phi^2} (s - 2m_\phi^2)} \right. \\
 &\left. \left. + \frac{8m_\chi^2 m_\phi^2 (8m_\chi^2 - 2m_\phi^2 - s)}{\sqrt{s - 4m_\chi^2} \sqrt{s - 4m_\phi^2} (s - m_\phi^2)} \right) \tanh^{-1} \left(\frac{\sqrt{s - 4m_\chi^2} \sqrt{s - 4m_\phi^2}}{s - 2m_\phi^2} \right) \right]. \quad (\text{D.11})
 \end{aligned}$$

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