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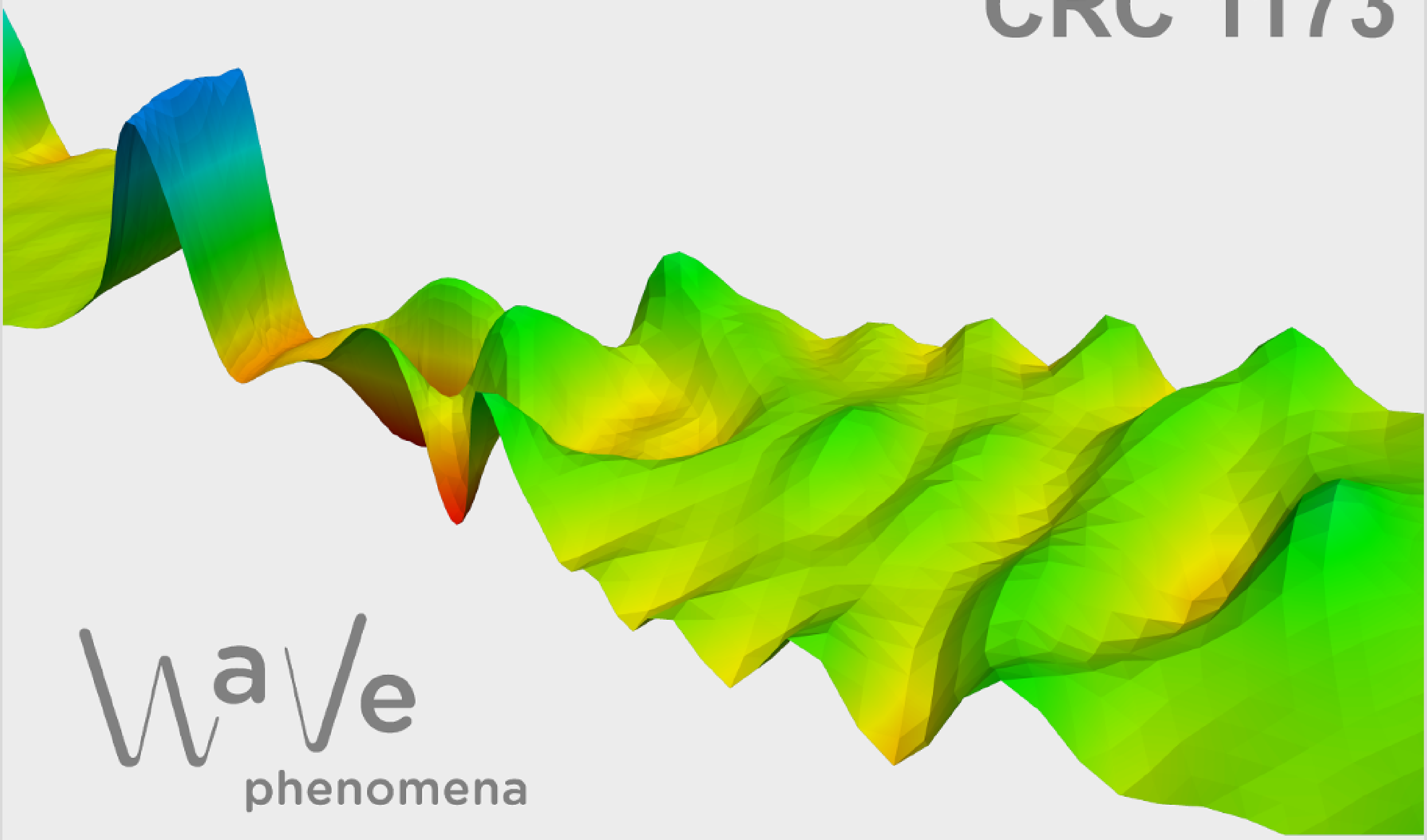

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VARIATIONAL GAUSSIAN APPROXIMATION FOR THE MAGNETIC SCHRÖDINGER EQUATION

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ABSTRACT. In the present paper we consider the semiclassical magnetic Schrödinger equation, which describes the dynamics of particles under the influence of a magnetic field. The solution of the time-dependent Schrödinger equation is approximated by a single Gaussian wave packet via the time-dependent Dirac–Frenkel variational principle. For the approximation we derive ordinary differential equations of motion for the parameters of the variational solution. Moreover, we prove L^2-error bounds and observable error bounds for the approximating Gaussian wave packet.

1. Introduction

In the present paper we study the semiclassical magnetic Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_0, \quad t \in \mathbb{R}, \tag{1.1a}$$

on $\mathbb{R}^d$ with magnetic Hamiltonian

$$H(t) = \frac{1}{2}\big(\mathrm{i}\varepsilon\nabla_x + A(t,x)\big)^2 + V(t,x), \tag{1.1b}$$

and initial value $\psi_0 \in L^2(\mathbb{R}^d)$ with semiclassical parameter $0 < \varepsilon \ll 1$. Here, A is a magnetic vector potential, and V is the electric potential. This equation arises in the modeling of the quantum dynamics of nuclei in a molecule subject to external magnetic fields. From a numerical point of view, solving this time-dependent partial differential equation raises three major problems. First, it is a high-dimensional problem, since the space dimension is typically given by $d = 3N$, where N is the number of nuclear particles in the system. Further, the computational domain $\mathbb{R}^d$ is naturally unbounded, and thus most numerical methods require truncation before discretization. For the method of lines (first discretize space, then time), high dimension combined with an unbounded domain leads to inadequately if not unattractably large systems that have to be integrated in time. Another challenge is given by the high oscillations induced by the small semiclassical parameter ε. For standard time integration schemes severe stepsize restrictions have to be imposed and leave these methods impracticable.

We consider the case that the initial value ψ_0 is strongly localized and given by a Gaussian wave packet,

$$\psi_0(x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\Big(\frac{1}{2}(x-q)^T\mathcal{C}(x-q) + (x-q)^T p + \zeta\Big)\Big),$$

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where $q, p \in \mathbb{R}^d$ are the packet's position and momentum center, $\mathcal{C} \in \mathbb{C}^{d\times d}$ is the width matrix of the envelope, and $\zeta \in \mathbb{C}$ a phase and weight parameter. For $A = 0$ it is well established that it is possible to reasonably approximate the solution by a Gaussian wave packet with parameters that are evolved according to ordinary differential equations. First studies in this direction are due to K. Hepp [21] and G. Hagedorn [13] from the perspective of mathematical physics, and E. Heller [19, 20] as well as R. Coalson, M. Karplus [6] with already an eye on numerical computation. The evolution equations for the parameters of all Gaussian wave packet approximations can be classified in two categories:

Variational: The variational approach relies on the time-dependent Dirac–Frenkel principle for deriving the parameter equations of motion. By the variational construction, the Gaussian wave packet automatically inherits several conservation properties of the exact solution.

Semiclassical: The semiclassical approach expands the wave packet ansatz with respect to the semiclassical parameter ε and derives ε independent parameter equations by matching terms with the same order.

Both types of ordinary differential equations have the advantageous property, that their solutions are non-oscillatory. Both approximations have the same convergence order with respect to the semiclassical parameter ε in L^2-norm, and both reproduce the exact solution for the special case of Schrödinger operators with linear magnetic potential A and quadratic electric potential V. For a further discussion, we refer to [5, Chapter 10.2] for a monograph that covers the semiclassical construction, to [25, Chapter II.4] or [24, Chapter 3] for a short book and a review presenting the variational case, and to [31] for a general presentation of Gaussian wave packet dynamics.

Contributions of the paper. Our main contribution in this paper is to first show that for the magnetic Schrödinger equation the variational approximation is still given by a system of ordinary differential equations for the parameters defining the Gaussian wave packet. Second, we prove rigorous error bounds for this approximation on finite time intervals $[0, T]$ in terms of the semiclassical parameter ε. The presented results generalize the bounds established in [24, 25] to non-vanishing magnetic potentials A and further allow for time-dependencies in both the electric and the magnetic potential. We also treat the more general case where the dynamics are generated by the Weyl quantization of a smooth and subquadratic Hamiltonian function. This includes convergence in the L^2-norm with order $\mathcal{O}(\sqrt{\varepsilon})$ as well as for expectation values of observables, which resemble certain measurable physical quantities of the wave function, with order $\mathcal{O}(\varepsilon^2)$. These estimates extend and improve the observable bound of [24, Theorem 3.5] and the result of [28] from the case of vanishing magnetic potential. Let us point out that the design and the analysis of time integrators for the magnetic variational equations of motion are currently under investigation.

Further wave packet results for $A = 0$. Hagedorn wave packets [13–15] are a multivariate anisotropic generalization of the Hermite functions. They are Gaussian wave packets with a polynomial prefactor, such that a family of them constitutes an orthonormal basis of $L^2(\mathbb{R}^d)$. In [1, 8, 10], time splitting integrators for Hagedorn wave packet approximations are proposed, that combine parameter propagation by ordinary differential equations with a Galerkin step. A spawning method for

Gaussian	L^2-norm	observables
semiclassical	$\mathcal{O}(\sqrt{\varepsilon})$	$\mathcal{O}(\varepsilon)$
variational	$\mathcal{O}(\sqrt{\varepsilon})$	$\mathcal{O}(\varepsilon^2)$

Table 1. Error bounds for the semiclassical and the variational approximation of magnetic Schrödinger dynamics according to Theorem 3.8 and Theorem 3.10. The variational observable error estimate extends and improves previously known results.

several families of Hagedorn wave packets is introduced in [29]. For variational Gaussian wave packets, a time splitting integrator, which is robust in the semiclassical parameter ε, is proposed in [9]. Recently in [28], T. Oshawa has analysed the expectation values of position and momentum for a variational Gaussian wave packet and proved $\mathcal{O}(\varepsilon^{3/2})$ accuracy. Our results here generalize and improve this error bound in two ways: First, we allow for general sublinear observables. Second, our method of proof shows $\mathcal{O}(\varepsilon^2)$ observable accuracy also for the case $A \neq 0$. It is worthwhile emphasizing, that from the perspective of the observable error variational Gaussians are more accurate than their semiclassical counterparts.

Related wave packet results for $A \neq 0$. The most general result for the semiclassical wave packet approach is given in [30, Theorem 21] of the monograph by D. Robert and M. Combescure. There, the propagation of Gaussian and Hagedorn wave packets is covered for a general class of time-dependent Hamiltonian operators $H(t)$, that includes the magnetic Schrödinger operator. The error analysis is with respect to the L^2-norm, but not for observables. The semiclassical construction there also receives corrections, such that it can be accurate to order $\mathcal{O}(\varepsilon^{k/2})$ for any $k \geq 1$. In [2], magnetic Schrödinger operators with polynomially bounded, time-independent magnetic fields and zero potential are considered. The initial coherent state has zero initial energy and its propagation is analysed for the long-time horizon $[0, T/\varepsilon]$. In [23], N. King and T. Ohsawa derive the equations of motion for variational Gaussians in the presence of a magnetic field. They conduct numerical experiments for the expectation value of the position and the momentum operator suggesting that the variational Gaussians are more accurate than the semiclassical ones. An extension of the Hagedorn Galerkin method [8] to the case of magnetic Schrödinger equations is studied in [34], including an error analysis with respect to the L^2-norm. However, no error bounds for the observables are investigated there. For linear magnetic potentials of a particular structure, in [11] a problem adapted splitting method for Hagedorn wave packets is derived but without error analysis. A slightly different approach, called the Gaussian wave packet transform, is proposed for the magnetic Schrödinger equation in [35]. There, the ordinary differential equations for the Gaussian parameters are the semiclassical ones except for an additional term for the scalar parameter ζ.

Outline of the paper. The rest of the paper is structured as follows. For our error analysis we introduce the analytical framework and the variational Gaussian wave packet ansatz in Section 2. We present our main results for the magnetic Schrödinger equation in Section 3, including the equations for the parameters, the conservation of different quantities, the convergence in the L^2-norm and the convergence of the observables. The proofs of the corresponding results are given in Sections 4 to 7.

Notation. Throughout the paper, we denote by $L^p(\mathbb{R}^d)$ the classical Lebesgue spaces, and by $\mathcal{S}(\mathbb{R}^d)$ the Schwartz space of rapidly decreasing functions. Further, we make use of the multiindex notation and let for $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$, $x \in \mathbb{R}^d$, $f \in \mathcal{S}(\mathbb{R}^d)$

$$|\alpha| \coloneqq \alpha_1 + \ldots + \alpha_d, \qquad x^\alpha \coloneqq x_1^{\alpha_1} \ldots x_d^{\alpha_d}, \qquad \partial^\alpha f \coloneqq \partial_1^{\alpha_1} \ldots \partial_d^{\alpha_d} f.$$

For a function $W \colon \mathbb{R}^d \to \mathbb{R}^L$, $L \geq 1$, we define the average

$$\langle W \rangle_u \coloneqq \langle u | W u \rangle = \int_{\mathbb{R}^d} W(x) |u(x)|^2 \, \mathrm{d}x,$$

if the integral exists. For a linear operator $\mathbf{A}$ acting on $L^2(\mathbb{R}^d)$, we denote

$$\langle \mathbf{A} \rangle_u \coloneqq \big\langle u | \mathbf{A} u \big\rangle = \int_{\mathbb{R}^d} \overline{u(x)} (\mathbf{A} u)(x) \, \mathrm{d}x,$$

whenever the integral is well-defined. We also use the dot product of $v, w \in \mathbb{C}^L$ as $v \cdot w \coloneqq v^T w = v_1 w_1 + \cdots + v_L w_L$.

2. General setting

We first discuss the analytic framework for our analysis and introduce the Gaussian wave packets. We further call some results on the wellposedness from the literature. For the vector potential we choose the Coulomb gauge, i.e. $\operatorname{div} A = 0$. In order to shorten notation, we rewrite the Hamiltonian in (1.1b) as

$$H(t) = -\frac{\varepsilon^2}{2} \Delta + \mathrm{i}\varepsilon A(t) \cdot \nabla + \widetilde{V}(t), \qquad \widetilde{V} \coloneqq \frac{1}{2} |A|^2 + V. \tag{2.1}$$

Throughout this paper we make the following smoothness and growth assumption on the potentials.

Assumption 2.1. *The scalar potential $\widetilde{V} \colon \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ and the vector valued potential $A = (A_j)_{j=1,\ldots,d} \colon \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ are infinitely often differentiable and in addition*

(a) *$\widetilde{V}$ is subquadratic, i.e. $\nabla^k \widetilde{V}$ is bounded for all $k \geq 2$, and*
(b) *A is sublinear, i.e. $\nabla^k A$ is bounded for all $k \geq 1$, and satisfies* $\operatorname{div} A = 0$.

If in addition to Assumption 2.1, we assume that $\partial_t A$ is sublinear, then it can be shown that the initial value problem (1.1a) is well posed for initial values in L^2, cf. [33, sec. 4] or the remarks after [30, Def. 1] or [27, Rem. 5.14]. In particular, the following wellposedness result on the unitarity of the time evolution guarantees that the norm of the solution of (1.1a) is the same as the one of the initial data. However, for our analysis here, only Assumption 2.1 will be used.

Theorem 2.2. *Let Assumption 2.1 hold and assume that $\partial_t A$ is sublinear. There exists a unitary evolution family $(U(t,s))_{t,s \in \mathbb{R}}$ on $L^2(\mathbb{R}^d)$ such that for all initial data $\psi_0 \in L^2(\mathbb{R}^d)$ the solution ψ of (1.1a) is given by*

$$\psi(t) = U(t, 0) \psi_0. \tag{2.2}$$

In the case of time-independent potentials the evolution family $(U(t,s))_{t,s\in\mathbb{R}}$ reduces to the unitary group $(e^{-it/\varepsilon H})_{t\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$, which which is given by the spectral theorem and commutes with the Hamiltonian.

Following [24, Chapter 3], we approximate the solution ψ of (1.1a) in the manifold $\mathcal{M}$ of Gaussian wave packets given by

$$\mathcal{M} = \Big\{ g \in L^2(\mathbb{R}^d) \;\big|\; g(x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\big(\frac{1}{2}(x-q)^T\mathcal{C}(x-q) + (x-q)^T p + \zeta\big)\Big), \\ q,\, p \in \mathbb{R}^d,\, \mathcal{C} = \mathcal{C}^T \in \mathbb{C}^{d\times d},\, \mathrm{Im}\,\mathcal{C} \text{ positive definite}, \zeta \in \mathbb{C}\Big\}. \tag{2.3}$$

The approximating Gaussian wave packet is characterized by the Dirac–Frenkel variational formulation, cf. [24,25]: seek $u(t) \in \mathcal{M}$ such that for all $t \in \mathbb{R}$ it holds

$$\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \quad \big\langle \mathrm{i}\varepsilon\partial_t u(t) - H(t)u(t) | v \big\rangle = 0 \quad \text{for all} \quad v \in \mathcal{T}_{u(t)}\mathcal{M},$$

with initial value $u(0) = u_0 \in \mathcal{M}$. Using the orthogonal projection $P_u : L^2(\mathbb{R}^d) \to \mathcal{T}_u\mathcal{M}$ we can equivalently write

$$\mathrm{i}\varepsilon\partial_t u(t) = P_{u(t)}\big(H(t)u(t)\big), \quad u(0) = u_0 \in \mathcal{M}. \tag{2.4}$$

We note that (2.4) can also be stated in terms of the symplectic projection onto the tangent space, see C. Lubich's blue book [25, II.1.3].

Remark 2.3. In the time-independent and non-magnetic case, one can also treat initial values $\psi_0 \notin \mathcal{M}$ using continuous superpositions of thawed and frozen Gaussians, see [24, Ch. 5]. The extension of these to the case (1.1b), however, is beyond the scope of the present work.

For the manifold $\mathcal{M}$ defined in (2.3) the tangent space $\mathcal{T}_u\mathcal{M}$ takes the following simple form.

Lemma 2.4 ([24, Lemma 3.1])**.** *For $u \in \mathcal{M}$ we have*

$$\mathcal{T}_u\mathcal{M} = \{\varphi u \,|\, \varphi \text{ } d\text{-variate complex polynomial of degree at most } 2\}\,.$$

The approximation by Gaussian wave packets seems appropriate due to the following exactness result, which is a consequence of Lemma 2.4 together with (2.4) and Theorem 2.2.

Proposition 2.5 ([24, Prop. 3.2])**.** *Let $V(t,\cdot)$ be quadratic and $A(t,\cdot)$ be linear in space for all $t \in \mathbb{R}$. If $\psi_0 \in \mathcal{M}$, then the variational approximation u defined by* (2.4) *is exact, i.e., $u(t) = \psi(t)$, where ψ denotes the solution of* (1.1a).

In the next section we derive a system of ordinary differential equations to determine parameters of the variational solution $u \in \mathcal{M}$ and present error bounds for the variational approximation.

3. Main results

In the remaining paper we consider (1.1a) and (2.4) for initial data satisfying

$$\psi_0 = u_0 \in \mathcal{M} \quad \text{and} \quad \|u_0\|_{L^2} = 1. \tag{3.1}$$

Our first step is to derive equations of motions for the parameters defining the variational solution u. Then we show that in the limit $\varepsilon \to 0$, these equations tend to classical equations of motions. Moreover, we study geometric properties of the solution and the variational approximation. Finally, we state error bounds for the solution in the L^2-norm and for averages of observables. Our work generalizes the results in [24] in the sense that we treat time-dependent, magnetic Hamiltonians. We also generalize the results of [23,28] from the position and momentum operator to sublinear observables in the sense of Assumption 2.1. For the sake of readability, we postpone the proofs to Sections 4 to 7.

3.1. **Variational equations of motion.** In order to write equations of motion for the parameters of a Gaussian wave packet $u \in \mathcal{M}$ we use the short notation

$$\begin{aligned} \mathcal{C}_{\mathrm{R}} &= \operatorname{Re}\mathcal{C}, & \mathcal{C}_{\mathrm{I}} &= \operatorname{Im}\mathcal{C}, \\ v &= (v_j)_{j=1}^d, & A &= (A_j)_{j=1}^d, \\ J_A &= \big(\partial_j A_k\big)_{j,k=1}^d, & (D^2_{A,v})_{k,l} &= \textstyle\sum_{j=1}^d \partial_l \partial_k A_j v_j. \end{aligned}$$

We start by deriving two equivalent sets of equations for $0 < \varepsilon \ll 1$. In the following section, we discuss the limit $\varepsilon \to 0$ and show that the two sets lead to the classical equations of motion for charged particles in a magnetic field given by the time-dependent Hamiltonian function

$$h(t,\widetilde{q},\widetilde{p}) = \frac{1}{2}|\widetilde{p}|^2 - A(t,\widetilde{q}) \cdot \widetilde{p} + \widetilde{V}(t,\widetilde{q}), \quad (t,\widetilde{q},\widetilde{p}) \in \mathbb{R} \times \mathbb{R}^{2d}, \tag{3.2}$$

cf. [12,18]. The first set of equations of motion reads:

Theorem 3.1. *Let u_0 satisfy (3.1) and be given by its parameters $q_0, p_0, \mathcal{C}_0, \zeta_0$ defined in (2.3). Then, the parameters of the solution $u \in \mathcal{M}$ of (2.4) satisfy*

$$\dot{q} = p - \langle A \rangle_u, \tag{3.3a}$$

$$\dot{p} = \frac{\varepsilon}{2}\left\langle \nabla \mathrm{tr}\left(J_A^T \mathcal{C}_{\mathrm{R}} \mathcal{C}_{\mathrm{I}}^{-1}\right)\right\rangle_u + \langle J_A \rangle_u^T p - \langle \nabla \widetilde{V} \rangle_u, \tag{3.3b}$$

$$\begin{aligned}\dot{\mathcal{C}} = &-\mathcal{C}^2 + \langle D^2_{A,p} \rangle_u + \langle J_A \rangle_u^T \mathcal{C} + \mathcal{C}\langle J_A \rangle_u - \langle \nabla^2 \widetilde{V} \rangle_u. \\ &+ \frac{\varepsilon}{2}\left\langle \nabla^2 \mathrm{tr}\left(J_A^T \mathcal{C}_{\mathrm{R}} \mathcal{C}_{\mathrm{I}}^{-1}\right)\right\rangle_u, \end{aligned}\tag{3.3c}$$

$$\begin{aligned}\dot{\zeta} = &\frac{1}{2}|p|^2 + \frac{\varepsilon}{2}\left\langle \mathrm{tr}\left(J_A^T \mathcal{C}_{\mathrm{R}} \mathcal{C}_{\mathrm{I}}^{-1}\right)\right\rangle_u + \frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C}) \\ &- \frac{\varepsilon}{4}\mathrm{tr}\Big(\mathcal{C}_{\mathrm{I}}^{-1}\big(\frac{\varepsilon}{2}\left\langle \nabla^2 \mathrm{tr}\left(J_A^T \mathcal{C}_{\mathrm{R}} \mathcal{C}_{\mathrm{I}}^{-1}\right)\right\rangle_u + \langle J_A \rangle_u^T \mathcal{C}_{\mathrm{R}} + \mathcal{C}_{\mathrm{R}} \langle J_A \rangle_u + \langle D^2_{A,p} \rangle_u\big)\Big) \\ &- \langle \widetilde{V} \rangle_u + \frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_{\mathrm{I}}^{-1}\langle \nabla^2 \widetilde{V} \rangle_u\big), \end{aligned}\tag{3.3d}$$

with initial data $(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0)$.

The proof of Theorem 3.1 is given in Section 4. We observe that in terms of the classical Hamiltonian function h defined in (3.2), the equations of motion (3.3) can be rewritten as

$$\dot{q} = \langle \nabla_p h \rangle_u, \tag{3.4a}$$

$$\dot{p} = -\langle \nabla_q h \rangle_u, \tag{3.4b}$$

$$\dot{\mathcal{C}} = -\langle \nabla_{qq} h \rangle_u - \langle \nabla_{qp} h \rangle_u \mathcal{C} - \mathcal{C}\langle \nabla_{pq} h \rangle_u - \mathcal{C}\langle \nabla_{pp} h \rangle_u \mathcal{C}, \tag{3.4c}$$

$$\dot{\zeta} = -\langle h \rangle_u + \frac{\varepsilon}{4}\,\mathrm{tr}(B\;{\mathcal{C}_{\mathrm{I}}}^{-1}) + p^T \langle \nabla_p h \rangle_u. \tag{3.4d}$$

with the matrix $B \in \mathbb{C}^{d\times d}$ given by

$$B = \big(\mathrm{Id}, \mathcal{C}\big)\,\langle \nabla^2 h \rangle_u \begin{pmatrix} \mathrm{Id} \\ \mathcal{C} \end{pmatrix}.$$

Later on, in Theorem 4.2 we extend these findings to the variational dynamics induced by a general a subquadratic Hamiltonian.

Remark 3.2. In order to solve (3.3) numerically, one might adapt the Boris algorithm originally proposed in [3] and recently analyzed in [16,17]. This algorithm is constructed for the classical equations of motion for charged particle systems. Details or an efficient numerical algorithm are ongoing work which will be presented elsewhere.

An alternative approach presented in [24] makes use of a factorization of the width matrix $\mathcal{C}$ due to Hagedorn. For the magnetic Schrödinger equation, it leads to differential equations for the factors of $\mathcal{C}$ instead of (3.3c). By [24, Lemma 3.16], we can write

$$\mathcal{C} = PQ^{-1} \quad \text{and} \quad \operatorname{Im}\mathcal{C} = (QQ^*)^{-1}, \tag{3.5}$$

with complex, invertible, and symplectic matrices P and Q. The latter means that for

$$Y := \begin{pmatrix} \operatorname{Re} Q & \operatorname{Im} Q \\ \operatorname{Re} P & \operatorname{Im} P \end{pmatrix} \qquad \text{and} \qquad J := \begin{pmatrix} 0 & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix} \in \mathbb{R}^{2d\times 2d} \tag{3.6}$$

it holds $Y^TJY = J$, or equivalently

$$Q^TP - P^TQ = 0, \tag{3.7a}$$

$$Q^*P - P^*Q = 2\mathrm{i}\,\mathrm{Id}. \tag{3.7b}$$

In fact, if Q and P are complex matrices satisfying (3.7), then Q and P are invertible and the matrix $\mathcal{C} = PQ^{-1}$ is symmetric with positive definite imaginary part $(QQ^*)^{-1}$. This allows us to write the Gaussian wave packet (2.3) as

$$u(\cdot, x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\Big(\frac{1}{2}(x-q)^TPQ^{-1}(x-q) + p^T(x-q) + \zeta\Big)\Big) \tag{3.8}$$

and to derive equations of motion for the parameters (q, p, Q, P, ζ).

Corollary 3.3. *Let u_0 satisfy (3.1) and be given by the parameters $q_0, p_0, \mathcal{C}_0, \zeta_0$. Then the Gaussian wave packet (3.8) with parameters (q, p, Q, P, ζ) solving*

$$\dot{Q} = P - \langle J_A \rangle_u Q, \tag{3.9a}$$

$$\dot{P} = \langle J_A \rangle_u^T P + \frac{\varepsilon}{2}\big\langle \nabla^2 \mathrm{tr}\left(J_A \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\right)\big\rangle_u Q + \big\langle D^2_{A,p}\big\rangle_u Q - \big\langle \nabla^2 \widetilde{V}\big\rangle_u Q, \tag{3.9b}$$

and (3.3a), (3.3b), and (3.3d) is the variational solution (2.4) with initial data

$$(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0).$$

If the initial matrices Q_0 and P_0 are symplectic, then $Q(t)$ and $P(t)$ are symplectic for all times $t \in \mathbb{R}$.

The proof of Corollary 3.3 is given in Section 4.

3.2. **Equations of motion in the limit $\varepsilon \to 0$.** The classical Hamiltonian function (3.2) induces the non-autonomous classical Hamiltonian system

$$\begin{aligned} \begin{pmatrix} \dot{\widetilde{q}}(t) \\ \dot{\widetilde{p}}(t) \end{pmatrix} &= J^{-1}\nabla h(t, \widetilde{q}(t), \widetilde{p}(t)) \\ &= \begin{pmatrix} \widetilde{p}(t) - A(t, \widetilde{q}(t)) \\ J_A^T(t, \widetilde{q}(t))\widetilde{p}(t) - \nabla \widetilde{V}(t, \widetilde{q}(t)) \end{pmatrix} \end{aligned} \tag{3.10}$$

with initial data $\widetilde{q}(s) = \widetilde{q}_s, \widetilde{p}(s) = \widetilde{p}_s$ and with J defined in (3.6). Since $A(t, \widetilde{q})$ and $\widetilde{V}(t, \widetilde{q})$ are sublinear and subquadratic with respect to $\widetilde{q}$, the right-hand side for the ordinary differential equation (3.10) is locally Lipschitz continuous. There is no blow-up, since

$$\begin{aligned}\frac{1}{2}\partial_t\big(\,|\widetilde{q}|^2 + |\widetilde{p}|^2\,\big) &= \widetilde{q}^T(\widetilde{p} - A(\widetilde{q})) + \widetilde{p}^T(J_A^T(\widetilde{q})\widetilde{p} - \nabla\widetilde{V}(\widetilde{q}))\\ &\le C\big(1 + |\widetilde{q}|^2 + |\widetilde{p}|^2\,\big),\end{aligned}$$

where the constant $C > 0$ depends on bounds of the potentials. By Gronwall's lemma, there is no finite time blow-up. This provides the existence of a unique global solution. The bound in [24, Lemma 3.15] states that $\langle\cdot\rangle_u$ tend to point evaluations at q as $\varepsilon \to 0$, i.e., $\langle A\rangle_u \to A(q)$. Hence, we observe that the magnetic equations of motion (3.3a) and (3.3b) tend to classical equations (3.10) as $\varepsilon \to 0$ and (3.3d) to

$$\dot{\zeta} = \frac{1}{2}|p|^2 - \widetilde{V}(\cdot, q).$$

In order to link the set of equations (3.9) to classical mechanics, we consider the linearization of (3.2) along the position and momentum parameters (q, p), i.e.,

$$\begin{aligned}\begin{pmatrix}\dot{Q}\\ \dot{P}\end{pmatrix} &= J^{-1}\nabla^2 h(\cdot, \widetilde{q}, \widetilde{p})\begin{pmatrix}Q\\ P\end{pmatrix}\\ &= \begin{pmatrix} P - J_A(\cdot, \widetilde{q})Q \\ \Big(D^2_{A(\cdot,\widetilde{q}),\widetilde{p}} - \nabla^2\widetilde{V}(\cdot, \widetilde{q})\Big)Q + J_A(\cdot, \widetilde{q})^T P\end{pmatrix}.\end{aligned} \tag{3.11}$$

By the same reasoning, we observe that the equations (3.9) tend to the linearized equations classical equations (3.11) as $\varepsilon \to 0$.

3.3. **Averages.** A further remarkable property of Gaussian wave packets is the conservation of several physical quantities. In the following, we recall the definitions of the linear and angular momentum for quantum dynamical systems.

Let $x = (x_1, \dots, x_N)$, where $x_k \in \mathbb{R}^3$, $k = 1, \dots, N$ and $d = 3N$, be position variables. We recall the follwoing definition given in [24, Chapter 3].

Definition 3.4. (a) The quantum mechanical total linear momentum operator is given by

$$\mathcal{P} := -\mathrm{i}\varepsilon\sum_{k=1}^{N}\nabla_{x_k}.$$

(b) The quantum mechanical total angular momentum operator is given by

$$\mathcal{L} := \sum_{k=1}^{N} x_k \times (-\mathrm{i}\varepsilon\nabla_{x_k}) = -\mathrm{i}\varepsilon\sum_{k=1}^{N}\begin{pmatrix} x_{k_2}\partial_{k_3} - x_{k_3}\partial_{k_2}\\ x_{k_3}\partial_{k_1} - x_{k_1}\partial_{k_3}\\ x_{k_1}\partial_{k_2} - x_{k_2}\partial_{k_1}\end{pmatrix}.$$

Next, we state sufficient conditions on the potentials A and V, which lead to the conservation of averages of the observables from Definition 3.4.

Definition 3.5. We call a potential $W = (W_j)_{j=1,\dots,d} : (\mathbb{R}^3)^N \to \mathbb{R}^d$

(a) translation invariant, if

$$W_j(x_1, \dots, x_N) = W_j(x_1 + r, \dots, x_N + r),$$

for all $r \in \mathbb{R}^3$ and $j = 1, \dots, d$,

(b) rotation invariant if for all orthogonal matrices $R \in \mathbb{R}^{3\times 3}$ with $\det R = 1$ it holds
$$W_j(x_1,\dots,x_N) = W_j(Rx_1,\dots,Rx_N),$$
where $j = 1,\dots,d$.

In the next lemma we provide a representation for the energy and state conservation properties of the momenta.

Lemma 3.6. *The following assertions hold.*

(a) We have $\|\psi(t)\|_{L^2} = \|u(t)\|_{L^2} = \|u_0\|_{L^2}$ *for all* $t \in \mathbb{R}$.

(b) If the potentials A and V are both time-independent, then
$$\langle H\rangle_{\psi(t)} = \langle H\rangle_{\psi_0} \quad \text{and} \quad \langle H\rangle_{u(t)} = \langle H\rangle_{u_0}.$$

(c) For $\varphi = \psi, u$ the energy $\langle H\rangle_\varphi$ is given by
$$\langle H(t)\rangle_{\varphi(t)} = \langle H(0)\rangle_{\varphi(0)} + \int_0^t \left\langle \mathrm{i}\varepsilon\partial_s A(s)\cdot\nabla\right\rangle_{\varphi(s)} + \left\langle \partial_s \widetilde{V}(s)\right\rangle_{\varphi(s)} \mathrm{d}s.$$

(d) For $\mathcal{P}$ and $\mathcal{L}$ from Definition 3.4 we have:

(i) If V and $A = (A_j)_{j=1}^d$ given in Assumption 2.1 are invariant under translations
$$\langle \mathcal{P}\rangle_{\psi(t)} = \langle \mathcal{P}\rangle_{\psi_0} \quad \text{and} \quad \langle \mathcal{P}\rangle_{u(t)} = \langle \mathcal{P}\rangle_{u_0}.$$

(ii) If $\widetilde{V}$ defined in (2.1) is invariant under rotations and $A(\cdot,x) = \alpha(\cdot)x$ for some $\alpha(\cdot) \in \mathbb{R}$, then
$$\langle \mathcal{L}\rangle_{\psi(t)} = \langle \mathcal{L}\rangle_{\psi_0} \quad \text{and} \quad \langle \mathcal{L}\rangle_{u(t)} = \langle \mathcal{L}\rangle_{u_0}.$$

The proof of Lemma 3.6 is given in Section 6.

3.4. **L^2-error bound.** In this section, we present the approximation property of the Gaussian wave packet with respect to the L^2-norm. Since our error bounds depend on parameters characterizing the Gaussian wave packet in (2.3), we first consider the boundedness of these parameters up to a fixed but arbitrary finite time $T > 0$ specified by ODE-theory.

Lemma 3.7. *For all times $T > 0$, the set of equations (3.3) is well posed on $[0,T]$ independently of ε. Furthermore, the solution parameters are bounded independently of ε, i.e.*
$$|\nu| \le c_{\nu_0}, \qquad \text{for all } \nu \in \{q, p, \mathcal{C}, \zeta\},$$
uniformly on $[0,T]$, where c_{ν_0} depends on the parameters of the initial Gaussian u_0, on the potentials V, A, and on T.

We note that by Corollary 3.3 the matrix $\mathcal{C}_\mathrm{I}$ is real symmetric, positive definite for all times t. To formulate the following results, we denote by $\rho > 0$ a lower bound on the smallest eigenvalue of $\mathcal{C}_\mathrm{I}$ on the finite time horizon $[0,T]$. For a discussion of relevant time scales on which ρ is sufficiently large compared to ε, called the Ehrenfest time, we refer to [24, Sec. 3.6]. With this, we can state our approximation result.

Theorem 3.8. *Let ψ, u be the solution of (1.1a) and (2.4), respectively, and let u_0 satisfy (3.1). Then the error bound*

$$\|\psi(t) - u(t)\|_{L^2} \le tc\sqrt{\varepsilon}, \qquad t \in [0,T],$$

holds with a constant c which depends on ρ, the bounds on the parameters from Lemma 3.7 and on the potentials, but is independent of ε and t.

We provide the details and the proof of the theorem in Section 5.

3.5. **Observable error bound.** In classical mechanics physical states are described by the position and momentum parameters $\widetilde{q}, \widetilde{p} \in \mathbb{R}^d$. Observables are functions depending smoothly on $(\widetilde{q}, \widetilde{p}) \in \mathbb{R}^d \times \mathbb{R}^d$, see, for example, [18, 32]. Classical mechanics can be linked to quantum mechanics via Weyl quantization, which asigns a classical observable to a quantum mechanical one using semiclassical Fourier transformation, cf. [7, Thm. 4.14] or [18, 26]. Formally, for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and an observable $\boldsymbol{a}$, we define

$$\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})\varphi(x) \coloneqq \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} \boldsymbol{a}\Big(\frac{x+\widetilde{q}}{2}, \widetilde{p}\Big) \mathrm{e}^{\mathrm{i}\widetilde{p}\cdot(x-\widetilde{q})/\varepsilon} \varphi(\widetilde{q}) \,\mathrm{d}(\widetilde{q}, \widetilde{p}).$$

The Weyl quantization of the projections to the first or second component of the classical variables are

$$\mathrm{op}_{\mathrm{Weyl}}(\widetilde{p})\varphi = -\mathrm{i}\varepsilon\nabla\varphi \quad \text{ and } \quad \mathrm{op}_{\mathrm{Weyl}}(\widetilde{q})\varphi = x\varphi.$$

Further examples of physically relevant observables stemming from classical symbols are

$$\mathrm{op}_{\mathrm{Weyl}}(|\widetilde{p}|^2)\psi(x) = -\varepsilon^2\Delta\psi(x)$$

and, due to $\operatorname{div} A = 0$,

$$\begin{aligned} \mathrm{op}_{\mathrm{Weyl}}(A(\widetilde{q}) \cdot \widetilde{p})\psi(x) &= \tfrac{1}{2}\left(A(x) \cdot (-\mathrm{i}\varepsilon\nabla) + (-\mathrm{i}\varepsilon\nabla) \cdot A(x)\right)\psi(x) \\ &= \left(A(x) \cdot (-\mathrm{i}\varepsilon\nabla)\right)\psi(x), \end{aligned}$$

and, of course,

$$\mathrm{op}_{\mathrm{Weyl}}(h(t))\psi(x) = H(t)\psi(x)$$

for the Hamiltonian function (3.2) and the magnetic Schrödinger operator (1.1b). An observable $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ defines for an L^2-normalised function $\varphi \in \mathcal{S}(\mathbb{R}^d)$ an expectation value,

$$\langle \varphi | \mathbf{A}\varphi \rangle = \int_{\mathbb{R}^d} \overline{\varphi(x)} (\mathbf{A}\varphi)(x) \mathrm{d}x,$$

and we investigate how expectation values issued by the variational approximation $u(t)$ differ from the ones of the true solution $\psi(t)$. For an error estimate relying on L^2 bounds, we have to restrict ourselves to sublinear classical observables.

Definition 3.9. The class of sublinear classical symbols is defined as smooth functions $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}$ such that for $\alpha \in \mathbb{N}_0^{2d}$ with $|\alpha| \ge 1$ there exists $C_\alpha > 0$

$$|\partial^\alpha \boldsymbol{a}(\widetilde{q}, \widetilde{p})| \le C_\alpha$$

for all $(\widetilde{q}, \widetilde{p}) \in \mathbb{R}^d \times \mathbb{R}^d$.

For the expectation values of classical sublinear observables, we obtain the following error estimate that generalizes and improves the findings of N. King and T. Ohsawa [23, 28], where asymptotic accuracy of the order $\varepsilon^{3/2}$ has been observed and proved for the variational position and momentum expectation value.

Theorem 3.10. *Let ψ, u be the solution of (1.1a) and (2.4), respectively, and let u_0 satisfy (3.1). Moreover, let $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ be an observable stemming from a classical sublinear observable $\boldsymbol{a}$ in the sense of Definition 3.9 such that $\boldsymbol{a} \circ \Phi^{t,s}$ is sublinear. Then we have the error bound*

$$\big|\langle \psi(t)|\mathbf{A}\psi(t)\rangle - \langle u(t)|\mathbf{A}u(t)\rangle\big| \le t\, c\, \varepsilon^2,$$

for all $t \in [0,T]$. The error constant c depends on the parameter bounds of Lemma 3.7 for the time-interval $[0,T]$, in particular on the bounds for the width matrix $\mathcal{C}$, on the potentials, and on $\boldsymbol{a}$, but is independent of ε and t.

Note that the convergence in the observables is of order ε^2, while the convergence in the L^2-norm presented in Theorem 3.8 is of order $\sqrt{\varepsilon}$. This is an improvement of the results obtained in [24, Theorem 3.5], where $\mathcal{O}(\sqrt{\varepsilon})$ norm accuracy and an $\mathcal{O}(\varepsilon)$ estimate for the non-magnetic observable error were proved. The rest of the paper is devoted to the proofs of the equations of motion and the error estimates presented in this section.

4. Equations of motions: proof of Theorem 3.1 and corollary 3.3

In this section we derive equations of motion for the parameters $(q, p, \mathcal{C}, \zeta)$ as well as for the factorization matrices Q and P. To do so, we compute both sides of (2.4) and compare the coefficients.

Proof of Theorem 3.1. In order to use the formula for the orthogonal projection derived in [24, Prop. 3.14] for (2.4), we observe that derivatives with respect to x of a Gaussian wave packet turn into scalar functions of x times u. For notational simplicity, we omit the time-dependence and in the potentials A and V we omit the space variable x. In particular, we have

$$\mathrm{i}\varepsilon A \cdot \nabla u = -A \cdot \big(\mathcal{C}(x-q) + p\big)u, \tag{4.1a}$$

$$-\frac{\varepsilon^2}{2}\Delta u = \Big(\frac{1}{2}(x-q)^T\mathcal{C}^2(x-q) + p^T\mathcal{C}(x-q) + \frac{1}{2}|p|^2 - \frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C})\Big)u, \tag{4.1b}$$

and for the time derivative it holds that

$$\mathrm{i}\varepsilon\partial_t u(\cdot, x) = \Big(-\frac{1}{2}(x-q)^T\dot{\mathcal{C}}(x-q) + \dot{q}^T\mathcal{C}(x-q) - \dot{p}^T(x-q) + p^T\dot{q} - \dot{\zeta}\Big)u. \tag{4.2}$$

Motivated by the classical magnetic Hamiltonian system (3.10), we eliminate one degree of freedom by setting $\dot{q} = p - \langle A\rangle_u$, see [12, 18]. Incorporating the above formulas, we compare the coefficients in x on both sides of (2.4) and arrive at equations of motions of the form

$$\begin{aligned}
\dot{q} &= p - \langle A\rangle_u,\\
\dot{p} &= \big\langle J_A^T\mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u + \big\langle J_A\big\rangle_u^T p - \big\langle\nabla\widetilde{V}\big\rangle_u,\\
\dot{\mathcal{C}} &= -\mathcal{C}^2 + \big\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\big\rangle_u + \big\langle D^2_{A,p}\big\rangle_u + \big\langle J_A\big\rangle_u^T\mathcal{C} + \mathcal{C}\big\langle J_A\big\rangle_u - \big\langle\nabla^2\widetilde{V}\big\rangle_u,\\
\dot{\zeta} &= \frac{1}{2}|p|^2 + \big\langle A^T\mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u + \frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C})\\
&\quad - \frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_{\mathrm{I}}^{-1}\big(\big\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\big\rangle_u + \langle J_A\rangle_u^T\mathcal{C}_{\mathrm{R}} + \mathcal{C}_{\mathrm{R}}\langle J_A\rangle_u + \langle D^2_{A,p}\rangle_u\big)\big)\\
&\quad - \langle\widetilde{V}\rangle_u + \frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_{\mathrm{I}}^{-1}\big\langle\nabla^2\widetilde{V}\big\rangle_u\big).
\end{aligned}$$

It remains to extract the additional power of ε from the terms that contain the difference $x-q$. From

$$|u(x)|^2 = \exp\Big(-\frac{1}{\varepsilon}(x-q)^T\mathcal{C}_{\mathrm{I}}(x-q) - \frac{2}{\varepsilon}\mathrm{Im}\,\zeta\Big)$$

we obtain the derivative

$$\nabla|u(x)|^2 = -\frac{2}{\varepsilon}\mathcal{C}_{\mathrm{I}}(x-q)|u(x)|^2, \tag{4.3}$$

and apply integration by parts to obtain

$$\begin{aligned}\big\langle A^T\mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u &= \big\langle A^T\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{I}}(x-q)\big\rangle_u\\ &= \int_{\mathbb{R}^d} A^T\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{I}}(x-q)|u(x)|^2\mathrm{d}x\\ &= \frac{\varepsilon}{2}\big\langle \mathrm{tr}\,\big(J_A^T\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\big)\big\rangle_u.\end{aligned}$$

Similarly, we gain an order of ε for

$$\big(\big\langle J_A^T\mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u\big)_i = \big(\big\langle J_A^T\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{I}}(x-q)\big\rangle_u\big)_i = \frac{\varepsilon}{2}\big\langle\partial_i\mathrm{tr}\,\big(J_A^T\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\big)\big\rangle_u,$$

as well as for

$$\big(\big\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\big\rangle_u\big)_{ij} = \frac{\varepsilon}{2}\Big\langle\sum_{k,l,m=1}^d \partial_m\partial_i\partial_j A_k\mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_{\mathrm{I}}^{-1})_{lm}\Big\rangle_u.$$

By the identity

$$\partial_{ij}\mathrm{tr}\,\big(J_A^T\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\big) = \sum_{k,m,l=1}^d \partial_{ij}\partial_m A_k\mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_{\mathrm{I}}^{-1})_{lm},$$

we conclude the equations of motion stated in (3.3). □

We now turn to the equations of motion for the Hagedorn factorization (3.5). The idea is to show that the product PQ^{-1} solves the same differential equation as $\mathcal{C}$ and conclude with the uniqueness of the variational solution u.

Proof of Corollary 3.3. We employ the differential identity

$$\partial_t(Q^{-1}) = -Q^{-1}\partial_t Q Q^{-1},$$

and the product rule to find that $\mathcal{C} = PQ^{-1}$ satisfies the differential equation

$$\dot{\mathcal{C}} = -PQ^{-1}\dot{Q}Q^{-1} + \dot{P}Q^{-1}$$

with $\partial_t Q = \dot{Q}$. Then, using (3.9), we see that this is the differential equation for $\mathcal{C}$ in (3.3c).

Concerning the symplectic relation in (3.7), we have

$$\partial_t(Q^TP - P^TQ) = \dot{Q}^TP + Q^T\dot{P} - \dot{P}^TQ - P^T\dot{Q},$$

and by inserting the differential equations of P,Q given in (3.9), we see that $Q^TP - P^TQ$ is constant. The same calculation holds for $\partial_t(Q^*P - P^*Q)$ with * replaced by ^{T}. Since p,q,A and V are real valued, we conclude

$$\partial_t(Q^*P - P^*Q) = \dot{Q}^*P + Q^*\dot{P} - \dot{P}^*Q - P^*\dot{Q} = 0,$$

which means that (3.7) holds true for all times. □

4.1. **Equations of motion for a general Hamiltonian.** The findings of Theorem 3.1 for the magnetic Schrödinger operator $H(t)$ extend to the dynamics for general Hamiltonian operators that are the Weyl quantization of a smooth function $h : \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$ of subquadratic growth, that is, for all $\alpha \in \mathbb{N}_0^{2d}$ with $|\alpha| \geq 2$ there exists $C_\alpha > 0$ such that

$$|\partial^\alpha h(t, \widetilde{q}, \widetilde{p})| \leq C_\alpha \tag{4.4}$$

for all $t \in \mathbb{R}$ and $(\widetilde{q}, \widetilde{p}) \in \mathbb{R}^{2d}$. Note that the classical magnetic Hamiltonian function (3.2) is not subquadratic, but our analysis works for both cases.

A first step for the generalization is the construction of a suitable orthonormal basis of the tangent space of a Gaussian wave packet, which is done in [24, Lemma 3.12 and Theorem 4.1] for the non-magnetic case, where only the modulus squared of the wave packet matters. For convenience, we state the representation formulas of the basis functions that we use. Consider a Gaussian wave packet $u \in \mathcal{M}$ of unit norm, $\|u\| = 1$. The family $\{\varphi_n\}_{|n|\leq 2}$ with

$$\varphi_0 = u, \tag{4.5a}$$

$$\varphi_{e_j} = \sqrt{\frac{2}{\varepsilon}}\ \left(Q^{-1}(x-q)\right)_j u, \tag{4.5b}$$

$$\varphi_{e_j+e_k} = \frac{1}{\sqrt{\delta_{kj}+1}} \left(\frac{2}{\varepsilon}\ \left(Q^{-1}(x-q)\right)_j\ \left(Q^{-1}(x-q)\right)_k - (Q^* Q^{-T})_{j,k} \right) u, \tag{4.5c}$$

is an orthonormal basis of the tangent space $\mathcal{T}_u\mathcal{M}$ of $\mathcal{M}$ at u. For calculating the orthogonal projection to the tangent space, we make use of another representation via the raising and lowering operators $\mathcal{A}_j^\dagger$ and $\mathcal{A}_j$. These are the jth component of the vector-valued operators

$$\mathcal{A}^\dagger = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} \left(P^* \mathrm{op}_{\mathrm{Weyl}}(\widetilde{q} - q) - Q^* \mathrm{op}_{\mathrm{Weyl}}(\widetilde{p} - p) \right),$$
$$\mathcal{A} = -\frac{\mathrm{i}}{\sqrt{2\varepsilon}} \left(P^T \mathrm{op}_{\mathrm{Weyl}}(\widetilde{q} - q) - Q^T \mathrm{op}_{\mathrm{Weyl}}(\widetilde{p} - p) \right),$$

respectively. Using the complete family of Hagedorn functions constructed by the infinite ladder process, we obtain that $\{\varphi_n\}_{|n|\leq 2}$ with

$$\varphi_0 = u, \quad \varphi_{e_j} = \mathcal{A}_j^\dagger u, \quad \varphi_{e_k+e_j} = \frac{1}{\sqrt{\delta_{kj}+1}}\ \mathcal{A}_j^\dagger\ \mathcal{A}_k^\dagger u, \tag{4.6}$$

see also [25, Chapter V.2] or [15, Theorem 3.3].

Equipped with the orthonormal basis (4.5) and (4.6), we can give an explicit formula for the quadratic polynomial generated by the orthogonal projection when acting on a general Hamiltonian operator.

Proposition 4.1 (Orthogonal projection)**.** *Let $h : \mathbb{R}^{2d} \to \mathbb{R}$ be smooth and of growth. Let $u \in \mathcal{M}$ be a Gaussian wave packet of unit norm, $\|u\| = 1$, with phase space center $z_0 = (q, p) \in \mathbb{R}^d \times \mathbb{R}^d$. Then,*

$$P_u(\mathrm{op}_{\mathrm{Weyl}}(h)u) = p_2 u,$$

where p_2 is the quadratic polynomial

$$p_2 : \mathbb{R}^d \to \mathbb{C},$$
$$p_2(x) = \beta + b^T(x-q) + \frac{1}{2}(x-q)^T B(x-q)$$

given by the complex coefficients

$$\begin{aligned}
\beta &= \langle h\rangle_u - \frac{\varepsilon}{4}\,\mathrm{tr}(B\ \mathcal{C}_{\mathrm{I}}^{-1}),\\
b &= \begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix}\langle\nabla h\rangle_u \in \mathbb{C}^d,\\
B &= \begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix}\langle\nabla^2 h\rangle_u \begin{pmatrix}\mathrm{Id}\\ \mathcal{C}\end{pmatrix} \in \mathbb{C}^{d\times d}.
\end{aligned}$$

The notation $\langle \boldsymbol{a}\rangle_u = \langle u \mid \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})u\rangle$ *refers to the expectation value of a quantized smooth observable* $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}^L$ *with respect to the Gaussian state* u*.*

Proof. We use the Hagedorn wave packets $\{\varphi_n\}_{|n|\le 2}$ associated with the Gaussian wave packet u as an orthonormal basis of the tangent space $\mathcal{T}_u\mathcal{M}$, see (4.5) and (4.6), and write the orthogonal projection as

$$P_u(\mathrm{op}_{\mathrm{Weyl}}(h)u) = \sum_{|n|\le 2} \langle \varphi_n \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle\ \varphi_n.$$

Starting with the contribution for $n = 0$, we have

$$\langle \varphi_0 \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle u \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle h\rangle_u.$$

For the following, it will be useful to introduce the slim rectangular matrix $Z = (Q; P) \in \mathbb{C}^{2d\times d}$ with column vectors $Z_1, \ldots, Z_d \in \mathbb{C}^{2d}$ and to write the ladder operators more compactly as

$$\mathcal{A}^\dagger = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}\ Z^* J\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z} - z), \qquad \mathcal{A} = -\frac{\mathrm{i}}{\sqrt{2\varepsilon}}\ Z^T J\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z} - z).$$

For $n = e_j$ we have by (4.5), [24, Lemmas 4.1, and 4.2] that

$$\langle \varphi_{e_j} \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle u \mid \mathcal{A}_j\mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle u \mid [\mathcal{A}_j, \mathrm{op}_{\mathrm{Weyl}}(h)]u\rangle.$$

Since the symbol of $\mathcal{A}_j$ is linear, we can use pseudodifferential calculus without remainders and obtain that the commutator satisfies

$$\begin{aligned}
[\mathcal{A}_j, \mathrm{op}_{\mathrm{Weyl}}(h)] &= -\frac{\mathrm{i}}{\sqrt{2\varepsilon}}\ \left[\mathrm{op}_{\mathrm{Weyl}}(Z_j^T J(\widetilde{z} - z)), \mathrm{op}_{\mathrm{Weyl}}(h)\right]\\
&= -\frac{\mathrm{i}}{\sqrt{2\varepsilon}}\frac{\varepsilon}{\mathrm{i}}\mathrm{op}_{\mathrm{Weyl}}(\{Z_j^T J(\widetilde{z} - z), h\})\\
&= \sqrt{\frac{\varepsilon}{2}}\ \mathrm{op}_{\mathrm{Weyl}}(Z_j^T \nabla h),
\end{aligned} \tag{4.7}$$

where we have calculated the Poisson bracket according to

$$\{Z_j^T Jz, h\} = \nabla(Z_j^T Jz)\cdot J\nabla h = -Z_j^T\nabla h.$$

Therefore,

$$\langle \varphi_{e_j} \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \sqrt{\frac{\varepsilon}{2}} Z_j^T \langle\nabla h\rangle_u.$$

After summation, we therefore obtain that

$$\begin{aligned}\sum_{j=1}^{d}\langle\varphi_{e_j}\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle\,\varphi_{e_j} &= \sum_{j=1}^{d}\langle\nabla h\rangle_u^T Z e_j e_j^T Q^{-1}(x-q)u\\ &= \langle\nabla h\rangle_u^T Z Q^{-1}(x-q)u\\ &= \langle\nabla h\rangle_u^T \begin{pmatrix}\mathrm{Id}\\ \mathcal{C}\end{pmatrix}(x-q)u,\end{aligned}$$

which concludes the computation of the first order contributions. For the second order wave packets, we analogously compute the projection coefficient as

$$\langle\varphi_{e_j+e_k}\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \frac{1}{\sqrt{\delta_{kj}+1}}\langle u\mid[\mathcal{A}_j,[\mathcal{A}_k,\mathrm{op}_{\mathrm{Weyl}}(h)]]u\rangle.$$

Using (4.7) twice, we obtain that the double commutator satisfies

$$\big[\mathcal{A}_j,[\mathcal{A}_k,\mathrm{op}_{\mathrm{Weyl}}(h)]\big] = \sqrt{\frac{\varepsilon}{2}}\,\big[\mathcal{A}_j,\mathrm{op}_{\mathrm{Weyl}}(Z_k^T\nabla h)\big] = \frac{\varepsilon}{2}\,\mathrm{op}_{\mathrm{Weyl}}(Z_j^T\nabla^2 h Z_k).$$

This implies for the coefficient that

$$\langle\varphi_{e_j+e_k}\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \frac{\varepsilon}{2\sqrt{\delta_{kj}+1}}\,Z_j^T\langle\nabla^2 h\rangle_u Z_k.$$

We now calculate the sum of all the second order contributions. We have

$$\begin{aligned}\sum_{|n|=2}\langle\varphi_n\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle\varphi_n &= \sum_{j=1}^{d}\sum_{k=1}^{j}\langle\varphi_{e_j+e_k}\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle\varphi_{e_j+e_k}\\ &= \sum_{j,k=1}^{d}\frac{\varepsilon}{2\sqrt{2}}\,Z_j^T\langle\nabla^2 h\rangle_u Z_k\;\frac{1}{\sqrt{2}}\mathcal{A}_j^\dagger\mathcal{A}_k^\dagger u,\end{aligned}$$

where the complete summation over the full square of indices is compensated by a change in normalisation of the contributions for $j\neq k$. For the part of the sum that generates a constant prefactor for the Gaussian, we have

$$\begin{aligned}-\frac{\varepsilon}{4}\sum_{j,k=1}^{d} Z_j^T\langle\nabla^2 h\rangle_u Z_k\;(Q^*Q^{-T})_{j,k} &= -\frac{\varepsilon}{4}\mathrm{tr}(Q^*Q^{-T}Z^T\langle\nabla^2 h\rangle_u Z)\\ &= -\frac{\varepsilon}{4}\mathrm{tr}(\begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix}\langle\nabla^2 h\rangle_u\begin{pmatrix}\mathrm{Id}\\ \mathcal{C}\end{pmatrix}QQ^*).\end{aligned}$$

For the quadratic prefactor, we similarly obtain

$$\begin{aligned}&\frac{1}{2}\sum_{j,k=1}^{d} Z_j^T\langle\nabla^2 h\rangle_u Z_k\;\big(Q^{-1}(x-q)\big)_j\;\big(Q^{-1}(x-q)\big)_k\\ &= \frac{1}{2}(x-q)^T\begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix}\langle\nabla^2 h\rangle_u\begin{pmatrix}\mathrm{Id}\\ \mathcal{C}\end{pmatrix}(x-q).\end{aligned}$$

□

Let $h:\mathbb{R}\times\mathbb{R}^{2d}\to\mathbb{R}$ be continuous with respect to time $t\in\mathbb{R}$, and smooth, and of subquadratic growth in the sense of (4.4). Denote $H(t)=\mathrm{op}_{\mathrm{Weyl}}(h(t))$. Then, the time-dependent Schrödinger equation

$$i\varepsilon\partial_t\psi(t) = H(t)\psi(t),\quad \psi(0)=\psi_0$$

has a unique solution $\psi(t) = U(t,0)\psi_0$ for all times $t \in \mathbb{R}$ for all square integrable initial data $\psi_0 \in L^2(\mathbb{R}^d)$, see [27] or [30, Def. 1]. The corresponding variational Gaussian wave packet obeys the following equations of motion.

Theorem 4.2 (Equations of motion for a general Hamiltonian). *Let $u_0 \in \mathcal{M}$ satisfy (3.1) and be given by its parameters $q_0, p_0, \mathcal{C}_0, \zeta_0$ defined in (2.3). Then, the parameters of the variational approximation*

$$\mathrm{i}\varepsilon\partial_t u(t) = P_{u(t)}(H(t)u(t)), \quad u(0) = u_0$$

satisfy the following set of ordinary differential equations (3.4) subject to initial data $(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0)$, where h is now the given general sub-quadratic classical Hamiltonian function. The Hagedorn parameter matrices of the variational wave packet satisfy:

$$\dot{P} = -\langle \nabla_{qq} h\rangle_u Q - \langle \nabla_{qp} h\rangle_u P, \qquad \dot{Q} = \langle \nabla_{pq} h\rangle_u Q + \langle \nabla_{pp} h\rangle_u P.$$

Moreover, the matrix factors Q, P are symplectic, provided that the initial matrices Q_0, P_0 of the factorization $\mathcal{C}_0 = P_0 Q_0^{-1}$ are symplectic.

Proof. We again use (4.2) and Proposition 4.1 and compare the coefficients with respect to the spatial variable x. We have one degree of freedom and set, inspired by (3.3a),

$$\dot{q} = \langle \nabla_p h\rangle_u.$$

Now, the claim follows by a direct calculation. □

The equations of motion given in Theorem 4.2 are indeed a generalization of the magnetic ones derived in Theorem 3.1 as we verify next.

Corollary 4.3. *In the special space of the magnetic Hamiltonian given in (3.2) we rediscover the equations of motion (3.3). Moreover, if $\varepsilon \to 0$ and averages tend to point evaluations at the center point q, then the equations (3.4a) and (3.4b) tend to classical equations of motion for a general classical Hamiltonian function h.*

Proof. We have that

$$\langle \nabla_p h\rangle_u = p - \langle A\rangle_u, \quad \text{and} \quad -\langle \nabla_q h\rangle_u = -\mathrm{i}\varepsilon\langle J_A^T \nabla\rangle_u - \langle \nabla \widetilde{V}\rangle_u.$$

Furthermore, it is

$$\nabla^2 h(\cdot, q, p) = \begin{pmatrix} \nabla^2 \widetilde{V}(\cdot, q) - D^2_{A(\cdot,q),p} & -J_A^T \\ -J_A & \mathrm{Id} \end{pmatrix},$$

such that the trace part appearing in (3.4d) contains the terms

$$\begin{aligned} -\langle \nabla_{qq} h\rangle_u &= \langle D^2_{A,-\mathrm{i}\varepsilon\nabla}\rangle_u - \langle \nabla^2 \widetilde{V}\rangle_u, & -\langle \nabla_{qp} h\rangle_u \mathcal{C} &= \langle J_A^T\rangle_u \mathcal{C}, \\ -\mathcal{C}\langle \nabla_{pq} h\rangle_u &= \mathcal{C}\langle J_A\rangle_u, & -\mathcal{C}\langle \nabla_{pp} h\rangle_u \mathcal{C} &= -\mathcal{C}^2. \end{aligned}$$

For the scalar contribution of the projection Proposition 4.1 we observe by (4.1),

$$\begin{aligned} \langle h\rangle_u &= -\frac{\varepsilon^2}{2}\langle \Delta\rangle_u + \mathrm{i}\varepsilon\langle A\cdot\nabla\rangle_u + \langle \widetilde{V}\rangle_u \\ &= \frac{1}{2}|p|^2 + \frac{\varepsilon}{4}\mathrm{tr}\Big((\mathcal{C}_\mathrm{R}{}^2 + \mathcal{C}_\mathrm{I}{}^2)\mathcal{C}_\mathrm{I}^{-1}\Big) - \langle A^T\big(\mathcal{C}_\mathrm{R}(x-q) + p\big)\rangle_u + \langle \widetilde{V}\rangle_u. \end{aligned}$$

Finally, we calculate the following trace, appearing in (3.4d), as

$$-\mathrm{tr}\Big((\mathcal{C}_\mathrm{R}{}^2 + \mathcal{C}_\mathrm{I}{}^2)\mathcal{C}_\mathrm{I}^{-1}\Big) + \mathrm{tr}\Big(\mathcal{C}^2\mathcal{C}_\mathrm{I}^{-1}\Big) = -2\,\mathrm{tr}(\mathcal{C}_\mathrm{I}) + 2\mathrm{i}\,\mathrm{tr}(\mathcal{C}_\mathrm{R}) = 2\mathrm{i}\,\mathrm{tr}(\mathcal{C}),$$

such that, together with

$$p^T \langle \nabla_p h \rangle_u = |p|^2 - p^T \langle A \rangle_u,$$

we obtain the differential equation (3.3d). □

5. L^2-error bound: proof of Lemma 3.7 and Theorem 3.8

This section is devoted to the wellposedness of the equations of motion (3.3) and the approximation quality of the variational solution in the L^2-norm.

We first state the following lemma which will be used frequently to obtain error bound with respect to ε. We recall that the lower bound on the eigenvalues of $\mathcal{C}_\mathrm{I}$ was denoted by $\rho > 0$.

Lemma 5.1 ([24, Lemma 3.8]). *For any $m \geq 0$ there exists a constant c_m such that for all $\varepsilon > 0$ it holds*

$$(\pi\varepsilon)^{-\frac{d}{4}} \det(\mathcal{C}_\mathrm{I})^{\frac{1}{4}} \Big(\int |x|^{2m} \exp\big(-\frac{1}{\varepsilon} x^T \mathcal{C}_\mathrm{I} x \big) \,\mathrm{d}x \Big)^{\frac{1}{2}} \leq c_m \Big(\frac{\varepsilon}{\rho} \Big)^{\frac{m}{2}},$$

where c_m is independent of ε and ρ.

We now prove the wellposedness result for (3.3) and show the boundedness of the parameters solving (3.3).

Proof of Lemma 3.7. We show that the right-hand side of (3.3) satisfies a local Lipschitz condition with Lipschitz constant independent of ε. To this end it is sufficient if the derivatives with respect to parameters $q, p, \mathcal{C}_\mathrm{R}, \mathcal{C}_\mathrm{I}, \zeta$ are bounded on a bounded domain. Then, we obtain a local solution and, as in Section 3.2, we can show that there is no blow-up.

The potentials in the averages of the equations of motion in (3.3) do not depend on ε. However, we need to carefully treat the absolute values of the Gaussian wave packet, since they contain ε in the denominator. By the chain rule, it is sufficient to first calculate the derivatives of averages of some arbitrary potential $\widehat{U}$, which is independent of the parameters. Then, the average has the form

$$\langle \widehat{U} \rangle_u = \frac{\sqrt{\det(\mathcal{C}_\mathrm{I})}}{(\pi\varepsilon)^{\frac{d}{2}}} \int \widehat{U}(x) \exp\left(-\frac{1}{\varepsilon} (x-q)^T \mathcal{C}_\mathrm{I} (x-q) \right) \mathrm{d}x,$$

from which we see that, in this case, the average only depends on q and $\mathcal{C}_\mathrm{I}$. Let u be a Gaussian wave packet with $\|u\|_{L^2} = 1$. By (4.3) we obtain

$$\begin{aligned}
&\frac{\sqrt{\det(\mathcal{C}_\mathrm{I})}}{(\pi\varepsilon)^{\frac{d}{2}}} \, \partial_q \exp\left(-\frac{1}{\varepsilon} (x-q)^T \mathcal{C}_\mathrm{I} (x-q) \right) \\
&= \frac{\sqrt{\det(\mathcal{C}_\mathrm{I})}}{(\pi\varepsilon)^{\frac{d}{2}}} \, \frac{2}{\varepsilon} \mathcal{C}_\mathrm{I}(x-q) \exp\left(-\frac{1}{\varepsilon} (x-q)^T \mathcal{C}_\mathrm{I} (x-q) \right) \\
&= -\nabla |u(x)|^2,
\end{aligned}$$

thus, using integration by parts, the derivative of the average with respect to to q is given by

$$\partial_q \langle \widehat{U}(x) \rangle_u = \langle \nabla \widehat{U}(x) \rangle_u.$$

We continue with derivatives with respect to $\mathcal{C}_\mathrm{I}$. For a differentiable matrix function $F : \mathbb{R}^{d\times d} \to \mathbb{R}$ and a general invertible, symmetric matrix $M = (m_{ij})_{i,j=1,\dots,d}$ we define the componentwise derivation matrix

$$\partial_M F(M) \coloneqq (\partial_{m_{ij}} F(M))_{i,j=1,\dots,d} \in \mathbb{R}^{d\times d}.$$

By [22, Part 0.8.10] we have

$$\partial_M a^T M b = ab^T \quad \text{ and } \quad \partial_M \det(M) = \det(M) M^{-1}$$

and consequently,

$$\partial_M \sqrt{\det(M)} = \frac{1}{2}\sqrt{\det(M)} M^{-1}.$$

Hence, it follows that

$$\partial_{\mathcal{C}_\mathrm{I}} \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I}(x-q)\right) = -\frac{1}{\varepsilon}(x-q)(x-q)^T \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I}(x-q)\right)$$

and

$$\partial_{\mathcal{C}_\mathrm{I}} \langle \widehat{U}(x)\rangle_u = -\frac{1}{\varepsilon}\big\langle (x-q)(x-q)^T \widehat{U}(x)\big\rangle_u + \frac{1}{2} I^{-1}\big\langle \widehat{U}(x)\big\rangle_u.$$

By Lemma 5.1 we have $\big|\big\langle (x-q)(x-q)^T \widehat{U}(x)\big\rangle_u\big| \le C\varepsilon$ for parameters on a bounded domain.

For potentials depending on the parameters, we use again that we are on a bounded domain and that the dependence on ε of the potentials in (3.3) is such that ε does not enter the denominator. □

We now turn to the L^2-error bound and adapt the proof of [24, Theorem 3.5] to the magnetic case and note that the multiplication potential $\widetilde{V}$ is already covered. In order to demonstrate the dependence of the constant in the error bound, we carry out the proof for the advection term.

Proof of Theorem 3.8. From the proof of [24, Theorem 3.5] we know that

$$\big\|\psi(t) - u(t)\big\|_{L^2} \le \int_0^t \frac{1}{\varepsilon}\big\|Hu - P_u(Hu)\big\|_{L^2}\,\mathrm{d}s.$$

(a) We write the action of the magnetic Schrödinger operator H on a Gaussian u with width $\mathcal{C}$ and phase space center (q, p) as

$$Hu = -\frac{\varepsilon^2}{2}\Delta u + Yu + \widetilde{V}u$$

with

$$Y_u \coloneqq -A\cdot(\mathcal{C}(x-q)+p). \tag{5.1}$$

We perform a second order Taylor expansion of the potentials Y_u and $\widetilde{V}$ around the point q and denote by W_q and $\widetilde{W}_q$ the respective remainders. Then,

$$(\mathrm{Id} - P_u)(Hu) = (\mathrm{Id} - P_u)(W_q u + \widetilde{W}_q u)$$

and

$$\big\|\psi(t) - u(t)\big\|_{L^2} \le \int_0^t \frac{1}{\varepsilon}\big\|W_q u + \widetilde{W}_q u\big\|_{L^2}\,\mathrm{d}s.$$

Since

$$W_q = \frac{1}{2}\sum_{|\alpha|=3}(x-q)^\alpha \int_0^1 (1-\theta)^2 \partial^\alpha Y_u\big(q + \theta(x-q)\big)\mathrm{d}\theta,$$

we bound $\left\|W_q u\right\|_{L^2}$ by finding a bound on $\partial^\alpha Y_u\big(q+\theta(x-q)\big)$, which then leads us to

$$|W_q(x)|^2 \le C|x-q|^6.$$

By norm conservation and Lemma 5.1 the claim that $\left\|W_q u\right\|_{L^2} = \mathcal{O}(\varepsilon^{3/2})$ follows. For the third derivative of $\partial_{lmn}Y_u$ where $l,m,n = 1,\dots,d$, we have

$$\begin{aligned}\partial_{lmn}Y_u &= (\partial_{lmn}A)^T\mathcal{C}(x-q) + (\partial_{lmn}A)^T p\\ &\quad + \big((\partial_{lm}A)^T\mathcal{C}\big)_n + \big((\partial_{ln}A)^T\mathcal{C}\big)_m + \big((\partial_{mn}A)^T\mathcal{C}\big)_l,\end{aligned} \tag{5.2}$$

where $\partial_{lmn}A$ is meant component wise. The term $x-q$ in (5.2) evaluated at $x = q+\theta(x-q)$ has the form

$$\theta(\partial_{lmn}A)^T\mathcal{C}(x-q).$$

By Lemma 5.1 we gain additional orders of ε, and we thus neglect the first summand in (5.2). The remaining terms are bounded again using Lemma 5.1.

(b) In the general subquadratic case, we use that the action of a semiclassical pseudodifferential operator on a Gaussian wave packet can be approximated by a polynomial prefactor, see [30, Lemma 14 in §2.3]. For any $\ell \in \mathbb{N}$ there exists a polynomial $\mathcal{Q}_\ell$ of degree ℓ, such that

$$Hu = \mathcal{Q}_\ell\, u + \mathcal{O}(\varepsilon^{(\ell+1)/2}),$$

i.e., we have

$$Hu - P_u(Hu) = W_{u,\ell}\, u + \mathcal{O}(\varepsilon^{(\ell+1)/2}), \tag{5.3}$$

with a remainder potential $W_{u,\ell}$. We now fix $\ell = 2$ and denote the corresponding cubic remainder potential $W_u = W_{u,2}$. The proof then works along the lines of the magnetic case. $\square$

6. Expectation values: proof of Lemma 3.6

In this section we adapt the proofs of [24, Section 3.2] on conservation properties to the time-dependent, magnetic case. Due to time-dependence, the energy will not be a conserved quantity.

Let ψ be the exact solution of (1.1a) and u the variational solution (2.4) such that (3.1) holds.

Proof of Lemma 3.6. The proof of norm conservation and the energy formula can be done in the same way as in [24]. We only show the conservation of total linear and angular momentum.

By [25, Theorem 1.3] or [9, Lemma 4.1] it is sufficient to show that $H(t)$ commutes with P and L, respectively, for each $t \in [0,T]$. By [24] it follows that $\mathcal{P}A_{k_j} = 0$ for all $k \in \{1,\dots,N\}$ and $j \in \{1,2,3\}$. We further calculate

$$\mathcal{P}(A\cdot\nabla)\psi = \sum_{k=1}^{N}\sum_{j=1}^{3}(\mathcal{P}A_{k_j})\partial_{k_j}\psi + A_{k_j}\mathcal{P}\partial_{k_j}\psi = (A\cdot\nabla)\mathcal{P}\psi.$$

Furthermore, a tedious calculation shows that $(A\cdot\nabla)\mathcal{L}\psi = \mathcal{L}(A\cdot\nabla)\psi$ if and only if

$$\sum_{l=1}^{N}\begin{pmatrix}A_{l_2}\partial_{l_3} - A_{l_3}\partial_{l_2}\\ A_{l_3}\partial_{l_1} - A_{l_1}\partial_{l_3}\\ A_{l_1}\partial_{l_2} - A_{l_2}\partial_{l_1}\end{pmatrix}\psi = \sum_{k=1}^{N}\sum_{j=1}^{3}\sum_{l=1}^{N}\begin{pmatrix}x_{l_2}(\partial_{l_3}A_{k_j})\partial_{k_j} - x_{l_3}(\partial_{l_2}A_{k_j})\partial_{k_j}\\ x_{l_3}(\partial_{l_1}A_{k_j})\partial_{k_j} - x_{l_1}(\partial_{l_3}A_{k_j})\partial_{k_j}\\ x_{l_1}(\partial_{l_2}A_{k_j})\partial_{k_j} - x_{l_2}(\partial_{l_1}A_{k_j})\partial_{k_j}\end{pmatrix}\psi$$

holds true. This condition is fulfilled if

$$\partial_{l_m} A_{k_j} = \alpha \delta_{l_m, k_j} \quad \text{und} \quad A_{l_n} = \alpha x_{l_n}$$

holds true for some $\alpha \in \mathbb{R}$, $j, n, m \in \{1, 2, 3\}$, and $k, l \in \{1, \dots, N\}$ and thus, if $A(\cdot, x) = \alpha(\cdot)x$ holds. □

7. Error bound for averages of observables: proof of Theorem 3.10

In this section we give the proof of Theorem 3.10. We proceed in three steps: First, we follow [24, Section 6.7] and establish an integral representation for the error that involves a commutator with the time-evolved observable. Second, we prove Egorov's theorem for the time-evolution of observables in the general context of magnetic Schrödinger operators. Third, we derive a semiclassical expansion of averages with respect to Gaussian wave packets. The combination of these steps then allows us to prove Theorem 3.10. We note that the semiclassical expansion of the averages is crucial for improving the observable estimate in [24, Theorem 3.5]. This section applies for both the magnetic and the general subquadratic hamiltonian case. For better readability, some arguments will be provided for the magnetic case only, but with natural slight modifications they also apply for the general subquadratic case.

7.1. Error representation.

We start with a useful a posteriori representation for the observable error. To this end, let $U(t, s)$ be the evolution family given by Theorem 2.2 and $\mathbf{A}$ an observable. We introduce the notation

$$\widetilde{\mathbf{A}}(t, s) \coloneqq U(s, t)\mathbf{A}U(t, s), \qquad t, s \in \mathbb{R}.$$

Lemma 7.1. *Let ψ be the solution of (1.1a) and u the solution of (2.4). If the initial value $\psi_0 = u_0 \in \mathcal{M}$ is a Gaussian wave packet with $\|u_0\|_{L^2} = 1$, then the error of the observables takes the form*

$$\begin{aligned} &\langle \psi(t) | \mathbf{A}\psi(t) \rangle - \langle u(t) | \mathbf{A}u(t) \rangle \\ &= \int_0^t \frac{1}{\mathrm{i}\varepsilon} \langle u(s) \Big| \left(\overline{W}_{u(s)} \widetilde{\mathbf{A}}(t, s) - \widetilde{\mathbf{A}}(t, s) W_{u(s)} \right) u(s) \rangle \, \mathrm{d}s, \end{aligned} \tag{7.1}$$

where the remainder potential $W_u : \mathbb{R}^d \to \mathbb{C}$ depends on the Gaussian wave packet u. In the general subquadratic case, it has been previously defined in (5.3). In the magnetic Schrödinger case, it satisfies

$$\begin{aligned} W_u = X_u(q) - \langle X_u \rangle_u + \frac{\varepsilon}{4} \mathrm{tr}({\mathcal{C}_{\mathrm{I}}}^{-1} \langle \nabla^2 X_u \rangle_u) + (\nabla X_u(q) - \langle \nabla X_u \rangle_u)^T (x - q) \\ + \frac{1}{2}(x - q)^T \left(\nabla^2 X_u(q) - \langle \nabla^2 X_u \rangle_u \right) (x - q) + R(X_u), \end{aligned} \tag{7.2}$$

with $X_u = Y_u + \widetilde{V}$ defined in (5.1) and (2.1), respectively, and $R(X_u)$ being the remainder potential of the quadratic Taylor expansion of X_u around the point q. For the non-magnetic Schrödinger case $A = 0$, we have $Y_u = 0$ and $W_u : \mathbb{R}^d \to \mathbb{R}$.

Proof. Let $U(t,s)$ be the evolution family, such that the exact solution of (1.1a) is given by (2.2). Using $\psi_0 = u_0$ and $U(t,t) = \mathrm{Id}$ we calculate

$$\begin{aligned}
&\langle u(t)|\mathbf{A}u(t)\rangle - \langle \psi(t)|\mathbf{A}\psi(t)\rangle \\
&\qquad = \langle u(t)|U(t,t)\mathbf{A}U(t,t)u(t)\rangle - \langle U(t,0)u(0)|\mathbf{A}U(t,0)u(0)\rangle \\
&\qquad = \langle u(t)|U(t,t)\mathbf{A}U(t,t)u(t)\rangle - \langle u(0)|U(0,t)\mathbf{A}U(t,0)u(0)\rangle \\
&\qquad = \int_0^t \frac{\partial}{\partial s}\langle u(s)|\underbrace{U(s,t)\mathbf{A}U(t,s)}_{=\widetilde{\mathbf{A}}(t,s)}u(s)\rangle \,\mathrm{d}s.
\end{aligned}$$

Employing the differential properties of the evolution family, that is, $\mathrm{i}\varepsilon\partial_t U(t,s) = H(t)U(t,s)$ and $-\mathrm{i}\varepsilon\partial_t U(s,t) = U(s,t)H(t)$, we obtain

$$\begin{aligned}
\frac{\partial}{\partial s}\widetilde{\mathbf{A}}(t,s) &= \frac{1}{\mathrm{i}\varepsilon}\big(H(s)U(s,t)\mathbf{A}U(t,s) - U(s,t)\mathbf{A}U(t,s)H(s)\big) \\
&= \frac{1}{\mathrm{i}\varepsilon}\big(H(s)\widetilde{\mathbf{A}}(t,s) - \widetilde{\mathbf{A}}(t,s)H(s)\big).
\end{aligned} \tag{7.3}$$

Since the variational evolution satisfies $\mathrm{i}\varepsilon\partial_t u(t) = P_{u(t)}H(t)u(t)$, we then have

$$\begin{aligned}
\frac{\partial}{\partial s}\langle u(s)|\widetilde{\mathbf{A}}(t,s)u(s)\rangle = \frac{1}{\mathrm{i}\varepsilon}\Big(&\langle(\mathrm{Id} - P_{u(s)})H(s)u(s)|\widetilde{\mathbf{A}}(t,s)u(s)\rangle\Big) \\
&-\langle u(s)|\widetilde{\mathbf{A}}(t,s)(\mathrm{Id} - P_{u(s)})H(s)u(s)\rangle\Big).
\end{aligned}$$

We arrive at (7.1), using that

$$(\mathrm{Id} - P_{u(s)})H(s)u(s) = X_{u(s)}u(s) - P_{u(s)}(X_{u(s)}u(s)) = W_{u(s)}u(s).$$

The claimed form of the remainder potential $W_{u(s)} : \mathbb{R}^d \to \mathbb{C}$ follows from [24, Proposition 3.14], since the proof of the projection formula there also applies for the potential function $X_{u(s)}$ even though it is complex-valued. □

7.2. **Egorov's theorem.** Further, to prove Theorem 3.10 we have to establish a variant of Egorov's theorem, which connects the time-evolved quantum observable $\widetilde{\mathbf{A}}(t,s)$, in case it originates from a Weyl-quantized $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$, with the evolution map of the classical Hamiltonian system. Recall that since A and $\widetilde{V}$ are sublinear and subquadratic, respectively, we obtain a unique global solution to the ordinary differential equation (3.10). We denote by

$$\Phi^{t,s} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}, \quad (\widetilde{q}_s, \widetilde{p}_s) \mapsto (\widetilde{q}_s(t), \widetilde{p}_s(t))$$

the classical propagator, which maps initial values at time s to the solution of (3.10) at time t. For any $\widetilde{z} = (\widetilde{q}, \widetilde{p})$, it satisfies the evolution equation

$$\begin{aligned}
\partial_t \Phi^{t,s}(\widetilde{z}) &= -J(\nabla_{\widetilde{z}} h)(t, \Phi^{t,s}(\widetilde{z})), \\
\Phi^{s,s}(\widetilde{z}) &= \widetilde{z}.
\end{aligned} \tag{7.4}$$

Both in the magnetic and the general subquadratic case, the classical propagator $\Phi^{t,\tau}$ is a diffeomorphism with inverse $(\Phi^{t,\tau})^{-1} = \Phi^{\tau,t}$. For time-independent, subquadratic Hamiltonians it is well-established that

$$\widetilde{\mathbf{A}}(t,0) = \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a} \circ \Phi^{t,0}\right) + \mathcal{O}(\varepsilon^2).$$

However, to the best of our knowledge, in the literature a proof of the Egorov approximation for the non-autonomous case is not available, and the proofs presented for example in [4], [36, Chapter 11], or [30, Thm. 12] assume time-independent or compactly supported Hamiltonians and thus do not cover our more general situation. The main difficulties are the time-dependence of the Hamiltonian operator $H(t)$, which prevents energy conservation, and the allowed sublinear growth of the observables.

Proposition 7.2 (time-dependent Egorov–theorem)**.** *Let* $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ *be a quantum observable stemming from a smooth, sublinear classical observable* $\boldsymbol{a}$ *in the sense of Definition 3.9. Further, let* $\widetilde{\boldsymbol{a}} : \mathbb{R}\times\mathbb{R}\times\mathbb{R}^{2d} \to \mathbb{R}$, $(t,s,\widetilde{z}) \mapsto \widetilde{\boldsymbol{a}}(t,s,\widetilde{z})$ *be defined by*

$$\widetilde{\boldsymbol{a}}(t,s,\widetilde{z}) = \boldsymbol{a} \circ \Phi^{t,s}(\widetilde{z}). \tag{7.5}$$

We consider two cases.

(a) *The Hamiltonian operator stems from a classical, subquadratic function h. Then, the observable given in (7.5) is sublinear and for all $\varphi \in L^2(\mathbb{R}^d)$ we have*

$$\left\| \big(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)\big)\varphi \right\|_{L^2} \le C\,\varepsilon^2\,\mathrm{e}^{C|t-s|}\,\|\varphi\|_{L^2}$$

for all $s,t\in\mathbb{R}$.

(b) *The Hamiltonian operator is a magnetic Schrödinger operator. We assume that the observable given in (7.5) is of time-exponential growth in the following sense. There exists a smooth nonnegative function $\Gamma(t,s)\ge 0$ such that for any $\alpha\in\mathbb{N}^{2d}$ there exists $C_\alpha>0$ with*

$$|\partial^\alpha_{\widetilde{z}}\widetilde{\boldsymbol{a}}(t,s,\widetilde{z})| \le C_{\boldsymbol{a},\alpha}\ \exp(|\alpha|\,\Gamma(t,s))$$

for all $\widetilde{z}\in\mathbb{R}^{2d}$ and all $t,s\in\mathbb{R}$. Then, for any $\varphi\in L^2(\mathbb{R}^d)$ such that $\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})\varphi \in L^2(\mathbb{R}^d)$, we then have

$$\left\| \Big(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)\varphi\Big) \right\|_{L^2} \le C\,\varepsilon^2\,\mathrm{e}^{C|t-s|}\,\left\|\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})\varphi\right\|_{L^2},$$

for all $s,t\in\mathbb{R}$.

The constant $C>0$ depends on derivative bounds of the potentials A, V and the observable $\boldsymbol{a}$, but not on ε,t,s. In particular, $C=0$ for A linear and V quadratic.

Proof. (1) We start by discussing the growth of the function $\widetilde{\boldsymbol{a}}(t,s,\widetilde{z})$ for case (a). For first order derivatives with respect to $(\widetilde{q},\widetilde{p})$ of the classical propagator we have

$$D\Phi^{t,s} = \mathrm{Id} + J^{-1}\int_s^t \nabla^2 h(\tau,\Phi^{\tau,s})\,D\Phi^{\tau,s}\,\mathrm{d}\tau,$$

and thus

$$\left\|D\Phi^{t,s}\right\|_\infty \le 1 + \int_s^t \sup_{\widetilde{z}\in\mathbb{R}^{2d}} \|\nabla^2_{\widetilde{z}} h(\tau,\widetilde{z})\|\,\|D\Phi^{\tau,s}\|_\infty\ \mathrm{d}\tau.$$

Since the Hamiltonian function $h(t,\cdot)$ is subquadratic, we have

$$\Gamma(t,s) \coloneqq \int_s^t \sup_{\widetilde{z}\in\mathbb{R}^{2d}} \|\nabla^2_{\widetilde{z}} h(\tau,\widetilde{z})\|\mathrm{d}\tau < \infty,$$

and by Gronwall's lemma

$$\left\|D\Phi^{t,s}\right\|_\infty \le \exp(\Gamma(t,s)).$$

Moreover, for any $\alpha \in \mathbb{N}^{2d}$ with $|\alpha| \geq 1$ there exists a constant $C_\alpha > 0$ such that

$$|\partial_{\widetilde{z}}^\alpha \Phi^{t,s}(\widetilde{z})| \leq C_\alpha \exp(|\alpha|\,\Gamma(t,s))$$

for all $t, s \in \mathbb{R}$ and all $\widetilde{z} \in \mathbb{R}^{2d}$, see [4, Lemma 2.2] for a proof that literally applies to the non-autonomous case. Then, the same argument as for [4, Lemma 2.4] yields that for every $\alpha \in \mathbb{N}^{2d}$ with $|\alpha| \geq 1$ there exists a constant $C_{\boldsymbol{a},\alpha} > 0$ such that

$$|\partial_{\widetilde{z}}^\alpha \widetilde{\boldsymbol{a}}(t,s,\widetilde{z})| \leq C_{\boldsymbol{a},\alpha}\ \exp(|\alpha|\,\Gamma(t,s))$$

for all $t, s \in \mathbb{R}$ and all $\widetilde{z} \in \mathbb{R}^{2d}$. In particular, $\widetilde{\boldsymbol{a}}(t,s,\cdot)$ is sublinear.

(2) Next we compare the operators $\mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}}(t,s))$ and $\widetilde{\mathbf{A}}(t,s) = U(s,t)\mathbf{A}U(t,s)$. Since on the diagonal $\widetilde{\boldsymbol{a}}(t,t,\cdot) = \boldsymbol{a}$ and $U(s,s) = \mathrm{Id}$, we obtain similarly as for (7.3)

$$\begin{aligned}
&\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\,(\widetilde{\boldsymbol{a}}(t,s)) \\
&= \int_s^t U(s,\tau)\Big(\frac{\mathrm{i}}{\varepsilon}\big[H(\tau), \mathrm{op}_{\mathrm{Weyl}}\,(\widetilde{\boldsymbol{a}}(t,\tau))\,\big] + \mathrm{op}_{\mathrm{Weyl}}\,(\partial_\tau \widetilde{\boldsymbol{a}}(t,\tau))\,\Big)U(\tau,s)\,\mathrm{d}\tau \\
&= \int_s^t U(s,\tau)\Big(\mathrm{op}_{\mathrm{Weyl}}(\{h(\tau), \widetilde{\boldsymbol{a}}(t,\tau)\}) + \mathrm{op}_{\mathrm{Weyl}}\,(\partial_\tau \widetilde{\boldsymbol{a}}(t,\tau))\,\Big)U(\tau,s)\,\mathrm{d}\tau + \rho(t,s),
\end{aligned}$$

where the last equation relies on the product rule of Weyl quantization [30, Theorem]. Here,

$$\{h(\tau), \widetilde{\boldsymbol{a}}(t,\tau)\} = \nabla_{\widetilde{z}} h(\tau) \cdot J \nabla_{\widetilde{z}} \widetilde{\boldsymbol{a}}(t,\tau)$$

denotes the Poisson bracket of $h(\tau)$ and $\widetilde{\boldsymbol{a}}(t,\tau)$. It remains to show that the integral vanishes and that the remainder $\rho(t,s)$ is of order ε^2.

(3) For the estimation of the remainder, we use that

$$\rho(t,s) = \varepsilon^2 \int_s^t U(s,\tau)\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{r}(t,\tau))U(\tau,s)\,\mathrm{d}\tau,$$

where $\boldsymbol{r}(t,\tau,\cdot)$ is a smooth function depending on the derivatives of the order ≥ 3 of the function $h(\tau,\cdot)$ and of the sublinear $\widetilde{\boldsymbol{a}}(t,\tau,\cdot)$. In order to estimate

$$\big\|\rho(t,s)\varphi\big\|_{L^2} \leq \varepsilon^2 \int_s^t \big\|\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{r}(t,\tau))U(\tau,s)\varphi\big\|_{L^2}\,\mathrm{d}\tau,$$

we investigate the above integrand.

(i) If h is subquadratic, then, due to the estimates given in (a), for all $\alpha \in \mathbb{N}_0^{2d}$ there exist $c_{1,\alpha}, c_{2,\alpha} > 0$ such that

$$|\partial_{\widetilde{z}}^\alpha \boldsymbol{r}(t,\tau,\widetilde{z})| \leq c_{1,\alpha} \exp(c_{2,\alpha}|t-\tau|)$$

for all $t, \tau \in \mathbb{R}$ and $\widetilde{z} \in \mathbb{R}^{2d}$, and the Calderón–Vaillancourt Theorem, see e.g. [30, Theorem 4], provides the claimed constant $C > 0$ for part (a).

(ii) In the magnetic case, we rewrite the remainder function

$$\boldsymbol{r}(\widetilde{q},\widetilde{p}) = \boldsymbol{r}(\cdot,\cdot,\widetilde{q},\widetilde{p}) = \boldsymbol{b}_0(\widetilde{q},\widetilde{p}) + \boldsymbol{b}(\widetilde{q},\widetilde{p})^T\widetilde{p},$$

where $\boldsymbol{b}_0 : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$ and $\boldsymbol{b} : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}^d$ are bounded with all their derivatives. For the first summand, we proceed as in the subquadratic case, using Calderón–Vaillancourt. For the second summand containing an unbounded linearity in $\widetilde{p}$, we use the product rule and obtain that

$$\mathrm{op}_{\mathrm{Weyl}}\big(\boldsymbol{r}_2(\widetilde{q},\widetilde{p})\big) = -\mathrm{op}_{\mathrm{Weyl}}\big(\boldsymbol{b}(\widetilde{q},\widetilde{p})\big) \cdot \mathrm{i}\varepsilon\nabla + \mathcal{O}(\varepsilon).$$

Then, the boundedness of $\boldsymbol{b}$ provides $C_{\boldsymbol{b}} > 0$ such that

$$\big\|\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{b}(t,\tau))\varepsilon\nabla\big(U(\tau,s)\varphi\big)\big\|_{L^2} \le C_{\boldsymbol{b}}\,\big\|\varepsilon\nabla\big(U(\tau,s)\varphi\big)\big\|_{L^2}.$$

In the next step, we analyse $\big\|\varepsilon\nabla\big(U(\tau,s)\varphi\big)\big\|_{L^2}$.

(4) Let $t \ge s$ and set $f(t) = \mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})U(t,s)\varphi$. We argue as in the proof for [5, Lemma 10.4] and observe that $f(t)$ solves the perturbed magnetic Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t f(t) = \mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})H(t)U(t,s)\varphi = H(t)f(t) + \delta(t)$$

with source term

$$\delta(t) = [\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z}), H(t)]U(t,s)\varphi = \frac{\varepsilon}{\mathrm{i}}\begin{pmatrix} \mathrm{op}_{\mathrm{Weyl}}(\widetilde{p} - A(\widetilde{q})) \\ \mathrm{op}_{\mathrm{Weyl}}\big(\nabla\widetilde{V}(\widetilde{q}) - \nabla A(\widetilde{q})\cdot\widetilde{p}\big)\end{pmatrix} U(t,s)\varphi,$$

where we used the product rule for the second equation. In the same spirit as in step (3), we estimate

$$\big\|\delta(t)\big\|_{L^2} \le C\varepsilon\big\|\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})U(t,s)\varphi\big\|_{L^2} = C\varepsilon\big\|f(t)\big\|_{L^2},$$

where we exploited the sublinearity of A and that $\widetilde{V}$ is subquadratic. By the variation of constants formula followed by Gronwall's lemma, we obtain that

$$\big\|f(t)\big\|_{L^2} \le \mathrm{e}^{C(t-s)}\big\|f(s)\big\|_{L^2} = \mathrm{e}^{C(t-s)}\big\|\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})\varphi\big\|_{L^2}.$$

(5) In the following step we show that $\widetilde{\boldsymbol{a}}$ satisfies the transport equation

$$\partial_\tau\widetilde{\boldsymbol{a}}(t,\tau) = -\{h(\tau), \widetilde{\boldsymbol{a}}(t,\tau)\}, \tag{7.6a}$$
$$\widetilde{\boldsymbol{a}}(t,t) = \boldsymbol{a} \tag{7.6b}$$

for $\tau \in [s,t]$. Then the integrand in question indeed vanishes, and we obtain

$$\widetilde{\mathbf{A}}(t,s) = \mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}}(t,s)) + \mathcal{O}(\varepsilon^2),$$

as claimed. We rewrite the transport equation (7.6) as

$$\begin{aligned} \partial_\tau\widetilde{\boldsymbol{a}}(t,\tau) &= J\nabla_{\widetilde{z}}h(\tau)\cdot\nabla_{\widetilde{z}}\widetilde{\boldsymbol{a}}(t,\tau), \\ \widetilde{\boldsymbol{a}}(t,t) &= \boldsymbol{a}. \end{aligned} \tag{7.7}$$

The following argument crucially uses that $\Phi^{t,\tau}$ is a diffeomorphism with inverse $(\Phi^{t,\tau})^{-1} = \Phi^{\tau,t}$. We observe that $\widetilde{\boldsymbol{a}}(t,\tau,\Phi^{\tau,t}(\widetilde{z})) = \boldsymbol{a}(\widetilde{z})$ for all $\widetilde{z} \in \mathbb{R}^{2d}$ and calculate

$$\begin{aligned} 0 &= \partial_\tau\boldsymbol{a}(\widetilde{z}) \\ &= \partial_\tau\widetilde{\boldsymbol{a}}(t,\tau,\Phi^{\tau,t}(\widetilde{z})) \\ &= (\partial_\tau\widetilde{\boldsymbol{a}})(t,\tau,\Phi^{\tau,t}(\widetilde{z})) - J(\nabla_{\widetilde{z}}h)(\tau,\Phi^{\tau,t}(\widetilde{z}))\cdot(\nabla_{\widetilde{z}}\widetilde{\boldsymbol{a}})(t,\tau,\Phi^{\tau,t}(\widetilde{z})), \end{aligned}$$

where, we used in the last step, the chain rule and (7.4). Since $\Phi^{\tau,t}$ is a diffeomorphism, this proves that $\widetilde{\boldsymbol{a}}(t,\tau)$ indeed solves the transport equation (7.7). $\square$

7.3. **Averages with respect to Gaussian wave packets.** The a posteriori error representation of Lemma 7.1 involves an average with respect to the variational solution. By Egorov's theorem, Proposition 7.2, the time-evolved quantum observable can be approximated by the Weyl-quantized classical observable evolved along the classical flow. We therefore derive an asymptotic expansion of averages of Weyl-quantized operators with respect to Gaussian wave packets. For obtaining this expansion, the following phase space moments will be useful.

Lemma 7.3 (Gaussian moments)**.** *We consider a Gaussian $u \in \mathcal{M}$ of unit norm, $\|u\| = 1$, with phase space center $z = (q,p) \in \mathbb{R}^{2d}$ and width matrix $\mathcal{C} \in \mathbb{C}^{d\times d}$. We denote by*

$$\rho_\ell(\mathcal{C}) = \pi^{-d} \int_{\mathbb{R}^{2d}} \widetilde{z}^\ell \exp(-\widetilde{z}\cdot G\widetilde{z})\,\mathrm{d}\widetilde{z} \qquad \textit{with} \qquad G = \begin{pmatrix} \mathcal{C}_\mathrm{I} + \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\mathcal{C}_\mathrm{R} & -\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1} \\ \mathcal{C}_\mathrm{I}^{-1}\mathcal{C}_\mathrm{R} & \mathcal{C}_\mathrm{I}^{-1} \end{pmatrix},$$

where $G \in \mathbb{R}^{2d\times 2d}$ is symmetric, positive definite and symplectic. Then, for any multi-index $\ell = (\ell_1,\dots,\ell_{2d}) \in \mathbb{N}_0^{2d}$, we have

$$\langle(\widetilde{z}-z)^\ell\rangle_u = \varepsilon^{|\ell|/2}\rho_\ell(\mathcal{C}).$$

If the length $|\ell|$ of the multi-index is odd, then we have $\langle(\widetilde{z}-z)^\ell\rangle_u = 0$.

Proof. The claimed representation becomes evident, when using the Wigner function of the Gaussian wave packet u. The Wigner function of a Gaussian wave packet centered in z satisfies

$$\mathcal{W}_u(\widetilde{z}) = (\pi\varepsilon)^{-d}\exp(-\tfrac{1}{\varepsilon}(\widetilde{z}-z)\cdot G(\widetilde{z}-z)),$$

where the matrix G is symplectic, symmetric, positive definite, see [24, Proposition 6.15]. The average of any Weyl-quantized observable can be written as the phase space integral of the symbol versus the Wigner function, see for example [24, Theorem 6.5]. In particular,

$$\begin{aligned}\langle(\widetilde{z}-z)^\ell\rangle_u &= \int_{\mathbb{R}^{2d}} (\widetilde{z}-z)^\ell\,\mathcal{W}_u(\widetilde{z})\,\mathrm{d}\widetilde{z} \\ &= (\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} (\widetilde{z}-z)^\ell \exp(-\tfrac{1}{\varepsilon}(\widetilde{z}-z)\cdot G(\widetilde{z}-z))\,\mathrm{d}\widetilde{z} \\ &= \pi^{-d}\varepsilon^{|\ell|/2}\int_{\mathbb{R}^{2d}} \widetilde{z}^\ell\exp(-\widetilde{z}\cdot G\widetilde{z})\,\mathrm{d}\widetilde{z},\end{aligned}$$

where we have used that symplecticity implies $\det(G) = 1$. We observe, that if the length $|\ell|$ of the multi-index is odd, then the above integral vanishes, and consequently $\langle(\widetilde{z}-z)^\ell\rangle_u = 0$ as well. □

We now use these moments for expanding Gaussian averages with respect to general observables.

Proposition 7.4 (Gaussian averages)**.** *We consider a Gaussian $u \in \mathcal{M}$ of unit norm, $\|u\| = 1$, with phase space center $z = (q,p) \in \mathbb{R}^{2d}$ and complex width matrix $\mathcal{C} \in \mathbb{C}^{d\times d}$. Then, for any smooth function $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}$ with bounded sixth order derivatives,*

$$\langle\boldsymbol{a}\rangle_u = \boldsymbol{a}(z) + \varepsilon f_2(\boldsymbol{a},\mathcal{C}) + \varepsilon^2 f_4(\boldsymbol{a},\mathcal{C}) + \rho^\varepsilon(\boldsymbol{a},\mathcal{C}),$$

where

$$f_k(\boldsymbol{a},\mathcal{C}) = \sum_{|\ell|=k}\frac{1}{\ell!}\,\partial^\ell\boldsymbol{a}(z)\,\rho_\ell(\mathcal{C}), \qquad k = 2,4.$$

The second order contribution satisfies

$$f_2(\boldsymbol{a},\mathcal{C}) = \tfrac{1}{4}\mathrm{tr}(\nabla^2\boldsymbol{a}(z)_{\mathcal{C}}\,{\mathcal{C}_{\mathrm{I}}}^{-1})$$

with

$$\nabla^2\boldsymbol{a}(z)_{\mathcal{C}} = \begin{pmatrix}\mathrm{Id} & \mathcal{C}^*\end{pmatrix}\nabla^2\boldsymbol{a}(z)\begin{pmatrix}\mathrm{Id}\\ \mathcal{C}\end{pmatrix} \in \mathbb{C}^{d\times d}. \tag{7.8}$$

The remainder satisfies $|\rho^\varepsilon(\boldsymbol{a},\mathcal{C})| \le C\varepsilon^3$ *with a constant* $C>0$ *that only depends on sixth order derivatives of* $\boldsymbol{a}$ *as well as on the width matrix* $\mathcal{C}$.

Proof. We start by Taylor expanding the symbol around z with sixth order remainder,

$$\boldsymbol{a}(\widetilde{z}) = \sum_{|k|\le 5}\frac{1}{k!}\partial^k\boldsymbol{a}(z)(\widetilde{z}-z)^k + \boldsymbol{r}_6(\widetilde{z};z),$$

where

$$\boldsymbol{r}_6(\widetilde{z};z) = \sum_{|k|=6} r_k(\widetilde{z};z)(\widetilde{z}-z)^k, \qquad r_k(\widetilde{z};z) = \frac{6}{k!}\int_0^1 (1-\vartheta)^5\partial^k\boldsymbol{a}(z+\vartheta(\widetilde{z}-z))\,\mathrm{d}\vartheta.$$

We have

$$\langle \boldsymbol{r}_6(\widetilde{z};z)\rangle_u = \sum_{|k|=6}\int_{\mathbb{R}^{2d}} r_k(\widetilde{z};z)\,(\widetilde{z}-z)^k\,\mathcal{W}_u(\widetilde{z})\,\mathrm{d}\widetilde{z}.$$

Therefore, using Lemma 7.3,

$$\langle\boldsymbol{a}\rangle_u = \boldsymbol{a}(z) + \varepsilon f_2(\boldsymbol{a},\mathcal{C}) + \varepsilon^2 f_4(\boldsymbol{a},\mathcal{C}) + \langle \boldsymbol{r}_6(\widetilde{z};z)\rangle_u,$$

and, with the same substitution as in the proof of Lemma 7.3, we bound

$$|\langle \boldsymbol{r}_6(\widetilde{z};z)\rangle_u| \le C(\boldsymbol{a},\mathcal{C})\,\varepsilon^3 \quad \text{with} \quad C(\boldsymbol{a},\mathcal{C}) = \sum_{|k|=6}\|r_k(\cdot;z)\|_\infty\;|\rho_k(\mathcal{C})|\,.$$

The constant $C(\boldsymbol{a},\mathcal{C})>0$ depends on fourth order derivatives of $\boldsymbol{a}$ and on the width matrix $\mathcal{C}$. It remains to rewrite the second order contribution as

$$\begin{aligned} f_2(\boldsymbol{a},\mathcal{C}) &= \pi^{-d}\sum_{|\ell|=2}\frac{1}{\ell!}\partial^\ell\boldsymbol{a}(z)\int_{\mathbb{R}^{2d}}(G^{-1/2}\widetilde{z})^\ell\exp(-|\widetilde{z}|^2)\,\mathrm{d}\widetilde{z}\\ &= \frac{1}{2}\,\pi^{-d}\int_{\mathbb{R}^{2d}}\widetilde{z}\cdot G^{-1/2}\nabla^2\boldsymbol{a}(z)G^{-1/2}\widetilde{z}\;\exp(-|\widetilde{z}|^2)\,\mathrm{d}\widetilde{z}\\ &= \frac{1}{4}\,\mathrm{tr}(\nabla^2\boldsymbol{a}(z)G^{-1}). \end{aligned}$$

Since G is symplectic and symmetric, its inverse satisfies

$$G^{-1} = JGJ^{-1} = \begin{pmatrix}\mathcal{C}_{\mathrm{I}}^{-1} & \mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{R}}\\ \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1} & \mathcal{C}_{\mathrm{I}}+\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{R}}\end{pmatrix}.$$

We decompose the Hessian $\nabla^2\boldsymbol{a}(z)$ in block form as

$$\nabla^2\boldsymbol{a}(z) = \begin{pmatrix} A & B\\ B^T & D\end{pmatrix}. \tag{7.9}$$

Using the cyclicity of the trace, we calculate that

$$\begin{aligned}\mathrm{tr}(\nabla^2\boldsymbol{a}(z)G^{-1}) &= \mathrm{tr}((A+B\mathcal{C}_{\mathrm{R}}+\mathcal{C}_{\mathrm{R}}B^T+\mathcal{C}_{\mathrm{I}}D\mathcal{C}_{\mathrm{I}}+\mathcal{C}_{\mathrm{R}}D\mathcal{C}_{\mathrm{R}})\mathcal{C}_{\mathrm{I}}^{-1})\\ &= \mathrm{tr}(\nabla^2\boldsymbol{a}(z)_{\mathcal{C}}\,\mathcal{C}_{\mathrm{I}}^{-1}),\end{aligned}$$

where $\nabla^2 \boldsymbol{a}(z)_{\mathcal{C}}$ was defined in (7.8) and has the form

$$\nabla^2 \boldsymbol{a}(z)_{\mathcal{C}} = A + B\mathcal{C} + \mathcal{C}^* B^T + \mathcal{C}^* D\mathcal{C},$$

which gives the claim. □

For our analysis of the observable error, we will use Proposition 7.4 also for observables that are products of two functions. One of the factors will have a controlled semiclassical expansion, when evaluated in the position center of the variational solution.

Corollary 7.5 (Gaussian averages)**.** *In the situation of Proposition 7.4 applied to a sublinear classical observable $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}$, we additionally consider a smooth and subquadratic function $b^\varepsilon : \mathbb{R}^d \to \mathbb{R}$, $x \mapsto b^\varepsilon(x)$. Then,*

$$f_2(b^\varepsilon, \mathcal{C}) = \tfrac{1}{4}\mathrm{tr}(\nabla^2 b^\varepsilon(q) {\mathcal{C}_{\mathrm{I}}}^{-1}).$$

(a) If the function satisfies

$$b^\varepsilon(q), \nabla b^\varepsilon(q) = \mathcal{O}(\varepsilon),$$

then

$$\langle \boldsymbol{a} b^\varepsilon \rangle_u = \boldsymbol{a}(z)\,(b^\varepsilon(q) + \varepsilon f_2(b^\varepsilon, \mathcal{C})) + \mathcal{O}(\varepsilon^2).$$

(b) If the function satisfies

$$b^\varepsilon(q) = \mathcal{O}(\varepsilon^2), \quad \nabla b^\varepsilon(q), \nabla^2 b^\varepsilon(q) = \mathcal{O}(\varepsilon),$$

then

$$\begin{aligned}\langle \boldsymbol{a} b^\varepsilon \rangle_u = \boldsymbol{a}(z)\,&\big(b^\varepsilon(q) + \varepsilon f_2(b^\varepsilon, \mathcal{C}) + \varepsilon^2 f_4(b^\varepsilon, \mathcal{C})\big) \\ &+ \varepsilon F_{1,1}(\boldsymbol{a}, b^\varepsilon, \mathcal{C}) + \varepsilon^2 F_{1,3}(\boldsymbol{a}, b^\varepsilon, \mathcal{C}) + \mathcal{O}(\varepsilon^3)\end{aligned}$$

with

$$F_{1,n}(\boldsymbol{a}, b^\varepsilon, \mathcal{C}) = \sum_{|\ell|=n+1} \sum_{\beta \le \ell, |\beta|=1} \frac{1}{(\ell-\beta)!}\ \partial^\beta \boldsymbol{a}(z)\ \partial^{\ell-\beta} b^\varepsilon(q)\ \rho_\ell(\mathcal{C}), \quad n = 1, 3.$$

Proof. For the trace formula, it is enough to observe that the matrices B and D in the block matrix (7.9) vanish, since b^ε only depends on x.

For proving the expansions of the averages, we crucially use the Leibniz formula for the ℓth derivative of the product, that is,

$$\partial^\ell(\boldsymbol{a} b^\varepsilon)(z) = \sum_{\beta \le \ell} \binom{\ell}{\beta}\ \partial^\beta \boldsymbol{a}(z)\ \partial^{\ell-\beta} b^\varepsilon(q)$$

for any multi-index $\ell \in \mathbb{N}_0^{2d}$.

(a) In the situation of statement (a), we only consider $|\ell| = 2$ and obtain

$$\varepsilon \partial^\ell(\boldsymbol{a} b^\varepsilon)(z) = \varepsilon \boldsymbol{a}(z) \partial^\ell b^\varepsilon(q) + \mathcal{O}(\varepsilon^2).$$

Then, Proposition 7.4 implies

$$\begin{aligned}\langle \boldsymbol{a} b^\varepsilon \rangle_u &= \boldsymbol{a}(z) b^\varepsilon(q) + \varepsilon f_2(\boldsymbol{a} b^\varepsilon, \mathcal{C}) + \mathcal{O}(\varepsilon^2) \\ &= \boldsymbol{a}(z)\,(b^\varepsilon(q) + \varepsilon f_2(b^\varepsilon, \mathcal{C})) + \mathcal{O}(\varepsilon^2).\end{aligned}$$

(b) In the situation of statement (b), we aim for a higher order expansion and need to consider second and fourth derivatives. In the same spirit as the proof of part (a), Proposition 7.4 implies the claimed expansion of the average $\langle \boldsymbol{a} b^\varepsilon \rangle_u$.

□

Remark 7.6. The estimates of Corollary 7.5 also apply to functions $b^\varepsilon(x)$ of the form $b^\varepsilon(x) = B^\varepsilon(x) \cdot (x-q)$, where $B^\varepsilon(x) \in \mathbb{R}^d$ is sublinear with uniform bounds in ε. A derivative $\partial^\alpha b^\varepsilon(x)$ additively decomposes into a bounded function and the function $\partial^\alpha B^\varepsilon(x) \cdot (x-q)$, which can be controlled by the arguments used in the proof of Theorem 3.8 (a).

7.4. **Proof of Theorem 3.10.** We now have everything at hand to estimate the error of observables and to conclude our final main result. In the following proof, we use Assumption 2.1 on the potentials and the representation (7.2) of the remainder potential W_u only to the extent that the arguments literally also apply to the dynamics induced by general subquadratic hamiltonians. Thus, the proof improves known observable error estimates in full generality.

Proof of Theorem 3.10. By Lemma 7.1 we only have to bound the commutator in the representation formula (7.1).

(a) We start by recalling, that in the proof of Theorem 3.8, we have estimated

$$\big\|W_{u(s)}u(s)\big\|_{L^2} = \big\|(\mathrm{Id} - P_{u(s)})H(s)u(s)\big\|_{L^2} \le C\varepsilon^{3/2}. \tag{7.10}$$

(b) We denote $\widetilde{\boldsymbol{a}}(t,s) = \boldsymbol{a} \circ \Phi^{t,s}$ and expand

$$\begin{aligned}
&\frac{1}{\mathrm{i}\varepsilon}\big\langle \overline{W}_{u(s)}\widetilde{\mathbf{A}}(t,s) - \widetilde{\mathbf{A}}(t,s)W_{u(s)}\big\rangle_{u(s)} \\
&= \frac{1}{\mathrm{i}\varepsilon}\big\langle \overline{W}_{u(s)}\mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)W_{u(s)}\big\rangle_{u(s)} + r_1(s,t).
\end{aligned}$$

Using first Cauchy-Schwarz and then (7.10) together with Proposition 7.2 and norm conservation, we bound the remainder by

$$|r_1(s,t)| \le \frac{2}{\varepsilon}\big\|W_{u(s)}u(s)\big\|_{L^2}\big\|\big(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)\big)u(s)\big\|_{L^2} \le c\,\varepsilon^{5/2}.$$

(c) As in the proof of Proposition 7.2, we use the product rule of Weyl calculus and expand the commutator. For notational simplicity, we suppress the dependence on t and s. We have by symmetry of the real part with respect to the L^2 scalar product and anti-symmetry of the Poisson bracket

$$\begin{aligned}
&\big\langle \overline{W}_u\,\mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}\right) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}\right)W_u\big\rangle_u \\
&= \frac{2}{\mathrm{i}}\big\langle \mathrm{Im}\,W_u\widetilde{\boldsymbol{a}}\big\rangle_u + \frac{\varepsilon}{\mathrm{i}}\big\langle\{\mathrm{Re}\,W_u, \widetilde{\boldsymbol{a}}\}\big\rangle_u + \frac{\varepsilon^2}{4\mathrm{i}}\big\langle \nabla^2\mathrm{Im}\,W_u J\nabla^2\widetilde{\boldsymbol{a}}J\big\rangle_u + \mathcal{O}(\varepsilon^3),
\end{aligned}$$

where the constant in $\mathcal{O}(\varepsilon^3)$ depends on phase space derivatives of the remainder potential $W_{u(s)}$ and of $\widetilde{\boldsymbol{a}}(t,s)$ of the order ≥ 3. Since $\widetilde{\boldsymbol{a}}(t,s)$ is sublinear and $W_{u(s)}$ consists of subquadratic summands and a non-subquadratic summand which can be handled by Remark 7.6, the Calderón–Vaillancourt Theorem applies for the remainder term. We will prove below that

$$\big\langle \mathrm{op}_{\mathrm{Weyl}}\left(\mathrm{Im}\,W_u\widetilde{\boldsymbol{a}}\right)\big\rangle_u = \mathcal{O}(\varepsilon^3), \tag{7.11a}$$

$$\big\langle \mathrm{op}_{\mathrm{Weyl}}\left(\{\mathrm{Re}\,W_u, \widetilde{\boldsymbol{a}}\}\right)\big\rangle_u = \mathcal{O}(\varepsilon^2), \tag{7.11b}$$

$$\big\langle \mathrm{op}_{\mathrm{Weyl}}\left(\nabla^2\mathrm{Im}\,W_u J\nabla^2\widetilde{\boldsymbol{a}}J\right)\big\rangle_u = \mathcal{O}(\varepsilon), \tag{7.11c}$$

which allows us to conclude that

$$\frac{1}{\mathrm{i}\varepsilon}\big\langle \overline{W}_u\widetilde{\mathbf{A}} - \widetilde{\mathbf{A}}W_u\big\rangle_u = \mathcal{O}(\varepsilon^2).$$

In order to do so, we first aim at the application of Corollary 7.5 statement (a) for $b^\varepsilon = \partial_j \mathrm{Re}\, W_u$ and statement (b) for $b^\varepsilon = \mathrm{Im}\, W_u$; see also Remark 7.6 for the non-subquadratic terms in W_u.

(d) From now on, we notationally focus on the magnetic Schrödinger case, but the analysis works the same for the general case. We denote the phase space center of the variational Gaussian u by $z = (q,p)$. The width matrix of u is $\mathcal{C}$ and has imaginary part $\mathcal{C}_{\mathrm{I}}$. We recall that the cubic remainder $R(X_u)$ in (7.2) vanishes together with its first and second derivatives when evaluated in q.

We first apply the analysis to the Poisson bracket that involves the real part of the remainder potential. For any $j = 1,\dots,d$, we use (7.2) and Proposition 7.4 and obtain $\partial_j \mathrm{Re}\, W_u(q) = \mathcal{O}(\varepsilon)$. Furthermore, by [24, Lemma 3.15] we have

$$\begin{aligned}
\nabla\partial_j \mathrm{Re}\, W_u(q) &= \nabla\partial_j \mathrm{Re}\, X_u(q) - \langle \nabla\partial_j \mathrm{Re}\, X_u\rangle_u = \mathcal{O}(\varepsilon),\\
\nabla^2\partial_j \mathrm{Re}\, W_u(q) &= \nabla^2\partial_j \mathrm{Re}\, R(X_u)(q) = \nabla^2\partial_j \mathrm{Re}\, X_u(q).
\end{aligned}$$

Hence, the function $b^\varepsilon = \partial_j \mathrm{Re}\, W_u$ fulfills the assumptions of statement (a) in Corollary 7.5, and together with Proposition 7.4, we obtain

$$\langle \partial_j \mathrm{Re}\, W_u \partial_{p_j}\widetilde{\boldsymbol{a}}\rangle_u = \mathcal{O}(\varepsilon^2).$$

After summation over j, we have proven (7.11b).

(e) Similarly, the first and second derivatives of $\mathrm{Im}\, W_u$ satisfy

$$\nabla \mathrm{Im}\, W_u(q),\ \nabla^2 \mathrm{Im}\, W_u(q) = \mathcal{O}(\varepsilon). \tag{7.12}$$

Moreover, Proposition 7.4 implies for the point evaluation of the imaginary part of the remainder potential that

$$\begin{aligned}
\mathrm{Im}\, W_u(q) &= \frac{\varepsilon}{4}\,\mathrm{tr}\Big(\big(\langle \nabla^2 \mathrm{Im}\, X_u\rangle_u - \nabla^2 \mathrm{Im}\, X_u(q)\big)\,{\mathcal{C}_{\mathrm{I}}}^{-1}\Big) + \mathcal{O}(\varepsilon^2)\\
&= \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{7.13}$$

At this point, a simple application of Proposition 7.4 and (7.12) yields (7.11c).

(f) The expansions in (7.12) and (7.13) show that $b^\varepsilon = \mathrm{Im}\, W_u$ satisfies the assumptions of statement (b) in Corollary 7.5. In order to prove (7.11a), we analyse the expansion obtained from Corollary 7.5 in two steps, aiming at

$$\mathrm{Im}\, W_u(q) + \varepsilon f_2(\mathrm{Im}\, W_u, \mathcal{C}) + \varepsilon^2 f_4(\mathrm{Im}\, W_u, \mathcal{C}) = \mathcal{O}(\varepsilon^3), \tag{7.14a}$$

$$\varepsilon F_{1,1}(\widetilde{\boldsymbol{a}}, \mathrm{Im}\, W_u, \mathcal{C}) + \varepsilon^2 F_{1,3}(\widetilde{\boldsymbol{a}}, \mathrm{Im}\, W_u, \mathcal{C}) = \mathcal{O}(\varepsilon^3). \tag{7.14b}$$

(g) We start with proving the first estimate (7.14a). For this, we need a slightly more accurate assessment of $\mathrm{Im}\, W_u(q)$ than developed previously. Using (7.2), Proposition 7.4, and (7.12), we have

$$\begin{aligned}
\mathrm{Im}\, W_u(q) &= -\,\varepsilon f_2(\mathrm{Im}\, X_u, \mathcal{C}) - \varepsilon^2 f_4(\mathrm{Im}\, X_u, \mathcal{C}) + \varepsilon f_2(\langle \mathrm{Im}\, X_u\rangle_u, \mathcal{C}) + \mathcal{O}(\varepsilon^3)\\
&= -\,\varepsilon^2 f_4(\mathrm{Im}\, X_u, \mathcal{C}) + \varepsilon^2 f_2(f_2(\mathrm{Im}\, X_u, \mathcal{C}), \mathcal{C}) + \mathcal{O}(\varepsilon^3).
\end{aligned}$$

Similarly, we obtain for the second term in (7.14a) that

$$\varepsilon f_2(\mathrm{Im}\, W_u, \mathcal{C}) = -\varepsilon^2 f_2(f_2(\mathrm{Im}\, X_u, \mathcal{C}), \mathcal{C}) + \mathcal{O}(\varepsilon^3).$$

Therefore, $\operatorname{Im} W_u(q)$ cancels both the contributions from the second and the fourth derivatives, and we have proven (7.14a).

(h) We next target the terms on the left hand side of equation (7.14b), that is,

$$\varepsilon F_{1,1}(\widetilde{\boldsymbol{a}}, \operatorname{Im} W_u, \mathcal{C}) = -\varepsilon^2 \sum_{|k|=2} F_{1,1}(\widetilde{\boldsymbol{a}}, \partial^k \operatorname{Im} X_u, \mathcal{C})\ \rho_k(\mathcal{C}) + \mathcal{O}(\varepsilon^3)$$

and

$$F_{1,3}(\widetilde{\boldsymbol{a}}, \operatorname{Im} W_u, \mathcal{C}) = F_{1,3}(\widetilde{\boldsymbol{a}}, \operatorname{Im} X_u, \mathcal{C}).$$

In Lemma A.1, we provide the combinatorial argument that shows (7.14b) as a consequence of Isserlis' theorem on the higher moments of multivariate normal distributions. Hence, we have proven $\langle \operatorname{Im} W_u \widetilde{\boldsymbol{a}} \rangle_u = \mathcal{O}(\varepsilon^3)$, that is, (7.11a). □

Remark 7.7. The crucial estimates of the previous proof, namely (7.11a) and (7.11b) are one order worse for the semiclassical Gaussian approximation, since it lacks the compensating averaging factors of the remainder potential. Therefore, for the semiclassical Gaussians only $\mathcal{O}(\varepsilon)$ observable accuracy can be expected.

Appendix A. Gaussian moments

By an application of Isserlis' theorem, the fourth order Gaussian moments can be written as sums of products of second order moments. That is, for a $2d$-dimensional Gaussian random vector

$$(X_1, \dots, X_{2d}) \sim \mathcal{N}(0, G)$$

with mean zero $0 \in \mathbb{R}^{2d}$ and covariance matrix $G \in \mathbb{R}^{2d \times 2d}$, the fourth order moments satisfy

$$\begin{aligned}
&\mathbb{E}(X_i^4) = 3 g_{ii}^2, \\
&\mathbb{E}(X_i^3 X_j) = 3 g_{ii} g_{ij}, \\
&\mathbb{E}(X_i^2 X_j^2) = g_{ii} g_{jj} + 2 g_{ij}^2 \\
&\mathbb{E}(X_i^2 X_j X_k) = g_{ii} g_{jk} + 2 g_{ij} g_{ik} \\
&\mathbb{E}(X_i X_j X_k X_\ell) = g_{ij} g_{k\ell} + g_{ik} g_{j\ell} + g_{i\ell} g_{jk}
\end{aligned}$$

with $i, j, k, \ell \in \{1, \dots, 2d\}$. We crucially use this for proving that the fourth order summations that appeared in the proof of Theorem 3.10 can be expressed in terms of second order summations.

Lemma A.1 (Resummation). *For any family $(a_{\beta,m})_{\beta,m}$ of real numbers, indexed by $m \in \mathbb{N}_0^{2d}$ and $\beta \le m$ with $|\beta| = 1$, we have*

$$\sum_{|m|=4} \sum_{\beta \le m, |\beta|=1} \frac{1}{(m-\beta)!}\ a_{\beta,m}\, \rho_m(\mathcal{C}) = \sum_{|k|=2} \sum_{|\ell|=2} \sum_{\beta \le \ell, |\beta|=1} \frac{1}{k!}\ a_{\beta,k+\ell}\, \rho_k(\mathcal{C}) \rho_\ell(\mathcal{C}).$$

Proof. We write a multi-index $m \in \mathbb{N}_0^{2d}$ of order $|m| = 4$ as

$$m = \langle j_1 \rangle + \langle j_2 \rangle + \langle j_3 \rangle + \langle j_4 \rangle$$

with coordinates $j_1, \dots, j_4 \in \{1, \dots, 2d\}$, where the bracket $\langle j \rangle = e_j$ denotes the jth canonical basis vector of $\mathbb{R}^{2d}$. We distinguish five different cases for the order four multi-index m.

(a) m has one non-zero component, that is, $m = 4\langle j\rangle$ with $j = 1, \ldots, 2d$. Then,

$$\begin{aligned}\frac{1}{(m-\beta)!}\, a_{\beta,m}\, \rho_m(\mathcal{C}) &= \frac{1}{3!}\, a_{\langle j\rangle,4\langle j\rangle}\, 3\rho_{2\langle j\rangle}(\mathcal{C})^2 \\ &= \frac{1}{k!}\, a_{\beta,k+\ell}\, \rho_k(\mathcal{C})\rho_\ell(\mathcal{C})\end{aligned}$$

with $k = 2\langle j\rangle = \ell$ and $\beta = \langle j\rangle$.

(b) m has two different non-zero components, that is, $m = 3\langle j_1\rangle + \langle j_2\rangle$ with $j_1 \neq j_2$. In this case, m dominates two multi-indices β of order one, and generates the terms

$$\begin{aligned}&\left(\frac{1}{2!}\, a_{\langle j_1\rangle,m} + \frac{1}{3!}\, a_{\langle j_2\rangle,m}\right) 3\rho_{2\langle j_1\rangle}(\mathcal{C})\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C}) \\ &= \frac{1}{2!}\left(a_{\langle j_1\rangle,m} + a_{\langle j_2\rangle,m}\right) \rho_{2\langle j_1\rangle}(\mathcal{C})\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C}) \\ &+ \frac{1}{1!}\, a_{\langle j_1\rangle,m}\ \rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C})\rho_{2\langle j_1\rangle}(\mathcal{C}).\end{aligned}$$

This amounts to the two (k, ℓ) pairs

$$\begin{aligned}&k = 2\langle j_1\rangle,\ \ell = \langle j_1\rangle + \langle j_2\rangle,\ \beta \in \{\langle j_1\rangle, \langle j_2\rangle\}, \\ &k = \langle j_1\rangle + \langle j_2\rangle,\ \ell = 2\langle j_1\rangle,\ \beta = \langle j_1\rangle.\end{aligned}$$

In a similar manner, we show that in the cases

(c) m has two identical non-zero components, that is, $m = 2\langle j_1\rangle + 2\langle j_2\rangle$ with $j_1 \neq j_2$,

(d) m has three non-zero components, that is, $m = 2\langle j_1\rangle + \langle j_2\rangle + \langle j_3\rangle$ with pairwise distinct j_1, j_2, j_3,

(e) m has four non-zero components, that is, $m = \langle j_1\rangle + \cdots + \langle j_4\rangle$ with distinct $j_1, \ldots, j_4$,

we obtain the appropriate format of the resulting summands, that is,

$$\frac{1}{k!} \sum_{\beta \le \ell, |\beta|=1} a_{\beta,k+\ell}\, \rho_k(\mathcal{C})\, \rho_\ell(\mathcal{C})$$

with $k, \ell \in \mathbb{N}_0^{2d}$ such that $|k| = |\ell| = 2$ and $k + \ell = m$. For concluding the proof, we have to verify that any possible (k, ℓ) pairing of order two multi-indices has appeared in one of the five cases (a)–(e). Let $i_1, \ldots, i_4 \in \{1, \ldots, 2d\}$ be such that

$$k = \langle i_1\rangle + \langle i_2\rangle, \quad \ell = \langle i_3\rangle + \langle i_4\rangle.$$

The combinatorics of this situation falls into the following five cases:

- (α) All four coordinates agree, that is, $i_1 = \cdots = i_4 =: j$. Then, $k + \ell = 4\langle j\rangle$, and we recognize the previous case (a).
- (β) Three of the four coordinates coincide with each other, which is case (b).
- (γ) The four coordinates form two different pairs, and we are in case (c).
- (δ) Two of the four coordinates agree, while the other two are different, which is case (d).

(ε) All four coordinates are distinct as in case (e).

Hence, the combinatorics of the order four multi-indices and the one of pairs of order two multi-indices are the same, and we have indeed proven that the two different summation formats yield the same result as claimed. □

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