

QUASIPARTICLES AND QUASIMOMENTUM

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ABSTRACT

Common and different properties of particles and quasiparticles are discussed and, in particular, the difference between real and quasimomentum is clarified.

I. INTRODUCTION

The concept of elementary excitations or quasiparticles has turned out to be an extraordinary powerful tool to describe the low lying excitations of condensed matter: In many cases the excited states can be viewed as a gas of approximately noninteracting particles with energies ϵ_α which contribute to total energy according to

$$E\{n_\alpha\} = \sum_{\alpha} \epsilon_{\alpha} n_{\alpha}. \quad (1)$$

α 's label single particle states and $\{n_\alpha\} = \{n_1, n_2, \dots\}$ denote the set of (nonnegative integer) occupation numbers. In many respects, these quasiparticles behave like ordinary particles, e.g. they are bosons or fermions with $n_{\mathbf{q}} = 0, 1, 2, \dots$ or $n_{\mathbf{q}} = 0, 1$, respectively.

Some authors reserve the name quasiparticle to cases where α has the property of momentum. Nevertheless, there are differences between particles and quasiparticles, in particular there is a subtle difference between momentum and quasimomentum which is not always fully respected.

The concept of quasiparticles was originally developed by Landau [1] who realized that there is a continuous mapping of the low energy excitation spectrum with interparticle interactions. Amazingly, this description holds even in relatively strong interacting systems like in metals or in superfluid helium.

A well known example of classical “quasiparticles” is the introduction of relative and center of mass coordinates of a two body problem interacting via a central force

$\mathbf{F}(\mathbf{r}) = f(|\mathbf{r}|) \mathbf{r}$, see Fig. 1. The two particles are located at positions $\mathbf{r}_i(t)$ ($i = 1, 2$)

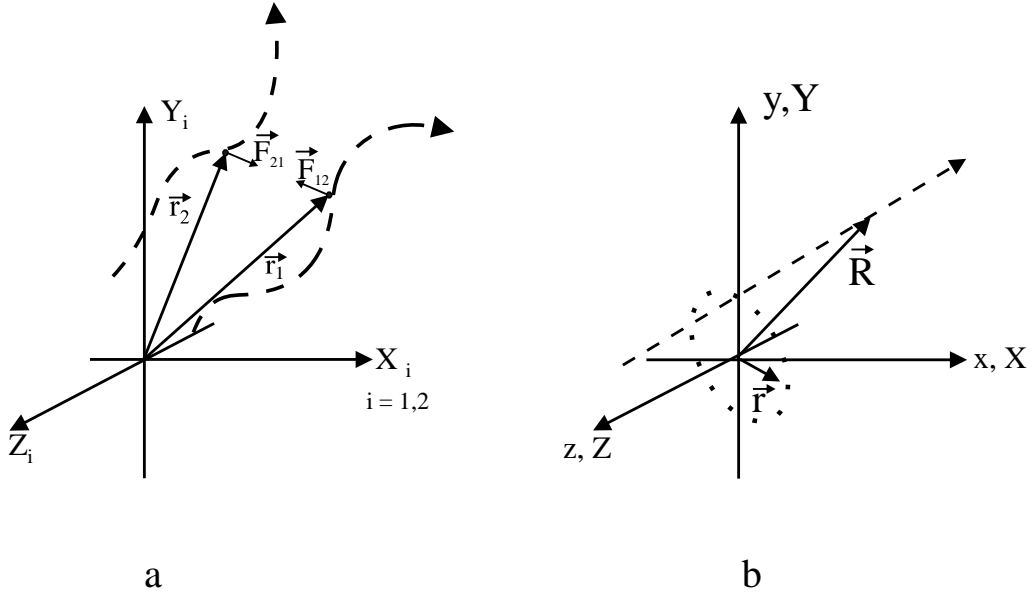


Fig. 1. (a) Classical two body system interacting via a central force \mathbf{F} and (b) the decoupled motion of the relative- and center of mass coordinates which describe the motion of two noninteracting “quasiparticles”. Dashed and dotted lines indicate possible trajectories.

and the forces between the particles obey Newton’s law actio=reactio. We omit for simplicity external forces and obtain:

$$m_1 \frac{d^2 \mathbf{r}_1}{dt^2} = f(|\mathbf{r}_1 - \mathbf{r}_2|) (\mathbf{r}_1 - \mathbf{r}_2), \quad (2)$$

$$m_2 \frac{d^2 \mathbf{r}_2}{dt^2} = f(|\mathbf{r}_2 - \mathbf{r}_1|) (\mathbf{r}_2 - \mathbf{r}_1). \quad (3)$$

By introduction of relative \mathbf{r} and center of mass coordinates \mathbf{R}

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}, \quad (4)$$

the dynamics of the two interacting particles at positions $\mathbf{r}_1, \mathbf{r}_2$ is transformed formally to the dynamics of a system of two noninteracting particles

$$m \frac{d^2 \mathbf{r}(t)}{dt^2} = f(|\mathbf{r}|) \mathbf{r}, \quad M \frac{d^2 \mathbf{R}(t)}{dt^2} = 0, \quad (5)$$

with reduced mass m and total mass M

$$m = \frac{m_1 m_2}{m_1 + m_2}, \quad M = m_1 + m_2. \quad (6)$$

We can call the two entities associated with \mathbf{r} and \mathbf{R} quasiparticles. In contrast to the original particles, however, these particles are not material bodies, i.e. there is no matter located at positions \mathbf{r} and \mathbf{R} so that there will be no collision at $\mathbf{R} = \mathbf{r}$. The procedure outlined above for a classical quasiparticle is obviously very similar to the one sketched in [2] when introducing the concept of quasiparticles in solids such as phonons, plasmons, magnons, or excitons.

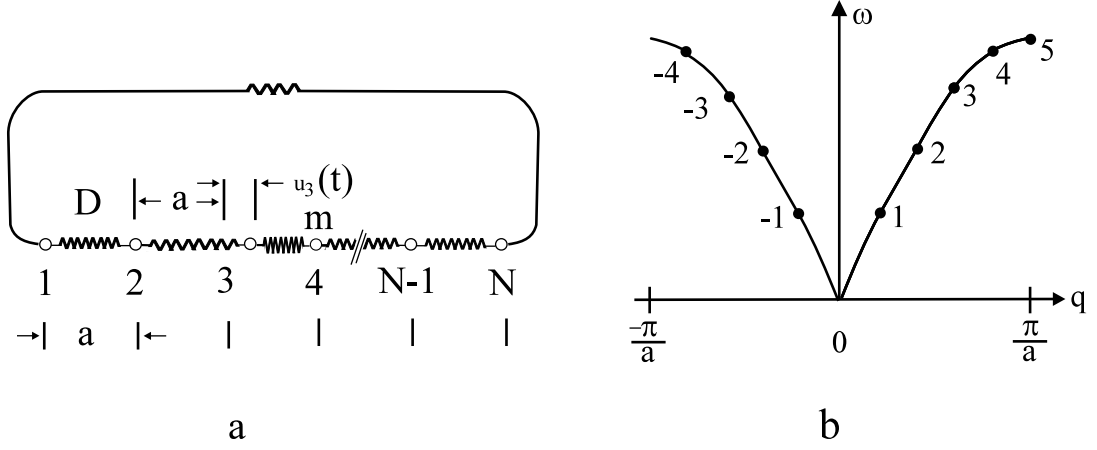


Fig. 2 (a) Linear monoatomic chain with equal masses m and nearest neighbour springs D and periodic boundary conditions, (b) frequency spectrum for $N = 10$ “atoms”.

The aim of this note is to discuss and to clarify the quasiparticle properties of condensed matter by using the linear chain as a prominent example in section II. Then, the equivalence of bosons and oscillators is sketched in section III. In Section IV we summarize common and different properties of particles and quasiparticles and give two examples.

II. LATTICE VIBRATIONS

As a prominent example for collective excitations in condensed matter we consider the vibrations of a linear chain, Fig. 2a. The longitudinal displacements u_j from the equilibrium positions $x_j^0 = ja, j = 1, 2, \dots, N$ where a denotes the lattice constant, obey the Newton-equation of motion:

$$m \frac{d^2 u_j(t)}{dt^2} = D(u_{j+1} - u_j) - D(u_j - u_{j-1}). \quad (7)$$

Imposing periodic boundary conditions $u_{N+1} = u_1$ we find two different types of solutions:

$$u_j^{cm}(t) = \bar{u} + \bar{v}t, \quad \text{independent of } j \quad (8)$$

$$u_j^\alpha(t) = \text{Re } A_\alpha e^{i(q_\alpha ja - \omega_\alpha t)}, \quad q_\alpha = \frac{2\pi}{Na} \alpha. \quad (9)$$

Eq.(8) describes the rigid motion of the chain, corresponding to the center of mass motion, counting as one degree of freedom whereas Eq.(9) describes $N - 1$ vibrations labeled by $\alpha = \pm 1, \pm 2, \dots, \pm[\frac{N}{2}]$. (For even N , $-\frac{N}{2}$ is excluded.) \bar{u} , \bar{v} are two real constants and A_α are complex constants which are fixed by the initial conditions. The frequency spectrum of the chain

$$\omega(q_\alpha) = 2\sqrt{\frac{D}{m}} \left| \sin \frac{q_\alpha a}{2} \right| \quad (10)$$

is depicted in Fig. 2b. Note, $\alpha = 0$ is definitely excluded because the corresponding solution $u_j^\alpha(t) = \text{const}$ is already contained in Eq.(8) as a special case with $\bar{v} = 0$ which describes a static displacement. Nevertheless, this property is often formulated in jargon, even in theoretical texts e.g. Kittel [4] p. 15

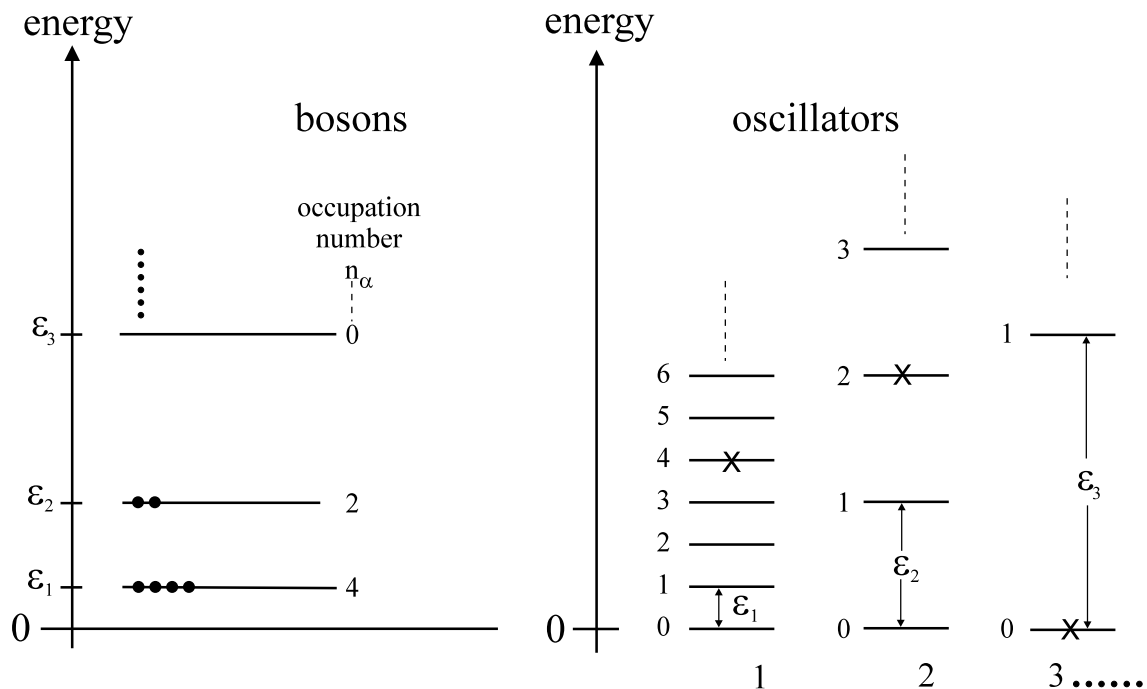


Fig. 3 *Equivalence of a system of N (noninteracting) bosons with single-particle energies ϵ_α and occupation numbers n_α and an infinite (uncoupled) set of harmonic oscillators with frequencies $\omega_\alpha = \epsilon_\alpha/\hbar$. Note that the zero-point energies of the oscillators are omitted. Dots symbolize particles, crosses excited states, respectively. $N = 6$.*

“The total momentum involves only the $q = 0$ mode which is a uniform translation of the system”.

Obviously, this statement is inappropriate as $u_j^\alpha(t)$ describes only the relative motion of the masses so that the total momentum is zero just by construction.

Quantization of the chain is almost trivial as each mode represents a harmonic oscillator. In particular, the total energy of the chain is

$$E\{n_q\} = \frac{p_{cm}^2}{2Nm} + \sum_q \hbar\omega_q \left(n_q + \frac{1}{2}\right), \quad n_q = 0, 1, 2, \dots, \quad (11)$$

where p_{cm} denotes the total (center of mass) momentum and, as usual, the $N - 1$ independent modes are conveniently described by a wave number in the first Brillouin zone, $|q| \leq \pi/a$

III. BOSONS AND OSCILLATORS

A harmonic oscillator has the unique property that the excitation spectrum is represented in terms of integer multiples of $\hbar\omega$ above the zero point energy $\frac{1}{2}\hbar\omega$. Equivalently, one might view the excited states as realized by adding hypothetical particles with energy $\hbar\omega$ to the “vacuum” state $|0\rangle$ as shown in Fig. 3. For a single oscillator the “life” of these particles is rather “dull” because these particles have no degrees of freedom.

If we have, however, a set of oscillators (or of quasiparticles) with different quantum numbers like those of the linear chain in Fig. 2b, then a quasi-particle may be forced to “jump” from one (single particle) state α to another one α' . This analogy can be put further and leads to the formulation of “second quantization” (occupation number representation) as sketched in Fig. 3.

Each N -boson state (described by a symmetric wave function) and each operator \mathcal{O} can be translated to the occupation number representation so that the expectation values are the same in both representations.

$$\Psi_{\alpha_1, \alpha_2, \dots}(\mathbf{r}_1, \mathbf{r}_2, \dots) \rightarrow |n_{\alpha_1}, n_{\alpha_2}, \dots\rangle, \quad (12)$$

$$\mathcal{O}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{p}_1, \mathbf{p}_2, \dots) \rightarrow \hat{\mathcal{O}}(\{a_\alpha, a_\alpha^\dagger\}). \quad (13)$$

Conveniently, operators $\hat{\mathcal{O}}$ are represented in terms of ladder operators $a_\alpha^\dagger, a_\beta$ with $a_\alpha|0\rangle = 0$ and commutation relations

$$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha, \beta}, \quad [a_\alpha, a_\beta] = 0, \quad [a_\alpha^\dagger, a_\beta^\dagger] = 0. \quad (14)$$

In “particle language”, the oscillator quantum numbers are termed occupation numbers, whereas, a_q^\dagger, a_q are called creation and annihilation operators for particles in the (single-particle) states labeled by α .

For example, the operator of total momentum is translated as

$$P = \sum_{j=1}^N p_j \rightarrow \hat{P} = \sum_{\alpha, \alpha'} \langle \alpha' | p | \alpha \rangle a_{\alpha'}^\dagger a_\alpha, \quad (15)$$

where \mathbf{p} is the momentum operator of a single particle, $\mathbf{p} = -i\hbar\nabla$.

However, the equivalence of bosons and oscillators is not one to one! The occupation number representation is more versatile than the traditional representation in terms of wave functions. The particle number is no longer just a parameter but becomes a dynamic variable described by the operator

$$\hat{N} = \sum_{\alpha} a_\alpha^\dagger a_\alpha. \quad (16)$$

The eigenvalues of $\hat{N}_\alpha = a_\alpha^\dagger a_\alpha$ are just $n_\alpha = 0, 1, 2, \dots$. As all \hat{N}_α commute, these operators have simultaneous eigenstates which are labeled by $\{n_\alpha\}$.

Operators which conserve the particle number, e.g. Eqs.(15,16), are composed of products with equal numbers of a_α^\dagger and a_β .

The equivalence theorem gives the possibility to go the other way and associates bosons with a set of oscillators, too. In the case of lattice vibrations, these bosons are called phonons. The displacement-operator of the chain (see [4] p.16), however,

$$u_j^\alpha = \sum_{q'} \sqrt{\frac{\hbar}{2Nm\omega_{q'}}} e^{iq'x_j^0} (a_{-q'}^\dagger + a_{q'}) \quad (17)$$

changes the phonon number by one and, thus, cannot be handled with wave functions. Fermionic systems may be mapped to two-level systems, where all commutators Eq.(14) are replaced by anticommutators. For details, we refer to standard textbooks, e.g. Kittel [4].

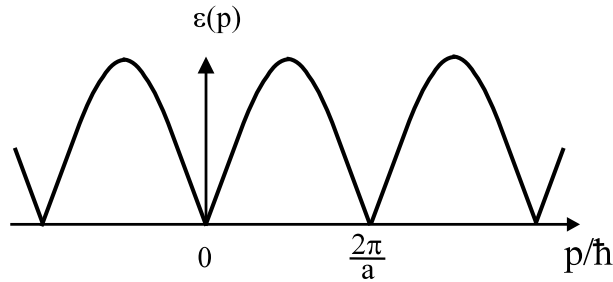


Fig. 4 The dispersion relation of (longitudinal) acoustic phonons extended over several Brillouin zones.

IV. QUASIPARTICLES

In particular cases, e.g. for vibrations of a crystalline lattice or for electrons in a periodic potential, α displays the characteristic properties of momentum. This is easiest recovered by using the extended zone scheme to define the crystal-momentum

$$\mathbf{p} = \hbar(\mathbf{q} + \mathbf{G}), \quad (18)$$

where \mathbf{q} is restricted to the first Brillouin zone and \mathbf{G} denotes an appropriate vector of the reciprocal lattice. Now $\epsilon(\mathbf{p})$ becomes a periodic function of \mathbf{p} which is a general property of excitations in crystals, as shown in Fig. 4 for acoustic phonons. The quantity \mathbf{p} is called quasi-, crystal- or pseudo-momentum and, in the “everyday laboratory jargon” often simply momentum. For most practical purposes a phonon (or other quasiparticles in crystals) acts as if \mathbf{p} is the momentum but there are subtle differences. In the following, we shall present aspects in which quasiparticles behave like real particles and also in which they are different.

As an exotic example, we present the collective excitations in superfluid and solid helium ^4He which both are of phonon-type at small \mathbf{q} . Interestingly, the “roton”-minimum in the liquid phase near $q \approx 2\text{\AA}^{-1}$ seems to be the remniscent of the longitudinal phonons in the crystalline phase near $\mathbf{q} \approx 0$ when shifted to the next Brillouin zone.

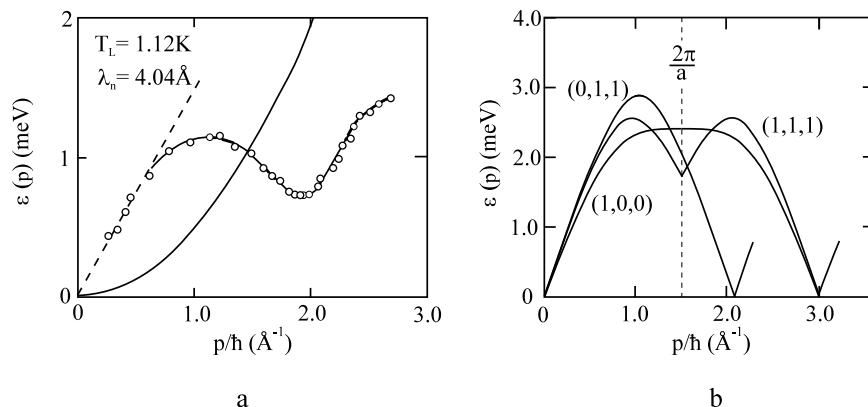


Fig. 5 Spectrum of (longitudinal) elementary excitations in helium ^4He : (a) superfluid and (b) bcc crystalline phase as determined by inelastic neutron scattering. According to Henshaw et al. [6] and Osgood et al. [7]. The parabola in (a) represents the kinetic energy of free ^4He atoms

A. Common properties of particles and quasiparticles

1. quasiparticles describe a transport of momentum and energy through condensed matter like ordinary particles do in vacuum. This transport is characterized by an energy - quasimomentum relation also called dispersion relation

$$\epsilon = \epsilon(\mathbf{p}). \quad (19)$$

For excitations in crystals, $\epsilon(\mathbf{p})$ is a periodic function of \mathbf{p} where \mathbf{p} is usually called crystal-momentum. For relativistic particles (in vacuum) there is a universal function

$$\epsilon(\mathbf{p}) = \sqrt{(m_0 c^2)^2 + (c\mathbf{p})^2}, \quad (20)$$

where c is the velocity of light in vacuum and m_0 is the rest mass.

2. The transport velocity of energy and momentum is given by

$$\mathbf{v}_T = \frac{\partial \epsilon(\mathbf{p})}{\partial \mathbf{p}}. \quad (21)$$

In the wave-picture this conforms with the group-velocity if ϵ and \mathbf{p} are substituted by $\hbar\omega$ and $\hbar\mathbf{k}$, respectively.

3. Interaction with (temporary and spatially) slowly varying external forces is governed by the equation of motion

$$\frac{d\mathbf{p}(t)}{dt} = \mathbf{F}_{ext}(t). \quad (22)$$

This equation is analogous to the Newton-equation in classical mechanics and it is valid provided the perturbation does not induce transitions between different branches of the quasiparticle spectrum (so-called quasiclassical dynamics).

4. Interaction with other particles (e.g. neutrons) or quasiparticles (e.g. phonons, Bloch electrons etc.) may create, destruct or scatter quasiparticles. These processes are governed by the conservation laws for energy and (quasi)momentum. For example, the creation of a phonon by a neutron scattered from \mathbf{P}_i to \mathbf{P}_f is governed by

$$\mathbf{P}_i - \mathbf{P}_f = \mathbf{p}, \quad E_i - E_f = \epsilon(\mathbf{p}). \quad (23)$$

Note, the participation of reciprocal lattice vectors is already included in Eqs.(23) by using the extended zone scheme.

5. quasiparticles are either bosons or fermions provided the interaction between them is weak i.e., the density of quasiparticles is low. Collective excitations, e.g. phonons, magnons or plasmons are (mostly) bosons and, thus, the change of their number is not restricted. Fermionic quasiparticles, however, can only be created or diminished in pairs as e.g., for electron-hole pair excitations near the Fermi-surface of a metal. In a semiconductor, such electron-hole pairs can form hydrogenic bound states (=excitons) which act as bosons at low density and if the excitation energy is smaller than the binding energy, see e.g., [2].
6. Quasiparticles are described by delocalized states, e.g., by plane waves or Bloch waves.

7. Quasiparticles have a finite life time τ . According to the energy - time uncertainty relation this life time causes a finite width $\Delta\epsilon = \hbar/\tau$ of the dispersion curve $\epsilon(\mathbf{p})$. A consistent quasiparticle description requires $\Delta\epsilon < \epsilon$.

Properties 1-7 strongly support the view that (real) momentum and quasimomentum describe – apart from the name – the same quantity. However, there are at least three subtle differences.

B. Differences between real momentum and quasimomentum

1. Symmetries and conservation laws [5].

Associated with every symmetry of a Hamiltonian is a conservation law. This is the famous Noether–theorem: The Hamiltonian of the linear chain (with periodic boundary conditions, see Fig. 2a) is invariant under (arbitrary) translations which are intimately connected to the conservation of total momentum. For example, scattering of a neutron with momentum \mathbf{P}_i to \mathbf{P}_f transfers (real) momentum to the crystal as a whole

$$\mathbf{P}_i - \mathbf{P}_f = \mathbf{p}_{\text{cm}} \quad (24)$$

which is carried by the center of mass degree of freedom.

The Hamiltonian of the linear chain is also invariant under the discrete transformation $x_j \rightarrow x_j + a$ which, – in contrast to the previously considered continuous transformation – would also be present if the masses would be tied to the “ground” by additional springs. This discrete symmetry (=renumbering of the atoms) leads to the conservation of crystal momentum of the interacting quasiparticles

$$\sum_j \mathbf{p}_j = 0 \pmod{\mathbf{G}}. \quad (25)$$

Of the two conservation laws Eqs.(24,25), crystal momentum is by far more important in solid state physics than ordinary momentum.

2. Transformation properties [8].

Energy ϵ and momentum \mathbf{p} of a non-relativistic particle with mass m can be changed by changing the frame of reference \mathcal{R} . If ϵ, \mathbf{p} are defined in \mathcal{R} , a Galilei–transformation to \mathcal{R}' (which moves with velocity $-\mathbf{V}$ with respect to \mathcal{R}) yields:

$$\epsilon' = \epsilon + \mathbf{p}\mathbf{V} + \frac{m}{2}\mathbf{V}^2, \quad \mathbf{p}' = \mathbf{p} + m\mathbf{V} \quad (26)$$

so that the relation between energy and momentum is form-invariant in all inertial systems: $\epsilon' = \epsilon(\mathbf{p}')$. This is the principle of classical relativity. Quasiparticles, however, transform differently:

$$\epsilon' = \epsilon + \mathbf{p}\mathbf{V}, \quad \mathbf{p}' = \mathbf{p}. \quad (27)$$

$\epsilon' - \mathbf{p}'\mathbf{V}$ and \mathbf{p}' are invariant with respect to Galilei-transformations. Eqs.(27) are closely related to the transformation properties of wave phenomena in material media

$$\omega' = \omega + \mathbf{q}\mathbf{V}, \quad \mathbf{q}' = \mathbf{q}. \quad (28)$$

The second equation of (28) states that (apart from relativistic effects) the wave length $\lambda = 2\pi/|\mathbf{q}|$ remains unchanged whereas the frequency is Doppler-shifted.

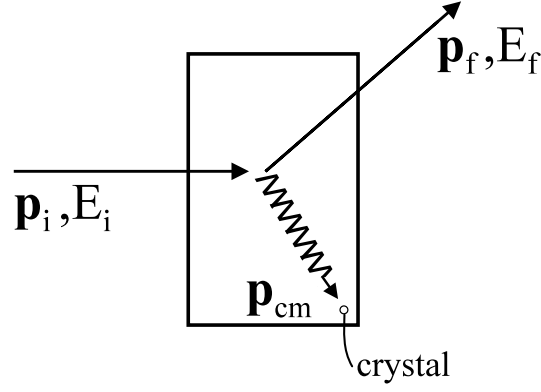


Fig. 6. Inelastic scattering of a neutron with momentum transfer $\mathbf{p}_{cm} = \mathbf{P}_i - \mathbf{P}_f$ to the crystal and the production of a phonon with wave vector $\mathbf{q} = \mathbf{p}_{cm} \bmod \mathbf{G}$.

3. For phonons, magnons, and other “lattice excitations” the number of modes is determined by the number of different wave vectors within a single Brillouin zone. For real particles, however, e.g. free electrons or photons, momentum is not restricted: There is a minimum wavelength a/π for lattice vibrations but not for free electrons or photons.

C. Example 1: Neutron scattering

As an illustration we first consider the excitation of phonons by neutron scattering as is discussed in Kittel [3], chapter 5. The following conservation laws hold:

$$\text{momentum: } \mathbf{P}_i = \mathbf{P}_f + \mathbf{p}_{cm}, \quad (29)$$

$$\text{crystal-momentum: } \mathbf{p} = \mathbf{p}_{cm}, \quad (30)$$

$$\text{energy: } E_i = E_f + \epsilon(\mathbf{p}) + \frac{\mathbf{p}_{cm}^2}{2Nm}. \quad (31)$$

The scattered neutron transfers momentum to the crystal, which is carried by the center of mass degree of freedom. Simultaneously, a phonon with wave number $\mathbf{q} = \mathbf{p} \bmod \mathbf{G}$ is created provided this process is allowed by the conservation of energy, see Fig. 6. A model calculation is sketched in appendix A whereas Fig. 7 gives some selected experimental results .

Fig. 7a displays the non-primitive cubic *bcc* unit cell, the first Brillouin zone, and the dispersion relations for (metallic) potassium. Since there is only one atom in the primitive cell there are only (three) acoustic branches. Note the different dispersion of the LA and TA branches along various directions in the Brillouin zone. Fig. 7b displays the neutron count rate of a certain (zone-boundary) optical phonon in (insulating) La_2CuO_4 at (reduced) wave number $(0.5, 0.5, 0)$ when excited in three different Brillouin zones: The maximum energy loss of the neutron is with about 15THz (or 65meV) always at the same frequency (or energy transfer) while the momentum transfer differs by reciprocal lattice vectors $(2, 2, 0)$, $(2, 2, 2)$, and $(2, 2, 4)$ (in units of $\frac{2\pi}{a}$, $\frac{2\pi}{b}$, $\frac{2\pi}{c}$, where a, b, c denote the lattice constants). Therefore, the same phonon may be created in different Brillouin-zones yet with different scattering cross sections. La_2CuO_4 crystallizes in the body centered orthorhombic structure so that the Brillouin zone boundary in $(1, 1, 0)$ direction is at $(0.5, 0.5, 0)$. The spectral width is due to the finite phonon life time as well as to the instrumental resolution. Note, *Sr*-doped La_2CuO_4 was the first *HTc* superconductor which was discovered by Bednorz and Müller [11] in 1986.

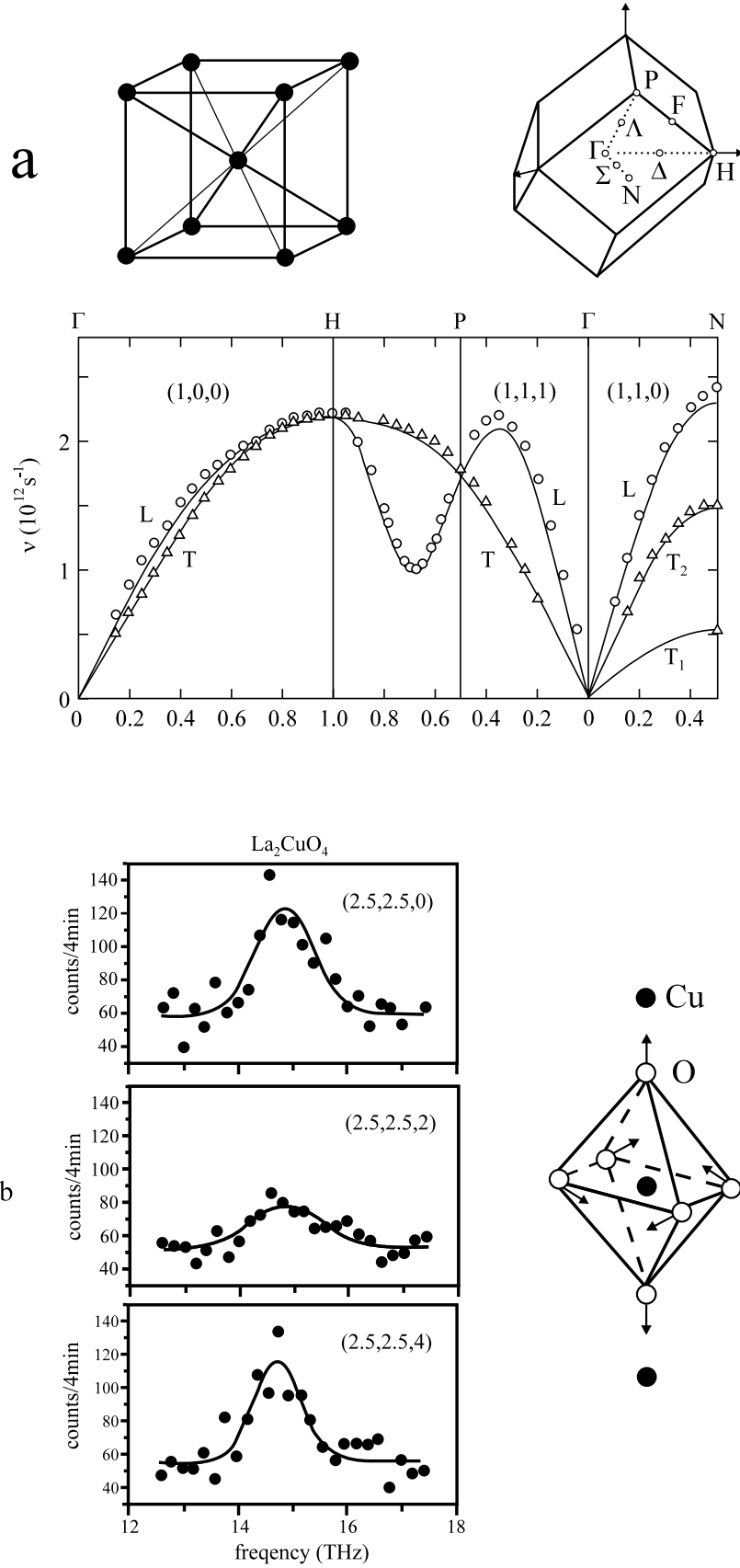


Fig. 7. (a) bcc structure, Brillouin zone, and phonon dispersion curves for potassium. Along the horizontal axis we plot q , $q/\sqrt{2}$, and $q/\sqrt{3}$ for the $(1,0,0)$, $(1,1,0)$, and $(1,1,1)$ directions, respectively. (b) excitation of a particular optical phonon (“scissor” mode) of La_2CuO_4 when excited with the participation of different reciprocal lattice vectors. According to Cowley et al.[9] and Pintschovius [10].

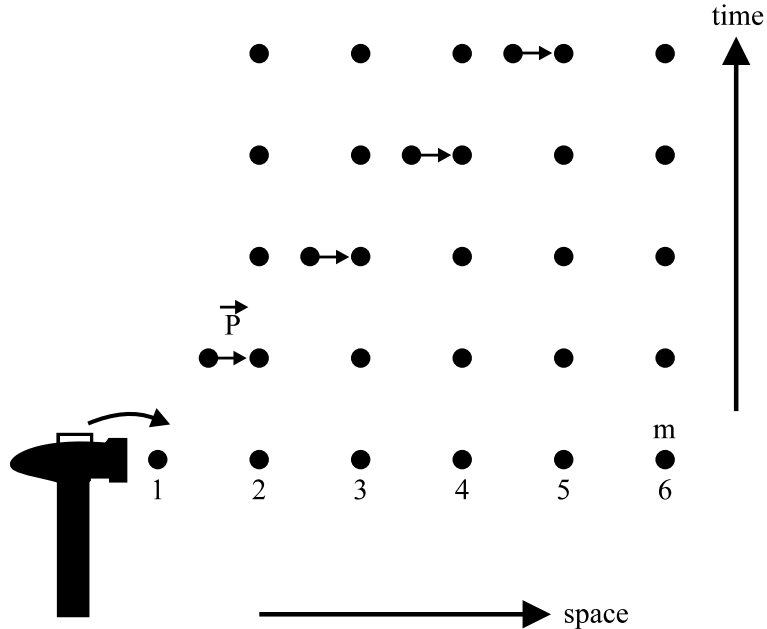


Fig. 8. *Transport of momentum and energy through a linear arrangement of masses which interact only by central collisions.*

D. Example 2: Transport of momentum and energy through a chain [8]

We consider the transport of momentum and energy through a piece of matter which is initially at rest. Next, we transfer a certain amount of momentum to one side e.g., by the hit of a hammer. The question arises how this momentum and the related energy will be passed from one volume element to the neighboring one. As a trivial example we consider the arrangement depicted in Fig. 8. The momentum p , which is transferred to particle # 1, will be transported by successive collisions. Although, this momentum is numerically equal to the total momentum of the chain, there is – in a naive view – no motion of the system as a whole at least for very large systems (see below). For a finite system the center of mass moves to the right however, with a speed proportional to the inverse of the number of masses involved. Yet, there is transport of momentum and energy with velocity $v_T = p/m$ through the system.

In another frame of reference \mathcal{R}' (moving with $-V$ with respect to \mathcal{R}) the total momentum and energy are transformed according to (see also Eq.(26)):

$$p'_{\text{tot}} = p + (Nm)V, \quad E'_{\text{tot}} = \frac{p^2}{2m} + pV + \frac{V^2}{2(Nm)}. \quad (32)$$

For fixed p the minimum of the energy can be reached in a frame of reference which moves with velocity V_0 .

$$V_0 = -p/Nm, \quad E_0 = \frac{p^2}{2m} \left(1 - \frac{1}{N}\right). \quad (33)$$

E_0 is the internal energy. For large systems, E_0 is almost identical with the energy in \mathcal{R} where, by definition, $V=0$. In all other frames of reference, however, the total energy as well as the total momentum scales to infinity with $N \rightarrow \infty$. A meaningful definition of the transported momentum and energy, however, must contain only those parts of Eqs.(32) which are independent of N in the limit of $N \rightarrow \infty$. These terms are:

$$\epsilon(p) = E_{\text{tot}} - N\mu = \frac{p^2}{2m} + pV, \quad p' = p. \quad (34)$$

The quantity $\mu = mV^2/2$, which is necessary to add a particle with mass m , is the chemical potential. The system defined by Eqs. (34) is again called a quasiparticle.

V. CONCLUSIONS

Concerning the transport of energy and momentum through matter, quasiparticles behave like ordinary particles and quasimomentum plays the part of ordinary momentum. Nevertheless, quasimomentum is not the generator of translations, and energy and momentum behave differently with respect to Galilei-transformations.

Although the quasiparticle description was originally developed for weakly interacting systems, this concept proved to be fruitful even for moderately strong interactions like real metals and liquid helium 3He and 4He at low temperatures. For strong interactions, however, new types of quasiparticles appear. For example the spin and charge degrees of freedom may separate (spinons, holons), charges may become fractional (as in the fractional Quantum Hall effect), or non Bose/Fermi statistics occurs (Anyons in two dimensional systems) [12].

The great advantage and success of the quasiparticle picture lies in the fact that thermodynamic as well as transport properties can be simply described. Examples are the temperature dependence of the specific heat in ordinary and Heavy-Fermion metals [13], de Haas van Alphen effect, cyclotron dynamics in semiconductors, or the Gunn-effect [3].

On the other hand, if a quasiparticle picture is inappropriate, like in amorphous solids or (normal) liquids, even a qualitative description is difficult. Fortunately, phonons still exist in the long wavelength limit where a continuum description always holds. For electrons in amorphous solids, on the other hand, all states become localized above a critical degree of disorder (=Anderson localization) [14]. The situation becomes even worse in (1-dimensional) quasicrystals, i.e. solids with nonperiodic but deterministic structure where the energy spectrum is not even continuous but is a Cantor-set [15].

In appendix B we try to sketch a similar chain of arguments as developed above for the quasimomentum for the angular momentum of quasiparticles.

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APPENDIX A

To establish the origin of the conservation laws stated in section IV we present a simple calculation of the phonon excitation rate upon neutron scattering. We consider a three dimensional harmonic crystal with one atom per unit cell which is described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2Nm} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}}. \quad (35)$$

$\hat{\mathbf{p}}, \hat{\mathbf{r}}$ are the center of mass momentum and coordinates of the crystal. To lighten the notation we have indicated only one of the three phonon branches $\omega(\mathbf{q})$. The external particle with mass M (“neutron”) is described by operators $\hat{\mathbf{P}}, \hat{\mathbf{R}}$ and Hamiltonian

$$\hat{H}_{ext} = \frac{\hat{\mathbf{P}}^2}{2M}. \quad (36)$$

Stationary states of the (uncoupled) system “neutron - crystal” are labeled by \mathbf{K} (=neutron momentum), \mathbf{k} (=total momentum of the crystal) with $\hbar\mathbf{k} = \mathbf{p}$, and $\{n_{\mathbf{q}}\}$,

$$|\mathbf{K}, \mathbf{k}, \{n_{\mathbf{q}}\}\rangle = \frac{e^{i\mathbf{K}\mathbf{R}}}{\sqrt{\Omega}} \frac{e^{i\mathbf{k}\mathbf{r}}}{\sqrt{\Omega}} |\{n_{\mathbf{q}}\}\rangle, \quad (37)$$

$$E(\mathbf{K}, \mathbf{k}, \{n_{\mathbf{q}}\}) = \frac{(\hbar\mathbf{K})^2}{2M} + \frac{(\hbar\mathbf{k})^2}{2Nm} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left(n_{\mathbf{q}} + \frac{1}{2}\right). \quad (38)$$

Ω is the volume of the crystal.

The interaction between the neutron and the crystal is:

$$\hat{H}_{int} = \sum_{j=1}^N V(\hat{\mathbf{R}} - (\hat{\mathbf{r}} + \mathbf{r}_j^0 + \hat{\mathbf{u}}_j)). \quad (39)$$

$V(\dots)$ denotes the interaction potential with a single atom of the crystal at position $\mathbf{r} + \mathbf{r}_j^0 + \mathbf{u}_j$, where \mathbf{r} gives the position of the center of mass of the crystal and $\hat{\mathbf{u}}_j$ the displacement of atom $\#j$ from its equilibrium position at \mathbf{r}_j^0 . According to the Golden Rule, \hat{H}_{int} induces transitions between stationary states Eq.(37) with a rate $\Gamma_{i \rightarrow f}$

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} \left| \langle i | \hat{H}_{int} | f \rangle \right|^2 \delta(E_i - E_f), \quad (40)$$

where the delta-function displays the conservation of energy.

As an initial state we chose a crystal at rest, i.e. $\mathbf{k} = 0$, $\{n_{\mathbf{q}} = 0\}$ for all \mathbf{q} . Then the transition matrix element becomes:

$$\langle f | \hat{H}_{int} | i \rangle = \int \frac{d^3\mathbf{R}}{\Omega} \int \frac{d^3\mathbf{r}}{\Omega} e^{i(\mathbf{K}_i - \mathbf{K}_f)\mathbf{R}} e^{-i\mathbf{k}\mathbf{r}} \sum_{j=1}^N \langle \{n_{\mathbf{q}}\} | V(\mathbf{R} - \mathbf{r} - \mathbf{r}_j^0 - \mathbf{u}_j) | 0 \rangle \quad (41)$$

which can be rewritten as:

$$\langle f | \hat{H}_{int} | i \rangle = \int e^{i(\mathbf{K}_i - \mathbf{K}_f - \mathbf{k})\mathbf{R}} \frac{d^3\mathbf{R}}{\Omega} \int V(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}} d^3\mathbf{r} \frac{1}{\Omega} \sum_{j=1}^N e^{i\mathbf{k}\mathbf{r}_j^0} \langle \{n_{\mathbf{q}}\} | e^{i\mathbf{k}\mathbf{u}_j} | 0 \rangle. \quad (42)$$

The first integral is nonzero only for

$$\mathbf{K}_i - \mathbf{K}_f = \mathbf{k} \quad (43)$$

which is the conservation of (total) momentum, Eq.(24). The second integral yields the Fourier-transform of the atomic potential, $V(\mathbf{k})$, which is called the structure factor of the atom.

For small displacements, we may expand the exponential operator

$$e^{i\mathbf{k}\mathbf{u}_j} = 1 + i\mathbf{k}\mathbf{u}_j \dots \quad (44)$$

The matrix element of the first term is nonzero only for $n_{\mathbf{q}} = 0$ which describes purely elastic (Bragg-) scattering:

$$\langle f | \hat{H}_{int} | i \rangle = \delta_{\mathbf{K}_i, \mathbf{K}_f + \mathbf{k}} \frac{N}{V} \sum_{\mathbf{G}} \delta_{\mathbf{k}, \mathbf{G}} V(\mathbf{k}). \quad (45)$$

The next term in the expansion changes the phonon number by one. To evaluate these matrix elements we use the representation of \mathbf{u}_j in terms of phonon creation and destruction operators $a_{\mathbf{q}}^\dagger$, $a_{\mathbf{q}}$, Eq. (17):

$$\mathbf{u}_j = \sum_{\mathbf{q}'} \sqrt{\frac{\hbar}{2Nm\omega_{\mathbf{q}'}}} e^{i\mathbf{q}'\mathbf{r}_j^0} \mathbf{e}_{\mathbf{q}} (a_{-\mathbf{q}'}^\dagger + a_{\mathbf{q}'}). \quad (46)$$

$\mathbf{e}_{\mathbf{q}}$ denotes the polarization vector (normalized eigenvector of the dynamical matrix). As a result, we obtain for elastic and single phonon excitation processes:

$$\langle f | \hat{H}_{int} | i \rangle = \delta_{\mathbf{K}_i, \mathbf{K}_f + \mathbf{k}} \frac{N}{\Omega} \sum_{\mathbf{G}} \left(\delta_{\mathbf{k}, \mathbf{G}} + i(\mathbf{k} \mathbf{e}_{\mathbf{q}}) \sqrt{\frac{\hbar}{2Nm\omega_{\mathbf{q}}}} \delta_{\mathbf{k}-\mathbf{q}, \mathbf{G}} \right) V(\mathbf{k}) \quad (47)$$

The first Kronecker-delta describes again the conservation of total momentum, Eq.(24), whereas the conservation of crystal momentum, Eq. (25), is captured by the Kronecker-deltas in the bracket. Note, that the one-phonon transition rate depends on the total transferred momentum - not on the wave number \mathbf{q} within the first Brillouin zone. For crystals with more than one atom in the primitive cell, $V(\mathbf{k})$ is replaced by the structure factor, see [3]. Higher order terms in the expansion (44) lead to multiphonon processes and to the Deye-Waller factor. Note further, that the transition rate $\Gamma_{i \rightarrow f}$ is proportional to N^2 which indicates that for Bragg-scattering as well as for inelastic phonon scattering all atoms of the crystal contribute coherently.

APPENDIX B

In the following, we try to explore if a similar chain of arguments as given above for the quasimomentum of quasiparticles can be found also for the angular momentum.

Free space has spherical symmetry i.e. it is invariant against any rotation around any axis. As a consequence (the Noether-theorem applies again) \mathbf{J}^2 and its projection onto a quantization axis (usually called z-axis) are conserved commuting quantities, i.e., their eigenvalues are “good” quantum numbers

$$\mathbf{J}^2 |j, j_z\rangle = j(j+1)\hbar^2 |j, j_z\rangle, \quad \mathbf{J}_z |j, j_z\rangle = j_z \hbar |j, j_z\rangle, \quad (48)$$

where $j = 0, \frac{1}{2}, 1, \dots$ and $j_z = -j, -j+1, \dots, j$.

The angular momentum \mathbf{J} of a particle can be decomposed into an orbital part $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and an inner part \mathbf{S} which is in some cases called spin. In a classical picture \mathbf{L} vanishes in a frame of reference in which the trajectory of the center of mass of the particle under consideration passes through the origin.

For the following discussion we consider only the inner part of angular momentum. In contrast to free space (see above), a crystalline solid is invariant only under rotations of $\pm \frac{\pi}{3}$, $\pm \frac{\pi}{2}$, $\pm \frac{2\pi}{3}$, and $\pm \pi$ around selected axes. Strictly speaking, angular momentum is therefore not a “good” quantum number for the classification of quasiparticles. The “good” quantum numbers follow from the irreducible representations of the point group of the solid (see e.g. [16]). However, the inspection of the compatibility tables of the full spherical group and of finite point groups of solids, shows that for crystals with high symmetry and in the vicinity of $\mathbf{k} = 0$ i.e. close to the Γ point and partly also along some directions of high symmetry, the angular momentum is up to $j = \frac{3}{2}$ with $j_z = \pm \frac{1}{2}, \pm \frac{3}{2}$ a “reasonably good” quantum number. Examples are the cubic point groups O_h and T_d . In uniaxial hexagonal systems like C_{6v} similar statements hold at

least for the projection of the angular momentum on the hexagonal axis. In an arbitrary direction in \mathbf{k} -space or in crystals of low symmetry, the concept of angular momentum cannot be used in solids. Within this limitation we discuss now the absorption of a photon with $\mathbf{q} \approx 0$ incident on a crystal with high symmetry in an analogous way, as we discussed the inelastic scattering of a neutron in chapter IV.C. We assume, that the photon is in a circularly polarized state σ^+ i.e., it carries an angular momentum \hbar in the direction of momentum. When the photon is absorbed in the crystal by creating an optical phonon, an exciton, a plasmon, or an optical magnon, the crystal as a whole carries the angular momentum $j_z = \hbar$ in analogy to Eq. (29) for the momentum. The rotational energy E_{rot} of the crystals as a whole, however,

$$E_{\text{rot}} = \frac{\mathbf{L}^2}{2\Theta} = \frac{\ell(\ell+1)\hbar^2}{2\Theta}, \quad (49)$$

tends to zero for a macroscopic crystal because of the large moment of inertia Θ . Simultaneously, the angular momentum of the absorbed photon appears as the quasi-, pseudo or crystal angular momentum of the created quasiparticle as for the quasimomentum in Eqs.(29), (30).

To elucidate this concept and assuming that the reader has some basic experience with group theory in solids [16], we give the following example. In a crystal with point group T_d i.e., with zincblende type crystal structure, the transitions from the crystal ground state with symmetry Γ_1 are dipole allowed only to excited states with symmetry Γ_5 in one-photon absorption processes. Simultaneously one finds in the above mentioned compatibility tables, that a state in vacuum with $j_z = 1$ is compatible with the irreducible representation Γ_5 .

In this sense we may say that a quasiparticle in a crystal carries energy, quasimomentum and even quasi angular momentum. The validity of the latter concept is, however, more restricted than that of quasimomentum. For example, there are $2s+1$ different internal states of a particle with spin s which have the same energy $\epsilon(\mathbf{p})$. Phonon, magnon etc. dispersion curves, however, split with increasing quasimomentum, in particular along low-symmetry directions, see Fig. 7a. Therefore, quasiangular momentum is not an internal degree of freedom of a quasiparticle so that it has to be used with more precautions than the concept of quasimomentum.