Quasiparticles in quantum crystals

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A new field of studies has recently arisen in solid-state physics—quantum crystals. The currently existing theoretical and experimental data indicate—leaving no doubt—that a quantum crystal is a new state of matter, which had been predicted theoretically by A. F. Andreev and I. M. Lifshitz. At low temperatures one has not too large a number of quasiparticles to deal with. This permits one to treat a quantum crystal as a "rarefied gas" of quasiparticles in the discrete space of the crystal lattice. Starting with the founding ideas of I. M. Lifshitz, a method is developed of describing the process of pairwise scattering of quasiparticles in the discrete space. The energy spectrum of the quantum crystal is discussed. The features of behavior of vacancions in solution are elucidated.

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INTRODUCTION

A new field of study has recently arisen in solid-state physics—quantum crystals. The currently existing theoretical and experimental data leave no doubt that a quantum crystal is a new state of matter, which has been predicted theoretically by Andreev and Lifshitz.[1]

The quantum theory of solids essentially assumes an identical order of magnitude among the distances between atoms. Here the minimum energy of the atomic system corresponds to an ordered and localized arrangement of the atoms in coordinate space, in which all the particles are at rest at certain equilibrium positions called the crystal-lattice nodes. The property of localization, which characterizes the crystal lattice, in this case is classical, since it does not take into account the quantum-mechanical indistinguishability of atoms and of their movement arising from tunneling.

In most crystals the thermal movement of the atoms at temperatures considerably below the melting point $(T \ll \Theta)$ has the character of small vibrations about the crystal-lattice nodes. The smallness of the vibrations implies that the mean thermal displacement of an atom from the node is very small in comparison with the lattice constant a, i.e., $\bar{u} \ll a$.

We can easily express the parameter $\bar{u}^2 / a^2 = \Lambda$ in terms of the characteristics of the atoms of the crystal. The characteristic frequency of vibration of the atoms is $\omega \sim \sqrt{(x/m)}$, where $x = U/a^2$ (U is the characteristic interaction energy of

the atoms). The Debye temperature is $\Theta \sim \hbar\omega = \hbar\sqrt{U/ma}$. The ratio of the Debye temperature to the quantity U is the parameter Λ. Hence we have

$$\Lambda = \frac{\hbar}{\sqrt{mUa}} .$$

In this form the parameter Λ is known as the de Boer parameter.

For most crystals the parameter Λ is actually very small. However, crystals exist for which Λ has large values arising from the smallness of m and the weakness of their interaction U. Thus, for example, ^{3}He has $\Lambda = 0.49$, ^{4}He has $\Lambda = 0.43$, H_2 has $\Lambda = 0.28$, Ne has $\Lambda \approx 0.1$, etc. There are other examples for which $\Lambda \gtrsim 1$. This refers to admixtures of light elements in matrices of heavy metals. Owing to their small mass and weak interaction with the atoms of the matrix, the atoms of the impurity are characterized by a parameter $\Lambda \gtrsim 1$. For example, this happens for hydrogen in matrices of niobium, zirconium, palladium, etc.

In all these cases the fundamental assumption of solid-state quantum theory that particles and crystal nodes correspond breaks down. Owing to the large values of the parameter Λ, i.e., the ratio of the amplitudes of the zero-point vibrations $\hbar/\sqrt{mU}$ to the lattice constant, the atoms of the crystal exist in a state of intense zero-point motion that leads to displacement of an atom from one node to another. On the other hand, the particles forming the crystal are generally

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identical. In quantum mechanics identical particles are indistinguishable. A situation arises in which a multitude of identical particles exists in a discrete crystal lattice, the wave functions of which overlap strongly owing to the large magnitudes of amplitudes of the zero-point vibrations. The overlap of the wave functions implies that the atoms are actually converted into moving quasiparticles in the space of the crystal lattice. One can no longer say that each particle corresponds to one definite lattice node. Any atom can exist at any node.

Evidently, two particles cannot exist simultaneously at the same lattice node. Therefore an infinitely large repulsion exists when the coordinates of two quasiparticles coincide. This is described by an "impenetrability" potential of quasiparticles at the same lattice node. Therefore it is important to take into account the correlation between particles as they approach one another.

Thus numerous crystals exist that clearly manifest the following features:

(a) the energy of the ground state of the crystal is altered by the presence of a large repulsion between the quasiparticles;

(b) the atoms are converted into moving quasiparticles in lattice space;

(c) the wave functions of the atoms overlap, leading to a finite probability of tunneling of atoms from one node to another.

The stated features lead to a physically new pattern possessing unique properties. This pattern corresponds to quantum crystals.

The fundamental ideas describing theis new state of matter have been presented by Andreev and Lifshitz[1] and have been studied theoretically and experimentally.[2-52,54,57-61,63]

At non-zero temperature the crystal tends to have a minimal free energy. Hence it can lose a little energy while slightly increasing in disorder. The conflict between this loss of energy and increase in disorder has the result that the free energy of the crystal is minimal when a certain number of vacancies exists—nodes not containing atoms. Owing to the large amplitudes of zero-point vibrations of the atoms, these vacancies become vacancions—quasiparticles characterized by a certain value of the energy ε and quasimomentum $\mathbf{p}$. Thus, a quantum crystal contains a gas of vacancions whose displacements are equivalent to the displacement of atoms.

Vacancions can exist even at absolute zero temperature—zero-point vacancions. In this case they also can move in the crystal in the equilibrium state. One can picture a quantum crystal as though it contained within itself a liquid consisting of zero-point vacancions, and hence capable of moving easily through the crystal lattice. The flow of this liquid is accompanied by mass transport of matter. In contrast to an ordinary liquid, here the direction of mass transport opposes the direction of flow of the vacancion liquid.[1,3] The vacancions lower the energy of the ground state of the crystal. The bottom of the vacancion band lies below the energy of the ground state of the crystal (Fig. 1). The width Δ of the vacancion band is proportional to the frequency of
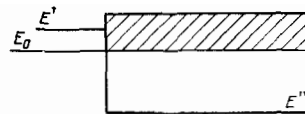

FIG. 1. Energy of a crystal containing a vacancion. E_0 is the energy of the ideal crystal; E' is the energy of the crystal containing a vacancy; E'' is the energy of the crystal containing a vacancion. The crystal with the vacancion can possess less energy than the ideal crystal.

tunneling of the atoms $(\Delta \sim J/\hbar)$. Hence the velocity of motion of a vacancion is $v \sim aJ$. In a certain sense, quantum crystals having zero-point vacancions are analogous to metals, i.e., crystals containing a liquid consisting of electrons. The electron liquid in a metal also can move easily through the crystal lattice. But every change in the electron density is accompanied by appearance of charge density, which gives rise to very strong electric fields, owing to which the spatial redistribution of mass of the material does not occur. A vacancy is an electrically neutral object. The flow of the vacancion liquid in a quantum crystal can be accompanied by a change in the spatial distribution of matter.

A light impurity atom in a quantum crystal also behaves like a quasiparticle—an impuriton or mass-fluctuation wave.[3,4]

Let us study a ^{4}He crystal containing one ^{3}He atom. This impurity atom becomes an impuriton. Owing to the ideal periodicity of the ^{4}He crystal, the energy of the impuriton is a certain periodic function of the quasimomentum $\mathbf{p}$. The width of the energy band of such an impuriton is $\Delta \lesssim 10^{-4}$ K, and the frequency of tunneling is $J \sim 1$ MHz. Hence the velocity of motion is $v \lesssim 10^{-1}$ cm/s.[3]

The width Δ of the band is considerably smaller than all the other energy characteristics of helium. Therefore the dynamics of impuritons is highly peculiar.[5-12,13,15] The ^{3}He atom possesses a nuclear spin 1/2. Hence the motion of the corresponding impuriton can be observed in NMR experiments.

These considerations on impurity particles also hold in the case of solutions of light particles in matrices of heavy metals. The light atoms become impuritons and have specific properties.[16-22]

Any defects in crystals in which the parameter Λ is not a small quantity in comparison with unity are delocalized and become quasiparticles—defectons, which are characterized by a certain value of the energy and quasimomentum.

A quantum crystal is a highly specific state of matter. As we have noted above, its density distribution is periodic in space. That is, in symmetry it resembles an ordinary crystal, but in the character of motion of quasiparticles it occupies a position intermediate between a liquid and a solid. A first form of motion has the property of motion in a liquid—this is the flow of the vacancion liquid with immobile lattice nodes. A second form of motion has the property of motion in solids, and involves displacement of crystal-lattice nodes. Evidently, when acted on by external forces, a quantum crystal does not conserve its shape. In a gravitational field a quantum crystal can flow from vessel to vessel analogously to liquids. However, the flow here is peculiar: the transfer of

matter from top to bottom is effected by flow of the vacancion liquid from bottom to top over the crystal-lattice nodes.

The motion of the above-stated quasiparticles is a quantum diffusion in lattice space, which has been found experimentally in Khar'kov (Grigor'ev, Esel'son, Mikheev, Shul'man) and in Sussex, England (Richards, Pope, Widom) in 1977.[6,7] The diffusion coefficient is an important, experimentally measurable characteristic of the gas of quasiparticles.

At finite temperatures the quasiparticles can collide with ordinary excitations, or photons. The scattering cross-section in collisions with phonons is proportional to the fourth power of the frequency. The diffusion coefficient in this region is proportional to T^{-9}.[1,3,12,13]

At low temperatures we can neglect the phonons, and scattering of quasiparticles by one another plays the main role. The diffusion coefficient in this region is proportional to the concentration of quasiparticles and is independent of the temperature.[3,16-18,50]

With rising temperature, the frequency of collisions with phonons increases, and during the time that a quasiparticle spends at a node, it comes into equilibrium with the lattice. In this case the localized quasiparticle diffuses by a random walk with a step equal to the lattice period. In this region the diffusion coefficient does not depend on the temperature.

Further increase in temperature leads to strong localization of the atoms in the potential wells of the crystal. In this case, diffusion is governed by superbarrier transitions from the excited state, and is described purely classically.

Evidently this pattern of motion has its own features depending on the type of quasiparticles (defectons, vacancions, impuritons, etc.). However, within the framework of this general pattern there are distinctive limiting situations.[19-27]

The highly unusual properties of impurity quasiparticles are preserved to a substantial degree even under conditions in which their mean free path is considerably smaller than the lattice period, as Kagan, Klinger, and Maksimov[12,13] have shown.

Depending on the statistics of the original atoms comprising the crystal, the quasiparticles in a quantum crystal obey either Bose-Einstein or Fermi-Dirac statistics. Both of these excitations can be found in a crystal in different concentrations or in the form of a solution of Fermi-Bose quasiparticles. A striking example of a quantum crystal is the ^{3}He–^{4}He solution. Phenomenological equations of hydrodynamics describing the macroscopic motions in quantum crystals have been proposed by Andreev and Lifshitz.[1] These equations enable one to study also solutions of quantum crystals (see, e.g., Ref. 49). The equations for a Fermi liquid have been derived by quantum field theory and studied for Fermi and Bose quantum crystals in the studies of Dzyaloshinskiĭ, Kondratenko, and Levchenkov.[11]

New quantum crystals have been postulated: ^{6}He and spin-oriented hydrogen.[34]

Experimental studies have recently appeared on the properties of two-dimensional quantum crystals—films of helium adsorbed on graphite.[42] At present such systems are being intensively studied by using well-known contemporary methods (neutron scattering, NMR, the Mössbauer effect, etc.).[57]

Vacancions exist in rather large concentration in an adsorbed two-dimensional helium crystal. This arises from an ordering phase transition in the field of the graphite substrate, which amounts to a network of shallow potential wells in the shape of regular hexagons covering the entire surface. Owing to the repulsion of atoms at close distances, this ordered state arises only at a density of covering at which one helium atom exists per three potential wells of graphite.

The study of periodicity and its influence on the properties of a two-dimensional crystal is the key to complete deciphering of the behavior of adsorbed systems. Both in these crystals and in those mentioned above, the phenomenon is predicted of superfluid motion—the crystal can flow practically without viscosity in thin capillaries.

This review treats a set of physical phenomena associated with the behavior of quasiparticles in quantum crystals. As we shall see below, precisely these phenomena manifest qualitatively new effects caused by the interaction of the quasiparticles with one another. The amplitude of two-quasiparticle scattering is calculated by the method of I. M. Lifshitz, which enables one to elucidate a number of interesting and unusual properties of the scattering pattern in the discrete crystal lattice.[32]

The motion of a pair of quasiparticles is described by the equation of I. M. Lifshitz, which allows one to associate the shape of the wave surface and the amplitude of the scattered quasiparticle with an arbitrary dispersion law.

The fundamental difference between the collisions of quasiparticles and those of particles in a vacuum is that the Galilean relativity principle in the usual sense is inapplicable to quasiparticles. If one identifies the quasimomentum with ordinary momentum, then it is convenient to picture that the crystal as a whole can gain momentum in definite portions.

Starting with the solution of the scattering problem, the method of calculating the increment to the free energy of the crystal caused by pair collisions of quasiparticles is then presented. Studies of the free energy of quantum crystals allow one to obtain the observed physical quantities.

The third part of the study treats a solution of pairwise-interacting Fermi-bose quasiparticles. The free energy of such a solution is calculated. This makes possible the construction of the state diagram and prediction of the properties of such crystals.

1. THEORY OF SCATTERING OF QUASIPARTICLES IN LATTICE SPACE

a) Exact solution of the problem of two-quasiparticle scattering

In the case being studied of pair collisions of quasiparticles, the method of I. M. Lifshitz enables one to construct a theory of scattering in lattice space without requiring that the interaction potential be small, as is characteristic of perturbation theory.[56]

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The construction of the theory of scattering of quasiparticles in lattice space involves calculating the effective cross-sections of the various processes that generally determine the behavior of the experimentally observed characteristics of a quantum crystal, such as the coefficient of quantum diffusion of impuritons, defectons, vacancions, or NMR times in systems of atoms possessing nuclear spin, etc. Examples of the scattering process are collisions of various quasiparticles with a classical impurity or defect in the quantum crystal, interaction of impuritons with one another, vacancions with impuritons, defectons, or with other quasiparticles. At low enough temperatures the concentration of the different quasiparticles is small. Hence pair collisions play the decisive role in creating the physical pattern. However, in contrast to the usual case of a pair collision in a vacuum, the problem of two-quasiparticle scattering does not reduce to the problem of scattering of one particle in the field of a motionless force center. The momentum of the center of gravity of the two quasiparticles is not eliminated by transforming their coordinates, since the motion of the quasiparticles is restricted by the crystal lattice. Hence the amplitude of pair scattering depends not only on the relative momentum of the quasiparticles, but also on the momentum of the center of gravity. Both these momenta determine the shape of the isoenergy surfaces of the scattering quasiparticles, whose dispersion laws are generally periodic functions of these momenta. Naturally, the laws of conservation of quasimomentum and energy are fulfilled in pair collisions ($p_i = p_e + 2\pi\hbar b$, $\varepsilon_i = \varepsilon_e$, where p_i and p_e are the sums of the quasimomenta before and after collision, b is an arbitrary reciprocal-lattice vector, and ε_i and ε_e are the energies of the quasiparticles before and after collision). One distinguishes normal processes ($b = 0$) and flipping processes ($b \neq 0$). However, this distinction is relative in character, since one can choose the unit cell of the reciprocal lattice arbitrarily.

In the crystal the quasiparticles migrate over the lattice nodes. Evidently two quasiparticles cannot exist simultaneously at the same node. This is ensured by the existence of an "impenetrability" potential (infinitely large potential when their coordinates coincide):

$$U_{RR'} = \begin{cases} V \to \infty, & R = R', \\ 0, & R \neq R'. \end{cases} \tag{1.1}$$

Here R and R' are discrete vectors corresponding to lattice nodes. This interaction can be rather large when the coordinates R and R' coincide. However, on the average it remains small, since it equals zero at other points, except for the nodes. In addition to this potential between the quasiparticles, a long-range attraction also acts. Its character depends on the type of quasiparticles and on the conditions under which they are manifested. Thus, for example, the theory of elasticity yields the following expression for the energy of elastic interaction of any type of point defects:

$$u(R - R') = V_0(n) \left(\frac{a}{|R - R'|} \right)^3. \tag{1.2}$$

Here $V_0(n)$ is the characteristic energy, which depends on the mutual orientation of the quasiparticles.

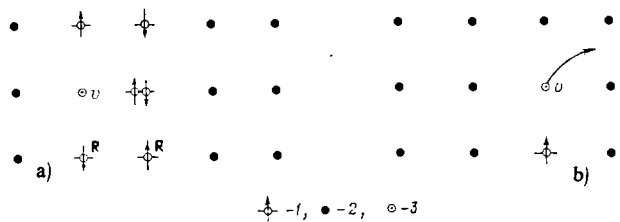FIG. 2. Scattering of quasiparticles. 1—^{3}He; 2—^{4}He; 3—vacancion (v).

In order to study the scattering process, let us first examine the simple case of the potential of (1.1). Let two quasiparticles with the momenta k_1 and k_2 and energies $\varepsilon(k_1)$ and $\varepsilon(k_2)$ interact via the impenetrability potential (Fig. 2a). The case in which the atoms do not change places in the treatment corresponds to "elastic" scattering. In "inelastic" scattering, the atoms of the target leave the given node to enter another (Fig. 2b). The process of two-quasiparticle scattering is described by the Lifshitz equation[31,32,44]:

$$\sum_{R''} A_{R_1 - R''} \varphi(R'', R_2) + \sum_{R''} A'_{R'' - R_2} \varphi(R'', R_1)$$
$$+ \sum_{R''} V(R_1, R_2) \varphi(R_1, R'') -$$
$$= z\varphi(R_1, R_2). \tag{1.3}$$

Here the magnitudes of the A_R correspond to the dispersion laws in the momentum representation:

$$\sum_R A_R \exp(ik_1 k) = \varepsilon(k_1), \quad \sum_R A'_R \exp(ik_2 R) = \varepsilon(k_2). \tag{1.4}$$

Also we have $z = E + i0$, where E is the total energy.

Generally this equation describes the different processes of scattering of quasiparticles in the discrete crystal-lattice space for different interaction potentials $V(R_1, R_2)$. In the case of interaction of (1.1), this equation will have the form

$$\sum_{R''} A_{R_1 - R''} \varphi(R'', R_2) + \sum_{R''} A'_{R'' - R_2} \varphi(R'', R_1)$$
$$+ V \sum_{R''} \delta_{R_1 R_2} \varphi(R_1, R'')$$
$$= z\varphi(R_1, R_2). \tag{1.5}$$

In this case Eq. (1.5) can be solved exactly, whereby one obtains the exact scattering wave function. The interaction operator of (1.1) satisfies the condition of degeneracy. That is, it can be represented as the sum of a finite number of projection operators onto the subspaces L^2. The canonical form of an arbitrary operator $\hat{A}$ that is degenerate is defined by the relationship[31]

$$(\hat{A}f, g) = \sum_{k=1}^{n} a_k l^{*(k)}(f) l^{(k)}(g). \tag{1.6}$$

Here the $l^{(k)}(f)$ are linear functionals, the a_k are real numbers, and f and g are arbitrary functions of L^2. The number of terms in the formula (1.6) is called the rank of the operator $\hat{A}$.

Having in mind below the study of the case of an arbitrary interaction operator, we shall start with the rather perspicuous case of a first-rank operator:

$$(\hat{A}f, g) = al^*(f) l(g). \tag{1.7}$$

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An example of such an operator is the "impenetrability" potential of quasiparticles, which expresses the fact that two particles cannot lie simultaneously at one node:

$$U_{R_1R_2} = V\delta_{R_1R} \cdot \delta_{R''R_2}. \qquad (1.8)$$

Here δ_{R,R_2} is the Kronecker δ symbol, and V is the characteristic interaction energy. The value of this function at another point $R = R_0$ is obtained by applying the operator l to the function $f(R)$. We can rewrite Eq. (1.5) as follows in operator form:

$$(\hat{L}_1 + \hat{L}_2 - \hat{\Lambda})\,\varphi = z\varphi. \qquad (1.9)$$

Here the terms $\hat{L}_{1\varphi}$ and $\hat{L}_{2\varphi}$ correspond to the first two terms of Eq. (1.5), which describe the transition from the node R_1 to the node R_2. Actually $\hat{L} = \hat{L}_1 + \hat{L}_2$ is the kinetic-energy operator of noninteracting quasiparticles, for which we can write the equation

$$(\hat{L}_1 + \hat{L}_2)\,\psi = \lambda\psi. \qquad (1.10)$$

Evidently, the functions ψ have the form of plane waves:

$$\psi = \exp(i\mathbf{k} \cdot \mathbf{R}). \qquad (1.11)$$

Equation (1.9) can be easily solved with allowance for the condition (1.8). Upon applying the operator $(\hat{L} - z)^{-1}$ to the equation, we have

$$\varphi = \int_{\varepsilon_1 + \varepsilon_2 = z} \frac{(\hat{\Lambda}\varphi_1\psi)\,\psi\,d\mathbf{k}}{\varepsilon_1 + \varepsilon_2 - z}. \qquad (1.12)$$

Let us introduce the notation:

$$\mathbf{p} = \mathbf{k}_2 - \mathbf{k}_1, \quad \mathbf{q} = \mathbf{k}_2 + \mathbf{k}_1, \quad \mathbf{q}' = \mathbf{q}_2 - \mathbf{q}_1, \quad z = E + i0,$$

$$E = \varepsilon\left(\mathbf{p} - \frac{\mathbf{q}'}{2}\right) + \varepsilon\left(\mathbf{p} + \frac{\mathbf{q}'}{2}\right).$$

Then the expression for φ will be:

$$\varphi(\mathbf{R}) = \tau V \int \frac{\exp(i\chi\mathbf{R})\,d\chi}{\varepsilon(\chi - (\mathbf{q}/2)) + \varepsilon(\chi + (\mathbf{q}/2)) - z}. \qquad (1.13)$$

Here we have $\tau = \varphi(0)$, and $\mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1$.

From the boundary condition for the wave function, which corresponds to the requirement that two quasiparticles cannot lie at one node, we obtain an equation that enables one to determine the eigenvalues of the energy:

$$1 = V \int \frac{d\chi}{-z + \varepsilon(\mathbf{p} - (\mathbf{q}/2)) + \varepsilon(\mathbf{p} + (\mathbf{q}/2))}. \qquad (1.14)$$

The quantity τ is an important characteristic of the scattering problem. We can derive the final expression from the complete form of the wave function for τ. The wave function as the sum of the incident and scattered waves will have the form

$$\varphi(\mathbf{R}) = \exp(i\mathbf{p} \cdot \mathbf{R}) + \tau V \int \frac{\exp(i\chi\mathbf{R})\,d\chi}{\varepsilon(\chi - (\mathbf{q}/2)) + \varepsilon(\chi + (\mathbf{q}/2)) - z}. \qquad (1.15)$$

Hence we have

$$\tau = \left[1 + V \int \frac{dx}{-\varepsilon(\chi - (\mathbf{q}/2)) - \varepsilon(\chi + (\mathbf{q}/2)) + z}\right]^{-1}. \qquad (1.16)$$

The integration in the latter equation is performed over the surface

$$\varepsilon\left(\chi + \frac{\mathbf{q}}{2}\right) + \varepsilon\left(\chi - \frac{\mathbf{q}}{2}\right) = E.$$

Thus Eqs. (1.14)–(1.16) describe the scattering process and allow one to find the exact magnitudes characterizing the collision of the quasiparticles when the first-rank interaction operator is degenerate. This case, which is important *per se* in a number of problems of scattering theory, is also essential because it suffices to approximate the interaction operator with degenerate operators for describing the overall scattering problem.

Let us examine the behavior for large $\mathbf{R}$ of the integral that enters into (1.15):

$$I(\mathbf{q}, E) = \int \frac{\exp(i\chi\mathbf{R})\,d\chi}{\varepsilon(\chi - (\mathbf{q}/2)) + \varepsilon(\chi + (\mathbf{q}/2)) - z}. \qquad (1.17)$$

Let $\mathbf{n}$ be the direction of propagation of the wave. We shall denote $\chi \cdot \mathbf{n} = u$, and perform the integration initially over a strip on the surface between $\mathbf{u}$ and $\mathbf{u} + d\mathbf{u}$, and then over the variable $\mathbf{u}$. This yields

$$I(\mathbf{q}, E) = \int f_{\mathbf{q}, E}(u)\exp(iuR)\,du. \qquad (1.18)$$

Here we have

$$f(u)\,du = \int_{\substack{\varepsilon(\chi - \frac{\mathbf{q}}{2}) + \varepsilon(\chi + \frac{\mathbf{q}}{2}) = E, \\ u < \chi\mathbf{n} < u + du}} \frac{d\Omega}{|\nabla\varepsilon(\chi - (\mathbf{q}/2)) + \nabla\varepsilon(\chi + (\mathbf{q}/2))|}. \qquad (1.19)$$

In the asymptotic expression of the integral of (1.18), terms of order of R^{-1} arise on integrating in the neighborhood of the discontinuities of the function $f(u)$, which are elliptic points of contact of the surface $\varepsilon(\chi - \mathbf{q}/2) + \varepsilon(\chi + \mathbf{q}/2) = E$ with the reference plane of the direction $\mathbf{n}$. These points are given by the equations

$$\varepsilon\left(\chi_\nu + \frac{\mathbf{q}}{2}\right) + \varepsilon\left(\chi_\nu - \frac{\mathbf{q}}{2}\right) = E,$$
$$\left[\mathbf{n}\left\{\nabla\varepsilon\left(\chi_\nu - \frac{\mathbf{q}}{2}\right) + \nabla\varepsilon\left(\chi_\nu + \frac{\mathbf{q}}{2}\right)\right\}\right] = 0. \qquad (1.20)$$

The discontinuities of the derivatives of the function $f(u)$ yield the terms of higher order of smallness, i.e., $O(R^{-2})$, which we shall neglect. At the points χ_ν the jumps Δ_ν are determined by the equation

$$\Delta_\nu\,du = d\Omega_{\chi_\nu}\cdot\left|\nabla\varepsilon\left(\chi_\nu - \frac{\mathbf{q}}{2}\right) + \nabla\varepsilon\left(\chi_\nu + \frac{\mathbf{q}}{2}\right)\right|^{-1}. \qquad (1.21)$$

Here $d\Omega_{\chi_\nu}$ is the area of the surface of the "hat" with its center at the point χ_ν and the height du:

$$d\Omega_{\chi_\nu} = 2\pi K_\nu^{-1/2}\,du.$$

Further, K_ν is the Gaussian curvature of the surface at the point ν. Finally we have

$$I = \frac{\exp(i\chi_\nu \cdot \mathbf{R})}{\sqrt{K_\nu R}}\frac{1}{|\nabla\varepsilon(\chi_\nu - (\mathbf{q}/2)) + \nabla\varepsilon(\chi_\nu + (\mathbf{q}/2))|}. \qquad (1.22)$$

The asymptotic expression for large $\mathbf{R}$ form Eqs. (1.15) and (1.22) will have the form

$$\varphi(\mathbf{R}) = \exp(i\mathbf{p} \cdot \mathbf{R}) + \tau V \sum_\nu f_\nu(\mathbf{p}, \mathbf{q}, \mathbf{q}')\frac{\exp(i\chi_\nu \cdot \mathbf{R})}{R}. \qquad (1.23)$$

Consequently,

$$f_\nu(\mathbf{p}, \mathbf{q}, \mathbf{q}') = \frac{\tau V}{|\nabla\varepsilon(\chi_\nu - (\mathbf{q}/2)) + \nabla\varepsilon(\chi_\nu - (\mathbf{q}/2))|\sqrt{K_\nu}}. \qquad (1.24)$$

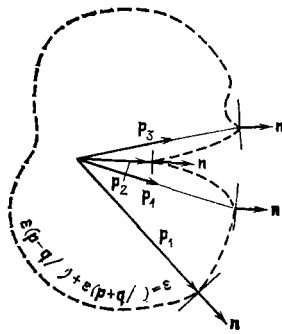719   Sov. Phys. Usp. **27** (9), September 1984

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FIG. 3. Isoenergy surface of scattered quasiparticles. The direction of scattering is n.

is here the amplitude of scattering of the two quasiparticles by one another.

The expression that we have found for the wave function (1.23) allows us to draw a number of conclusions regarding the character of the scattered waves.

In most cases the wave function of a scattered quasiparticle in a quantum crystal amounts to a superposition of several waves, whose number equals the number of possible solutions of Eq. (1.20). Each of these waves has its own form and its own rate of propagation (Fig. 3).

Each term in Eq. (1.24) determines the cross-section of a process in which the quasiparticles after scattering have a definite value of the quasimomentum for a given value of q.

In the case of open isoenergy surfaces, directions can also exist in the crystal along which scattering is "forbidden". The event of scattering in this direction will occur only if one of the quasiparticles goes over into another concavity of the surface $\varepsilon(\chi_\nu - q/2) + \varepsilon(\chi_\nu + q/2) = E$ for the fixed value of q.

b) Scattering of a vacancion by a defecton

The energy of a vacancion is a periodic function of the quasimomentum. The form of this function is determined by the structure of the lattice and by its symmetry. For example, in the strong-coupling approximation in a simple cubic lattice, the dispersin law has the form

$$\varepsilon\ (\mathbf{k}) = \varepsilon_0 + \Delta_v\ (\cos k_x a$$
$$+ \cos k_y a + \cos k_z a).$$

Here ε_0 is the energy of formation of a vacancion (in bcc ^{4}He at pressures $P \sim 25$ atm we have $\varepsilon_0 \sim 5$ K, and in hcp ^{4}He $\varepsilon_0 \sim 15$ K), and Δ_v is the width of the vacancion band $(\Delta_v \sim 10$ K).

Figure 4 shows the form of the isoenergy surface constructed by machine calculation in the case in which $\cos k_x a + \cos k_y a + \cos k_z a = 0.9$. As we pointed out above, the scattering direction is determined by the form of the isoenergy surface. In this case scattering occurs in four directions in the crystal corresponding to the convexities of the isoenergy surface.

The width of the energy band of a vacancion considerably exceeds the width of the defecton band Δ_i. Hence we can treat the interaction of these quasiparticles as a process of elastic scattering of a vacancion by a classical defect in the
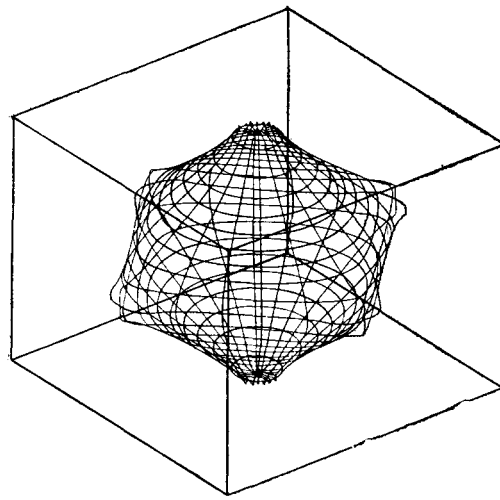

FIG. 4. Isoenergy surface in the case of a cubic crystal.

quantum crystal, neglecting the intrinsic tunneling of the defect.[3] This scattering process is described by the Lifshitz equation[44]:

$$\sum_{\mathbf{R}'} A_{\mathbf{R}-\mathbf{R}'}\varphi\ (\mathbf{R}') - z\varphi\ (\mathbf{R}) = V\delta_{\mathbf{R}\mathbf{R}'}\varphi\ (\mathbf{R}'). \tag{1.25}$$

Here

$$\varepsilon\ (\mathbf{k}) = \sum_{\mathbf{R}} A_{\mathbf{R}} \exp\ (i\mathbf{k}\cdot\mathbf{R}) \tag{1.26}$$

is the dispersion law of a vacancion, and V is the characteristic interaction energy $(V \sim 10^3\ \Delta_v)$.

By using the boundary condition that a vacancion cannot exist at the same node as an impurity, we find from the expression for the wave function

$$\varphi\ (\mathbf{R}) = \exp\ (i\mathbf{p}\mathbf{R}) + \tau V \int \frac{\exp\ (i\chi\mathbf{R})\,d\mathbf{x}}{\varepsilon\ (\chi) - z} \tag{1.27}$$

that

$$\tau = \Big[1 - V \int \frac{d\chi}{\varepsilon\ (\chi)\ -z}\Big]^{-1}. \tag{1.28}$$

The eigenvalues of the scattering energy $E\ (z = E + i0)$ are determined by an equation that stems from Eq. (1.14)

$$1 = V \int \frac{d\chi}{\varepsilon\ (\chi) - z}. \tag{1.29}$$

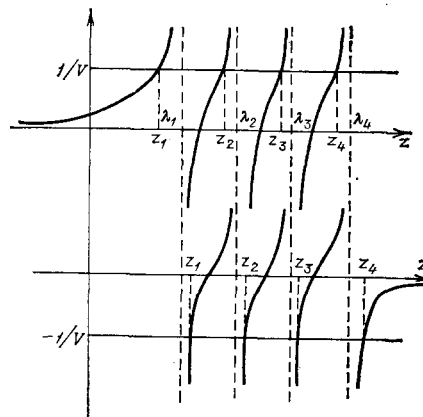Figure 5 shows graphically the solution of Eq. (1.29). The

FIG. 5. Graphic solution of Eq. (1.29).

sequence of eigenvalues z_p alternates with the sequence λ_k. In additiion to the scattering states, in special cases Eq. (1.29) has a solution corresponding to bound states of the quasiparticles. Outside each of the intervals of the continuous spectrum of values of E, Eq. (1.29) has no more than one solution. These roots split off, either only from the right-hand boundaries of the intervals, or only from the left-hand boundaries, depending on the sign of V, and they correspond to localized states.

Upon studying the asymptotic values of φ for large $\mathbf{R}$, we obtain from Eq. (1.27):

$$\varphi(\mathbf{R}) = \exp(i\mathbf{p}\mathbf{R}) + \frac{\tau V}{R} \sum_\nu f_\nu \exp(i\chi_\nu \mathbf{R}).$$

Here f_ν is the amplitude of scattering by a vacancion:

$$f_\nu = \frac{\tau V}{|\nabla \varepsilon(\chi_\nu)\sqrt{K_\nu}|}.$$

Also, K_ν is the Gaussian curvature of the surface $\varepsilon(\chi) = E$ at the point of contact of this surface with the plane of the scattering direction $\mathbf{n}$.

Consequently the total scattering cross-section will be

$$\sigma = \frac{V^2}{v(\mathbf{k}_0)\,v(\mathbf{k}_\nu)\,K_\nu}\left(1 + V\int \frac{d\chi}{z - \varepsilon(\chi)}\right)^{-2}. \quad (1.30)$$

After scattering, the vacancion will be a superposition of several waves whose number equals the number of sheets of the isoenergy surface $\varepsilon(\chi) = E$.

In analyzing the process of scattering of a vacancion, we must bear in mind the fact that a vacancion at low enough temperatures lies near the bottom of the band where its energy is minimal. In this case the dispersion law will be quadratic: $\varepsilon(\chi) = \hbar^2\chi^2/2m^*$ (m^* is the effective mass of the vacancion: $m^* \sim \hbar^2\Delta a^2$). According to Eq. (1.27), the wave function of the vacancion in this case will be

$$\varphi(\mathbf{R}) = \exp(i\mathbf{p}\cdot\mathbf{R}) - \frac{m^* a^3 \tau V}{2\pi\hbar^2}\frac{\exp(i\cdot 2m^* ER/\hbar^2)}{R}. \quad (1.31)$$

Consequently, in scattering in the field of a repulsive potential, the vacancion remains all the time inside a single reciprocal-lattice cell. When the energy is close to the maximum, the vacancion goes over into the adjacent reciprocal-lattice cell.

In scattering in the field of an attractive potential, the pattern will be the reverse. The situation here is analogous to the motion of electrons in metals,[53] but with allowance for the fact that the vacancion, owing to the periodicity of the dispersion law in the general case, can be reflected not only from the point at which the energy reaches a maximum, but also from the point at which the energy is minimal, since at this point the velocity also vanishes.

c) Scattering of a vacancion by an impuriton

The phenomenon of scattering of a vacancion by an impuriton is substantially important for explaining the experimental facts on spin diffusion.[4,7–9] Here we must distinguish the cases of "elastic" and "inelastic" scattering—the impuriton does not move from its node in the scattering process, or shifts to an adjacent node. First let us examine the graphic example of one-dimensional scattering. Let the vacancion be

scattered by an impuriton whose intrinsic tunneling is a sufficiently small quantity. Consequently, during the time of interaction the impuriton succeeds only in being displaced by a distance of the order of a reciprocal-lattice period, while the vacancion is scattered by this impurity. Whenever the impact parameter of the scattering is large enough, the vacancion after scattering cannot become a nearest neighbor of the impuriton. This rules out the possibility of simultaneous exchange of places of these quasiparticles.

Let the interaction potential of the vacancion with the impuriton have the form

$$V_{R_\nu R_1} = \frac{V_0 a}{R_\nu - R_1},$$

Here V_0 is the characteristic interaction energy, and R_ν and R_i are the one-dimensional position vectors of the interacting quasiparticles. We examine the case in which $R_i \ll R_\nu$. Thus, for example, within the time of interaction, the impuriton is displaced from the coordinate origin only by the amount a or $-a$. The Lifshitz equation for this process has the following form:

$$\sum_{R'} A_{R_\nu - R'}\varphi(R', R_1) - z\varphi(R_1, R_\nu) = \sum_{R'} V_{R_\nu - R_1}\varphi(R', R_\nu). \quad (1.32)$$

The interaction potential $V_{R_\nu R_i}$ under the condition $R_i \ll R_\nu$ is approximated in terms of the degenerate potential in the form of a finite series. Substitution of the latter into Eq. (1.32) yields

$$\sum_{R'} A_{R_\nu - R'}\varphi(R', R_1) - z\varphi(R_1, R_\nu)$$

$$= \sum_{R'} V_0 a\left(\frac{1}{R_\nu} + \frac{R_1}{R_\nu^2}\right)\varphi(R', R_\nu). \quad (1.33)$$

Equation (1.33) allows us to determine the cross-section of the scattering process being discussed. In order to do this, as we have pointed out in Sec. 1a, we must find the asymptotic expression of the wave function of (1.33), which leads to the following expression for the scattering amplitude:

$$f_{00} = \frac{V_0 a\varepsilon}{|\partial\varepsilon/\partial\chi|}\left(1 + V_0\varepsilon a\int \frac{d\chi}{-\varepsilon(\chi) + z}\right)^{-1}. \quad (1.34)$$

Here $\varepsilon = \sum_{R_\nu}\exp(i\chi R_\nu)/R_\nu$. Analogously one determines the scattering amplitude of the process in which the impuriton is displaced to the nearest neighboring node.

In the process of "inelastic" scattering of a vacancion by an impuriton, exchange of places occurs as soon as these quasiparticles lie at adjacent nodes. For example, this phenomenon in a dilute solution of a strongly polarized ^{3}He–^{4}He crystal gives rise to spin diffusion, which is observed experimentally.

The Lifshitz equation describing the stated scattering process can be written in the form

$$\sum_{\substack{\mathbf{a}, \\ R_1 \neq R_\nu}} A_{R_1, R_\nu + \mathbf{a}}\varphi(R_1, R_\nu + \mathbf{a}) - z\varphi(R_\nu, R_1)$$

$$= t\sum_{\mathbf{a}}\{\varphi(R_1, R_\nu) - \varphi(R_i, R_\nu + \mathbf{a})\}\delta_{R_1 R_\nu + \mathbf{a}}. \quad (1.35)$$

Here $\mathbf{R}_i$ and $\mathbf{R}_\nu$ are respectively the discrete coordinates of

the impuriton and the vacancion, and t is proportional to the probability of transition of the vacancion from a node to an adjacent node.

For simplicity we shall assume that the impuriton lies at the coordinate origin. The scattering amplitude is determined from the asymptotic expression of the solution of Eq. (1.35), and will be

$$f = \frac{t}{|\nabla \varepsilon (\chi_v)| \sqrt{K_v}} [\varphi(-\mathbf{a}) - \varphi(0)]. \qquad (1.36)$$

Here we have

$$\varphi(0) = \frac{\int \dfrac{d\chi}{\varepsilon(\chi) - z}}{\int A_\chi \, d\chi / [\varepsilon(\chi) - z]},$$

$$\varphi(-\mathbf{a}) = \frac{\int \exp(-i\chi \mathbf{a}) \, d\chi / [\varepsilon(\chi) - z]}{\int A_\chi \, d\chi / [\varepsilon(\chi) - z]},$$

$$A_\chi = \sum_\mathbf{a} e^{i\chi \mathbf{a}}.$$

One determines the scattering amplitude in a completely analogous way when the impuriton does not lie at the coordinate origin. In this case one uses the expression $\delta_{\mathbf{R}_i,\mathbf{R}_v + \mathbf{a}} = \Sigma_\mathbf{R} \cdot \delta_{\mathbf{R}_i\mathbf{R}} \cdot \delta_{\mathbf{R}\cdot\mathbf{R}_v + \mathbf{a}}$ in Eq. (1.35)

Let us calculate the spin diffusion in the case of a Boltzmann gas of vacancions while using the expression (1.36) that we have derived for the scattering amplitude. The mean velocity of motion of a reversed spin owing to scattering by it of vacancions is written as follows[14,63]:

$$\mathbf{u} = \sum_\mathbf{a} \mathbf{a} W_\mathbf{a} = \sum_\mathbf{a} \mathbf{a} \int d\mathbf{k} \sigma_\mathbf{a}(\mathbf{k}) \, v(\mathbf{k}) \, [n(\varepsilon) - n(\varepsilon + \mathbf{F} \cdot \mathbf{a})]. \qquad (1.37)$$

Here $W_\mathbf{a}$ is the probability of displacement of the reversed spin by the vector $\mathbf{a}$, $\mathbf{F}$ is the force acting on it, and $n(\varepsilon)$ is the distribution function of the vacancions. For example, if we use Eq. (1.36) with $\mathbf{F} \cdot \mathbf{a} \sim t$, we have

$$\mathbf{u} = \sum_\mathbf{a} \mathbf{a} \alpha(\mathbf{a}) \int v(\varepsilon) \exp\left(-\frac{\varepsilon}{T}\right) \left[1 - \exp\left(-\frac{t}{T}\right)\right] d\varepsilon. \qquad (1.38)$$

Here we define

$$\alpha(\mathbf{a}) = t^2 [\varphi(-\mathbf{a}) - \varphi(0)] |\nabla \varepsilon(\mathbf{k}_0) \sqrt{K_v}|^{-1}.$$

The latter expression enables one to study spin diffusion for various dispersion laws of the vacancions, i.e., for various $\alpha(\mathbf{a})$ and densities of state $v(\varepsilon)$. For example, in the case $v(\varepsilon) \sim (\varepsilon - \varepsilon_0)^{-1/2}$, one obtains well known results[14,61,63] that coincide with the experimental data (see the review on the NMR experiments in Ref. 4, and also Refs. 6–9).

d) Scattering of like quasiparticles

As low enough temperatures the experimentally observable characteristics (quantum-diffusion coefficient, heat capacity, NMR relaxation times, etc.) are governed by the pair collisions of quasiparticles with one another.[3,9] To elucidate the fundamental features of pair collisions in the lattice space of the crystal, let us study the scattering of a vacancion by a vacancion and of an impuriton by an impuriton.

From the standpoint of experimental studies, the process of scattering of a vacancion by a vacancion seems interesting for studying the problem of formation of bound states of vacancions in a crystal.

The features of the bound states of different quasiparticles in a quantum crystal that are accessible to experimental verification have been predicted in the studies of Andreev.[3,17] These features include, for example, the correlation of vacancions, or of two quasiparticles, caused by the finite width of their bands. The total kinetic energy of two vacancions cannot vary more than by the width of the band Δ_v. The interaction energy is also bounded by the magnitude of Δ_v. Therefore two vacancions cannot approach or separate from one another by an arbitrary distance. The distance between them is determined by the condition that the interaction energy is of the order of Δ_v. However, such a pair of quasiparticles can move freely in the crystal, but only along certain special directions. Consequently two- or one-dimensional quasiparticles arise in the three-dimensional quantum crystal. The existence in the crystal of crystallographically equivalent points for finding such a pair implies the possibility of its motion as a whole.

Crystal-lattice symmetry can be taken into account in detail in the process of formation of bound states by employing the founding study of Pitaevskiĭ,[41] which showed that bound states of various quasiparticles can be formed in the crystal at certain special lattice points when the interaction between the quasiparticles is arbitrarily weak.

The formation of bound states of vacancions is described within the framework of the Lifshitz equation, whose solution allows one to determine the wave functions and energies of the new excitations.

Let us write the Lifshitz equation for vacancions being scattered:

$$\sum_{\mathbf{R}'} A_{\mathbf{R}_v - \mathbf{R}'} \varphi(\mathbf{R}', \mathbf{R}_v) + \sum_{\mathbf{R}'} A'_{\mathbf{R}' - \mathbf{R}_v} \varphi(\mathbf{R}_v, \mathbf{R}')$$
$$+ t \sum_{\mathbf{R}'} V_{\mathbf{R}_v \mathbf{R}'} \varphi(\mathbf{R}', \mathbf{R}_v) = z\varphi. \qquad (1.39)$$

Here t is an arbitrary real parameter, while V is the first-rank interaction operator. In particular, if we allow for the fact that vacancions cannot approach to distances less than $\mathbf{R}_0$, we can represent the interaction in the form

$$V = V_0 \delta_{\mathbf{R}\mathbf{R}_0}.$$

Here V_0 is the characteristic interaction energy, while $R_0 \sim a(V_0/\Delta)^{1/3}$.[1] This representation of the potential is important only for simplicity of presentation, and does not restrict the generality.

We obtain the following equation to determine the eigenvalues of the energy from Eq. (1.39) with account taken of the boundary condition on the wave function, which consists in the idea that two vacancions cannot lie at a single node (see Sec. 1a):

$$1 = tV_0 \int \frac{d\chi}{\varepsilon(\chi - (q/2)) + \varepsilon(\chi + (q/2)) - z}. \qquad (1.40)$$

This equation, along with the eigenvalues of the scattering energy, also defines the energies of the bound states of vacan-

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[1] If the vacancions interact via the potential $V = V_0(a/R)^3$, then the condition $V \sim \Delta$ yields the stated value of R_0.

cions. The wave functions corresponding to these states are determined by solving Eq. (1.39) (Sec. 1a).

For example, let the crystal have a sixfold symmetry axis. Then, as Pitaevskiĭ[41] showed, bound states can be formed near the symmetry axis when $t \to 0$. This arises from the fact that special points exist near the symmetry axis for which the integrand in Eq. (1.40) diverges. Owing to this, the equation has a solution for infinitesimally small t. The integrand in Eq. (1.40) can be represented in the form of the following series lacking second-order terms:

$$\varepsilon\left(\chi - \frac{q}{2}\right) + \varepsilon\left(\chi + \frac{q}{2}\right) = 2\varepsilon\left(\frac{q_0}{2}\right) + b\chi_\perp^4. \qquad (1.41)$$

Here q_0 is a certain point on the symmetry axis.

At this point the coefficient of the expansion, e.g., that of $\chi_\perp^2$ vanishes, where $\chi_\perp$ is the momentum perpendicular to the symmetry axis. This condition is the definition of the point q_0.

Upon substituting the expansion (1.41) into Eq. (1.40), we find the following expression for the binding energy $\delta_0 = 2\varepsilon(q_0/2) - E$:

$$\delta_0 = \frac{\pi^2 \Lambda^2 t V_0}{16b}. \qquad (1.42)$$

Here Λ is a quantity of the order of the reciprocal-lattice period.

Whenever the crystal has two- or fourfold symmetry axes, second-order terms will also exist in the expansion of the total energy. The energy of the bound vacancions in such cases is calculated analogously on the basis of Eqs. (1.39) and (1.40).

Depending on the way in which they are formed, vacancions can obey either Bose or Fermi statistics. In the case of Fermi vacancions, pairs of quasiparticles can be formed near the Fermi surface (analogously to Cooper pairs in superconductors).[56]

A rarefied impuriton gas exists in a dilute ^{3}He–^{4}He solution at low enough temperatures. As is indicated by the theoretical and experimental studies,[3,7-9] the diffusion coefficient of the impuritons is inversely proportional to the concentration of the latter:

$$D \approx \frac{Ja^4}{\sigma x}. \qquad (1.43)$$

Here J is the frequency of tunneling, and σ is the scattering cross-section of an impuriton by an impuriton, which is determined by Eq. (1.24) with various impuriton dispersion laws. In the case of a simple cubic lattice, the scattering cross-section of impuritons, according to Eq. (1.24) ($q = 0$) will be[2]

$$\sigma = \frac{16\pi^2 a^2}{\Lambda^2 I^2(0)},$$

$$I(0) = \int d\mathbf{k} \left[2\varepsilon_0 - E + (2\Delta \cos k_x a + \cos k_y a + \cos k_z a)\right]^{-1}. \qquad (1.44)$$

As was shown in the experimental study of Richards and Owers-Bradley,[40] at temperatures below 5 K and covering densities from 0.7 to 1.0 (with respect to the covering density

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[2] Integrals of the type of $I(0)$ have been tabulated in Ref. 63.

of a filled monolayer), the processes of quantum tunneling that occur in the two-dimensional system make the fundamental contribution to the fluctuations of the local field. The scattering cross-section, and hence the quantum diffusion coefficient, are obtained by using two-dimensional analogs of Eqs. (1.24) and (1.44).

e) Scattering by an arbitrary potential

The interaction of quasiparticles alters the values of the equilibrium characteristics of the gas of quasiparticles, and this means also the characteristics of the solid: the heat capacity, the thermal expansion coefficient, the diffusion coefficient, etc. The collisions also give rise to relaxation processes in the crystal, kinetic phenomena, resonance phenomena, etc.

In order to study the overall pattern of interaction of quasiparticles with one another on the basis of the method of I. M. Lifshitz, let us first examine the problem of interaction in operator form. This allows us to treat various concrete cases as depending on the type of potential.

Let the kinetic-energy operator for one of the quasiparticles be $\hat{L}_1$, and $\hat{L}_2$ for the other. The interaction of the quasiparticles is described by the operator $\hat{\Lambda}$. Then the equation corresponding to their mutual scattering will be

$$(\hat{L}_1 + \hat{L}_2 + \hat{\Lambda})\varphi - z\varphi = \hat{F}. \qquad (1.45)$$

Here $\hat{F}$ is the operator corresponding to some external force.

Let us denote $\hat{L} = \hat{L}_1 + \hat{L}_2$. Equation (1.45) with $\hat{\Lambda} = 0$ gives the wave function ψ and the eigenvalues of the interacting quasiparticles:

$$(\hat{L}_1 + \hat{L}_2)\psi - z\psi = \hat{F}. \qquad (1.46)$$

Let us study the class of degenerate operators that satisfy the condition

$$\Lambda\varphi = T\psi. \qquad (1.47)$$

This actually defines the new operator T, whose action on ψ yields $\Lambda\varphi$.

In configuration space Eq. (1.47) leads to the following conclusion. At small distances between the two quasiparticles, where the potential Λ is infinite, the exact wave function must vanish, while the product $\Lambda\varphi$ will remain finite. Moreover, the unperturbed wave function ψ vanishes nowhere. Therefore the operator T must be regular throughout space.

Upon substituting Eq. (1.47) into Eq. (1.45), we have

$$(\hat{L} - z)\varphi + \hat{T}\psi = \hat{F}. \qquad (1.48)$$

Let us introduce the resolvents of the operators L and Λ:

$$(\hat{L} - z)^{-1} = \hat{R}_z, \quad (\hat{L} + \hat{\Lambda} - z)^{-1} = \tilde{R}_z. \qquad (1.49)$$

Upon applying the resolvent $\hat{R}_z$ to Eq. (1.48), we obtain

$$\varphi = \hat{R}_z \hat{F} - \hat{T} \hat{R}_z \psi. \qquad (1.50)$$

According to the condition (1.49), the magnitude of T is determined by the expression

$$T = \tau(\varphi, \psi). \qquad (1.51)$$

Here τ defines the interaction.

Upon substituting the value of the wave function φ into Eq. (1.51), we obtain the following expression from (1.50):

$$T = \frac{\tau\,(\hat{F},\ R_z^{*}\psi)}{1+\tau\,(\hat{R}_z\psi,\ \psi)}. \tag{1.52}$$

Let us find finally the function φ from Eq. (1.52) by using Eq. (1.50):

$$\overset{\approx}{R}_z\hat{F} - \hat{R}_z\hat{F} = -\frac{\tau\,(\hat{F}\hat{R}_z\varphi,\ R_z\varphi)}{1+\tau\,(R_z\varphi,\ \varphi)}. \tag{1.53}$$

Finally, we have the following expression for the wave function:

$$\varphi = \psi + \frac{\tau\,(R_z\psi,\ \psi)}{1+\tau\,(R_z\psi,\ \psi)}. \tag{1.54}$$

We note that mathematical methods are well known that enable one to approximate any interaction operator with degenerate operators.[62] Thus, the approximation of an arbitrary interaction operator with degenerate operators gives an effective method for solving Eq. (1.3) or (1.45) in a broad class of cases, and it enables one to associate the form of the wave surface and the amplitude of the scattered quasiparticles with their dispersion law.

2. ENERGY SPECTRUM OF A QUANTUM CRYSTAL

a) Contribution to the free energy of a quantum crystal

Actually, at low temperatures the calculation of the free energy of a crystal reduces to calculating the free energy of the gas of the corresponding elementary excitations, which behave as a sort of quasiparticles moving in the space occupied by the crystal, and which possess definite values of energy and momentum. When the concentration of quasiparticles is small, the approximation of the virial expansion, in which the energy is expressed in terms of the pair scattering amplitude $f(\mathbf{k},\mathbf{k}')$, proves to be quite sufficient in this calculation. The terms quadratic in the scattering amplitude are small when the collisions of the quasiparticles can be described in the Born approximation.

Therefore the contribution of these terms to the free energy is inessential. However, at low enough temperatures the interaction becomes strong. This complicates the situation, both because of the quadratic terms and because of the anisotropy of the crystal. An example of such a system is a crystal in which the quasiparticles are scattered by immobile impurities. For this case I. M. Lifshitz first proposed a method for calculating the increment to the free energy of the crystal caused by the presence of the impurities.[31] This method does not employ the Born approximation, and hence it does not require smallness of the interaction potential of the quasiparticles with the impurities.

We shall examine below an analogous method of calculating the increment to the free energy caused by pair collisions of quasiparticles with one another.[32,51] For example, such collisions are realized in quantum crystals. However, the result in the present treatment is not expressed in terms of the scattering amplitude, but in terms of a characteristic of the problem associated with it, but simpler, the so-called spectral function, which contains the features pointed out above of the interacting quasiparticles.

Let us assume that the number of quasiparticles is small enough that we can consider not more than one pair of quasiparticles to be colliding at the same time. Evidently, in a system of N quasiparticles the number of such pairs will be of the order of N^2. The intereaction between the quasiparticles will be strong whenever any two of them lie very close to one another, i.e., practically tend to occupy the same lattice node. This interaction will be infinitely large and repulsive when the coordinates of the two particles coincide exactly in the crystal lattice. This corresponds to the potential (1.1) with the wave function (1.15). Let us examine the variation of the free energy of the crystal using the example of this interaction potential.

Along with the solutions describing the scattering of the quasiparticles, Eq. (1.8) also has solutions corresponding to bound states. If the concentration of quasiparticles is c, then the concentration of bound states will be proportional to c^2. As a function of the variable $q/2$, the eigenvalues $\varepsilon(q/2)$ represent new excitation branches corresponding to bound states.

Let us represent z in Eq. (1.14) in the form

$$z = E + \alpha\xi\,(E) + O\,(\alpha^2). \tag{2.1}$$

We have

$$1 = V \int \frac{d\chi}{\varepsilon\,(\chi - (q/2)) + \varepsilon\,(\chi + (q/2)) - E - \alpha\xi\,(E)}. \tag{2.2}$$

For simplicity, let us study the sequence of operators with purely discrete spectrum $\hat{L}_\alpha$, which converges as $\alpha \to 0$ to the value $\hat{L}$. The eigenvalues of the opeator $\hat{L}_a$ will be the numbers $E_n = n\alpha$, each of them infinitely multiple. As I. M. Lifshitz[31] showed, for an operator with a multiple spectrum, addition of the first-rank operator $\hat{A}$ of (1.1) reduces the multiplicity of each eigenvalue of the spectrum to unity. Here the points E_n remain, while the eigenvalues z_n that are split off are shifted and lie between the values E_n and E_{n+1}. Thus, the eigenvalues of the operator $\hat{L}_\alpha + \hat{A}$ that are split off are represented in the form (2.1) or

$$z_n = E_n + \alpha\xi\,(E_n) + O\,(\alpha^2).$$

In the case of such a discrete spectrum, the integral in (2.2) is converted into a summation over the numbers n. Here, upon substituting $d\chi = d\Omega\,dE$ (where $d\Omega$ is an element of solid angle), we have

$$1 = V \sum_m \frac{\nu\,(E_m,\ q)\,\Delta E_m}{E_m - E_n - \alpha\xi\,(E_n)}. \tag{2.3}$$

Here we have

$$\nu\,(E_m,\ q) = \int\limits_{E_m}^{E_m + \Delta E_n} \frac{d\Omega}{|\,\nabla\varepsilon\,(\chi - (q/2)) + \nabla\varepsilon\,(\chi + (q/2))\,|}. \tag{2.4}$$

Upon taking the limit in Eq. (2.3) as $\alpha \to 0$ and $n \to \infty$, so that $E_n = E$ remains in place, we have

$$\tilde{\xi}(E) = \int \xi\,(E,\ q)\,dq,$$

$$\xi\,(E,\ q) = \frac{1}{\pi}\,\text{arctg}\,\frac{\pi V \nu\,(E,\ q)}{1 + V \int \dfrac{\nu\,(\varepsilon,\ q)\,d\varepsilon}{E - \varepsilon}}. \tag{2.5}$$

Thus we determine from the scattering problem the spectral

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shift, a knowledge of which enables us to determine the change in free energy of the crystal

$$\widetilde{\xi}(E) = \int \xi(E, \mathbf{q})\, d\mathbf{q}, \quad \xi(E, \mathbf{q}) = \frac{1}{\pi} \operatorname{arctg} \frac{\pi v(E, \mathbf{q})}{\displaystyle\int \frac{v(\varepsilon, \mathbf{q})\, d\varepsilon}{E - \varepsilon}} \cdot$$
(2.6)

Let the free energy in the unperturbed case be $F_0 = \mathrm{Sp}\,\Phi(\widehat{L})$, where

$$\Phi(\varepsilon) = T \ln(1 - e^{-\varepsilon/T}) + \varepsilon_0,$$
(2.7)

while the free energy of the perturbed crystal is

$$F_1 = \mathrm{Sp}\,\Phi(\widehat{L} + \widehat{\Lambda}).$$
(2.8)

Then the change in the free energy caused by the perturbation will be

$$\Delta F = \lim_{\alpha \to 0} \sum_n [\Phi(E_n + \alpha \widetilde{\xi}(E_n)) - \Phi(E_n)].$$
(2.9)

Hence we have

$$\Delta F = \int_{\Gamma} \widetilde{\xi}(E)\, \Phi'(E)\, dE.$$
(2.10)

Here the integral is taken over the region Γ of the continuous spectrum.

Together with the expressions (2.5) and (2.6), the formula derived here enables one to find the contribution to the free energy of the interacting quasiparticles.

Let us examine some special cases by using Eq. (2.10). The quantity $v(E, \mathbf{q})$ that enters into (2.5) and (2.6) has the meaning of the density of states and in all cases is well known. Thus, for example, in the case of a lattice of cubic symmetry, $v(E)$ equals:

$$v(E) = \mathrm{const} \cdot E^{-1/4}.$$
(2.11)

For simplicity we shall assume that $v(E, \mathbf{q}) = v(E)f(\mathbf{q})$, where $f(\mathbf{q})$ is a certain function of $\mathbf{q}$ alone. Then, upon substituting the value of (2.11) into Eq. (2.6), we have

$$\xi = \frac{1}{4}.$$
(2.12)

Analogously, we can easily find from the same formulas that the following expression holds near the boundaries of the band, when $v(E) = \mathrm{const} \cdot E^{-1/2}$:

$$\xi = \frac{1}{2}.$$
(2.13)

Consequently, we have the following in these cases from Eq. (2.10) for a system of quasiparticles:

$$\Delta F = \frac{N^2 T}{V} \frac{a^3 \ln 2}{4},$$
(2.14)

$$\Delta F = \frac{N^2 T}{V} \frac{a^3 \ln 2}{2}.$$
(2.15)

Thus the contribution to the pressure will be of the order of Nb/V (where b is the constant defined in Eqs. (2.14) and (2.15) in the region in which the infinitely large repulsion between the pairs of quasiparticles is significant.

b) Heat capacity of a two-dimensional crystal

The experimental studies of Bretz and others have shown that the heat capacity of a two-dimensional crystal of helium adsorbed on graphite shows anomalous behavior at
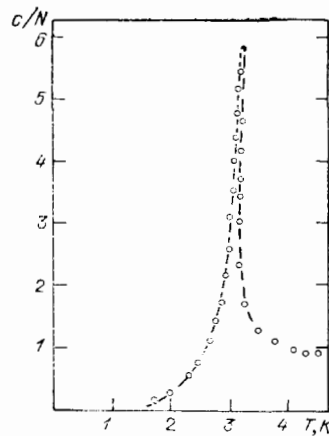

FIG. 6. Heat capacity of a two-dimensional crystal of ${}^4\mathrm{He}$.[42]

temperatures of the order of 1 K—a sharp maximum.[42] In the range of relative covering densities from 0.7 to 1.0 in the given system, one helium atom is present for every three potential wells of the substrate (Fig. 6) upon ordering; owing to the repulsive forces of atoms at short distances. In such a system attractive forces exist between the next-nearest neighboring atoms. The appearance of vacancies in rather large concentratiion leads to the possibility in principle of discovering a superfluid phase of the crystal.

Calculation of the heat capacity by Eqs. (2.5) and (2.10) yields the relationship $C \sim |t|^{-\alpha}$, where $t = (T_c - T)/T_c$. This agrees qualitatively with the stated experimental result. Thus, the given system behaves like a two-dimensional quantum crystal containing vacancions (see also Ref. 40). Interestingly, in such a system, as the monolayer transforms into a measurable phase, the frequency of sound at which effective absorption can occur decreases, since the increment to the free energy of the crystal caused by collisions of quasiparticles leads to an increase in the relaxation time of the parameters characterizing the phase transition.[48]

As the results of Refs. 33, 48, and 54 imply, the vacancions in a two-dimensional crystal in a certain temperature region have a specific behavior (see also Sec. 3b) that leads to a distinctive temperature contribution to the heat capacity.

c) Nonideal Bose gas of quasiparticles

In the general case the statistics of quasiparticles is determined by the number of particles that must be annihilated or created to form the corresponding excitation. Each quasiparticle is characterized by the quasimomentum $\mathbf{k}$, the corresponding energy $\varepsilon(\mathbf{k})$, and the spin s. The process of quantum-mechanical tunneling requires that the existence of the spins must not violate the periodicity of the lattice, For this reason, they must all be oriented in the same direction.

The pair collisions of quasiparticles obeying Bose statistics give rise to a rearrangement of the energy spectrum of the system. It is characteristic of such a system that the relativity principle of Galileo is inapplicable to quasiparticles directly, since the latter require the presence of the medium in which they move. This fact leads to a distinctive phenomenon in the rearrangement of the energy spectrum. The

Bose condensate that arises does not have zero momentum, as in the case of an ordinary Bose gas, but has a finite momentum of motion as a whole. Consequently, there are two privileged systems of reference, respectively associated with the condensate and with the lattice. Evidently, each quasiparticle in the condensate is characterized by a quasimomentum and energy that correspond to this quasimomentum.

Let the velocity $\mathbf{v}$ of the condensate correspond to the quasimomentum $\mathbf{p}_0 (\nabla \varepsilon(\mathbf{k})|_{\mathbf{k}=\mathbf{p}_0} = \mathbf{v})$.

Let us construct the energy spectrum of such a system, whose Hamiltonian has the form[32,55,56]

$$\hat{H} = \sum_{\mathbf{R}, \mathbf{R}'} A_{\mathbf{R}-\mathbf{R}'} \hat{a}_{\mathbf{R}}^+ \hat{a}_{\mathbf{R}'} + \sum_{\mathbf{R}, \mathbf{R}'} U_{\mathbf{R}, \mathbf{R}'} \hat{a}_{\mathbf{R}}^+ \hat{a}_{\mathbf{R}'}^+ \hat{a}_{\mathbf{R}'} \hat{a}_{\mathbf{R}} = \hat{H}_0 + \hat{H}_{\text{int}}. \tag{2.16}$$

Here $\hat{a}_{\mathbf{R}}^+$ and $\hat{a}_{\mathbf{R}}$ are the operators for creation and annihilation of quasiparticles at the node $\mathbf{R}$, while $U_{\mathbf{RR}'}$ is the interaction potential of the quasiparticles, and we have

$$A_{\mathbf{R}} = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \exp(i\mathbf{k}\mathbf{R}). \tag{2.17}$$

The operators $\hat{a}_{\mathbf{R}}^+$ and $\hat{a}_{\mathbf{R}}$ satisfy the usual commutation relationships[56]:

$$\hat{a}_{\mathbf{R}} \hat{a}_{\mathbf{R}'}^+ - \hat{a}_{\mathbf{R}'}^+ \hat{a}_{\mathbf{R}} = \delta_{\mathbf{RR}'}. \tag{2.18}$$

Pair collisions between quasiparticles via the "impenetrability" potential of (1.1) do not satisfy the condition of applicability of the Born approximation. The attractive potential of (1.2) satisfies this condition, and hence can be taken into account in (2.16) in the term H_{int} by using perturbation theory.

In order to describe the system under discussion in the momentum representation, we must take into account the property characteristic of a quantum crystal—motion of the quasiparticles over the nodes alone, and the impossibility of finding more than one particle at one node. This becomes possible if one takes into account the exact wave function (1.6) of the quasiparticles in transforming to the momentum representation. Thus, let us transform the weak attractive potential to the momentum representation as follows:

$$U_{\mathbf{p}-\mathbf{q}/2, \mathbf{p}+\mathbf{q}/2}^{\mathbf{p}-\mathbf{q}'/2, \mathbf{p}+\mathbf{q}'/2} = \sum_{\mathbf{R}, \mathbf{R}'} U_{\mathbf{RR}'} \varphi(\mathbf{R}, \mathbf{R}'). \tag{2.19}$$

The Hamiltonian (2.16) in the momentum representation will have the form

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}}$$
$$+ \sum_{\mathbf{k}, \mathbf{q}, \mathbf{q}'} U(\mathbf{k}, \mathbf{q}, \mathbf{q}') \hat{a}_{\mathbf{k}-(\mathbf{q}/2)}^+ \hat{a}_{\mathbf{k}+(\mathbf{q}/2)}^+ \hat{a}_{\mathbf{k}+(\mathbf{q}'/2)} \hat{a}_{\mathbf{k}-(\mathbf{q}'/2)}. \tag{2.20}$$

The summation in the last term is performed over all values of the momenta of the quasiparticles, while conforming to the law of conservation of momentum in a pair collision.

Let us study the case of the gas approximation $ka \ll 1$. Then we obtain the following equation from (2.19) with allowance for (1.15):

$$U(\mathbf{p}_0) = \tau V \int \frac{d\chi}{\varepsilon(\chi - \mathbf{p}_0) + \varepsilon(\chi + \mathbf{p}_0) - 2\varepsilon(\mathbf{p}_0)}. \tag{2.21}$$

Application of perturbation theory in the Hamiltonian of

(2.20) now implies formally the expansion of the fourfold summation as a power series in the small quantities $\hat{a}_{\mathbf{k}}^+$ and $\hat{a}_{\mathbf{k}}$. The zero-order term of the expansion is the number:

$$\hat{a}_{\mathbf{p}_0}^+ \hat{a}_{\mathbf{p}_0}^+ \hat{a}_{\mathbf{p}_0} \hat{a}_{\mathbf{p}_0} = N_{\mathbf{p}_0}^2. \tag{2.22}$$

Here $N_{\mathbf{p}_0}$ is the number of quasiparticles in the condensate. The second-order terms will be:

$$a_{\mathbf{p}_0}^2 \sum_{\mathbf{k} \neq 0} (\hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} + \hat{a}_{\mathbf{k}}^+ \hat{a}_{-\mathbf{k}}^+ + 2\hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}}). \tag{2.23}$$

Since the number of quasiparticles in the condensate is large, we can treat the operators as ordinary numbers neglecting their noncommutativity. Thus we have the following from (2.20), (2.22), and (2.23):

$$\hat{H} = \frac{N_{\mathbf{p}_0}^2 U(\mathbf{p}_0)}{2V} + \frac{N_{\mathbf{p}_0} U(\mathbf{p}_0)}{2V} \sum_{\mathbf{k} \neq 0} (\hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} + \hat{a}_{\mathbf{k}}^+ \hat{a}_{-\mathbf{k}}^+ + 2\hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}})$$
$$+ \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}}. \tag{2.24}$$

In order to determine the energy spectrum, we must convert the Hamiltonian to diagonal form, which is done by the Bogolyubov transformation. Finally we have

$$\hat{H} = E_0 + \sum_{\mathbf{k}} \varepsilon'(\mathbf{k}) \hat{b}_{\mathbf{k}}^+ \hat{b}_{\mathbf{k}}. \tag{2.25}$$

Here E_0 is the energy of the ground state ($\hat{b}_{\mathbf{k}}^+$ and $\hat{b}_{\mathbf{k}}$ are the new Bose operators):

$$E_0 = \frac{N_{\mathbf{p}_0}^2}{2} c^2(\mathbf{p}_0) - \beta N_{\mathbf{p}_0} U(\mathbf{p}_0) \varepsilon_0 + \varepsilon_0, \quad \varepsilon_0 = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}), \tag{2.26}$$

while $c(\mathbf{p}_0)$ is the velocity of sound:

$$c(\mathbf{p}_0) = \sqrt{2U(\mathbf{p}_0) \frac{N_{\mathbf{p}_0}}{V}}. \tag{2.27}$$

The new dispersion law for $\varepsilon'(\mathbf{k})$ has the form

$$\varepsilon'(\mathbf{k}, \mathbf{p}_0) = \left\{ \frac{1}{2} [\varepsilon(\mathbf{k} - \mathbf{p}_0) + \varepsilon(\mathbf{k} + \mathbf{p}_0) - 2\varepsilon(\mathbf{p}_0)] \right.$$
$$\left. + \frac{1}{2} c^2(\mathbf{p}_0) [\varepsilon(\mathbf{k} - \mathbf{p}_0) + \varepsilon(\mathbf{k} + \mathbf{p}_0) - 2\varepsilon(\mathbf{p}_0)] \right\}^{1/2}. \tag{2.28}$$

The quantity $\hat{b}_{\mathbf{k}}^+ \hat{b}_{\mathbf{k}} = n_{\mathbf{k}}$ amounts to the number of quasiparticles having the momentum $\mathbf{k}$, while Eq. (2.28) defines the relationship of their energy to the quasimomentum. According to Eq. (2.28), the energy of the quasiparticles depends also on the momentum $\mathbf{p}_0$, which corresponds to the velocity $\mathbf{v}$ of motion of the superfluid Bose condensate.

The quantity $c(\mathbf{p}_0)$ coincides with the velocity of sound in the system of quasiparticles, since the pressure is $P = -(\partial E / \partial V)_T$, while $c^2(\mathbf{p}_0) = \partial P / \partial \rho$, where $\rho = N_{\mathbf{p}_0} / V$. It would be of interest in principle to observe a dependence of the velocity of sound on $\mathbf{p}_0$.

3. THEORY OF THE FERMI-BOSE QUANTUM CRYSTAL

a) Free energy of a solid solution

The method developed in Sec. 2 is applicable, e.g., for calculating the free energy of a solid solution. The increment in the free energy owing to pair collisions is finite in the limit of unlimited enlargement of the crystal. Therefore, in calculating the change in free energy with respect to a classical

crystal, one can treat the limiting case of an infinite crystal, for which the energy spectrum is continuous.

The free energy of the solution is changed by the amount ΔF by one event of pair scattering. Then, in the presence of impuritons in the concentration c, the free energy is represented in the form

$$F = F_0 + Nc\,\Delta F. \tag{3.1}$$

Here F_0 is the free energy of the pure crystal, and N is the total number of atoms.

Evidently the present statements are true in collisions of any type of quasiparticles with one another. If, for example, Fermi-Fermi, Bose-Bose, and Fermi-Bose particle collisions can occur in a solution of Fermi and Bose quasiparticles, this leads to the following contribution to the free eneregy of the solution:

$$\Delta F = \Delta F_B N_B^2 + \Delta F_F N_F^2 + \Delta F_{FB} N_F N_B. \tag{3.2}$$

Here N_F and N_B are the numbers of Fermi and Bose quasiparticles, ΔF_i (i = F, B, or FB) is the increment to the free energy [see Eqs. (2.5) and (2.10)] respectively in collisions of Fermi-Fermi, Bose-Bose, and Fermi-Bose quasiparticles.

Equations (2.5) and (2.10) also allow one to calculate the contribution to the free energy arising from bound states of quasiparticles. As was shown in Sec. 1, bound states arise in a quantum crystal near special points in quasimomentum space when the interaction between them is arbitrarily small ($t \rightarrow 0$). In this case the formula for ΔF will have the form

$$\Delta F = \int \frac{\nu(\varepsilon)\,V\,t}{1 + Vt \displaystyle\int \frac{\nu(\mu)\,d\mu}{\mu - \varepsilon}} \frac{d\varepsilon}{e^{\varepsilon/T} - 1}. \tag{3.3}$$

At the concentration c, the concentration of bound pairs of quasiparticles will be of the order of c^2. Hence the contribution to the free energy will be $c^2\,\Delta F$.

b) Phase separation in a ^{3}He–^{4}He solid solution

In solutions of quantum crystals, quasiparticles obeying both Fermi and Bose statistics can exist simultaneously. Let us examine the properties of a crystal that contains $N_3 = n_3 V$ Fermi quasiparticles and $N_4 = n_4 V$ Bose quasiparticles. The concentration of Fermi quasiparticles is $c = N_3/N$, where $N = N_3 + N_4$.

Experimentally the problem of phase separation arose in studying the ordering of the nuclear spins of ^{3}He when the specimen contained an appreciable amount of the impurity ^{4}He.[4,59] Edwards, McWilliams, and Dount found that a large anomalous heat capacity appears at a certain temperature that depends on the concentration of the impurity. The large heat capacity indicates that some ordering process is occurring. Such an anomaly can arise from the decomposition of a solid solution into two phases.

To elucidate the problem of phase separation, let us first treat the case of zero temperature. We shall write the expression for the free energy for a ^{3}He–^{4}He solution in the following form[1,44] [see (3.2)]:

$$F = \lambda \frac{V_0 - V}{V_0} N_4 + \frac{\pi a}{m_4^*} \frac{N_4^2}{V} - \frac{V}{5\pi^{1/3}m_3^*} \left(\frac{N_3}{V}\right)^{5/3}$$
$$+ \frac{\pi a'}{m_3^*} \frac{N_3^2}{V} + 2\pi a_0 \left(\frac{1}{m_3^*} + \frac{1}{m_4^*}\right) \frac{N_3 N_4}{V}. \tag{3.4}$$

Here a, a', and a_0 are respectively the scattering lengths for Bose-Bose, Fermi-Fermi, and Fermi-Bose quasiparticles (see Sec. 1), and m_3^* and m_4^* are the effective masses of the quasiparticles ($m_3^* \sim \hbar^2/\Delta_3 a^2$, $m_4^* \sim \hbar^2/\Delta_4 a^2$). Further, V_0 is the value of the volume at which vacancions are formed.

One can determine by the generally known formulas of statistical physics[56] the pressure and chemical potential of the quasiparticles. This enables one to determine the region of stratification of the solution into two phases. One can be easily convinced from the conditions of phase equilibrium that zereo-point impuritons, i.e., impuritons existing at zero temperature, do not contribute substantially to the pressure in the region of small concentrations:

$$P = \frac{n\lambda V}{V_0} + \frac{\pi a n^2}{m^*} + 2\pi a_0 \left(\frac{1}{m_3^*} + \frac{1}{m_4^*}\right) n^2 c. \tag{3.5}$$

Thus the impuritons have a rather high mobility, for otherwise the crystal could remain in a metastable state upon lowering the temperature. The experimental facts confirm these results.[59,61]

Now let us examine a solution of Fermi-Bose quasiparticles in lattice space in the presence of equilibrium vacancions and at nonzero temperature. The existence in the solution of vacancions alters the physical pattern. The vacancions possess high mobility, owing to which certain phenomena can appear that are characteristic of liquid solutions.

The Hamiltonian of the solution being studied in the second-quantization representation has the form

$$\hat{H} = \sum_{R, R'} A_{R-R'} \hat{a}_R^+ \hat{a}_{R'} + \sum_{R, R'} B_{R-R'} \hat{b}_R^+ \hat{b}_{R'}$$
$$+ \frac{1}{2} \sum_{R, R'} U_{RR'}^1 \hat{a}_R^+ \hat{a}_{R'}^+ \hat{a}_{R'} \hat{a}_R$$
$$+ \frac{1}{2} \sum_{R, R'} U_{RR'}^2 \hat{b}_R^+ \hat{b}_{R'}^+ \hat{b}_{R'} \hat{b}_R + \sum_{R, R'} U_{RR'}^3 \hat{a}_R^+ \hat{a}_R \hat{b}_R^+ \hat{b}_R. \tag{3.6}$$

Here

$$U_{RR'}^i = \begin{cases} V \rightarrow \infty, & R = R', \\ -v^i(R - R'), & R \neq R' \end{cases} \tag{3.7}$$

is the interaction between Bose-Bose ($i = 1$), Fermi-Fermi ($i = 2$), and Fermi-Bose ($i = 3$) quasiparticles. Here $\hat{a}_R^+$, $\hat{a}_R$, $\hat{b}_R^+$, and $\hat{b}_R$ are creation and annihilation operators, respectively for Bose and Fermi quasiparticles at the point R of lattice space. The number of quasiparticles is smaller than the number of crystal-lattice nodes. Each lattice node can be occupied either by a boson or by a fermion or by a vacancion. This is analogous to the idea that each node can exist in three different states. Let us introduce three vectors that correspond to these states: $(1, 0, 0)$ is a state occupied by a boson, $(0, 1, 0)$ is a state occupied by a vacancion, and $(0, 0, 1)$ is a state occupied by a fermion.

These vectors are the eigenvectors of the z-component of the unitary spin operator σ^z corresponding to the eigenvalues 1, 0, and -1. We can easily convince ourselves that, e.g., a Bose quasiparticle is created whenever the operator

$\sigma^z \sigma^+$ acts on a state having $\sigma^z = 0$. Consequently the boson creation operator can be expressed in terms of the spin operator multiplied by the corresponding projection operator[56]:

$$\hat{a}_R^+ = \frac{1}{\sqrt{2}} \sigma_R^z \sigma_R^+, \quad \hat{a}_R = \frac{1}{\sqrt{2}} \sigma_R^- \sigma_R^z. \tag{3.8}$$

Analogously one can introduce the operators for fermion creation and annihilation:

$$\hat{b}_{R+}^+ = \frac{1}{\sqrt{2}} \sigma_R^z \sigma_R^-, \quad \hat{b}_R = \frac{1}{\sqrt{2}} \sigma_R^+ \sigma_R^z. \tag{3.9}$$

We can easily verify that the usual commutation relationships remain in force here.

Owing to translational symmetry, σ does not depend on the index R. The molecular-field approximation states that the field at the Rth node coincides with the mean field $\overline{U}$ and does not depend on the orientation of the spin σ_R.[58] In a quantum crystal the spins are all oriented in the same direction in order that the system be periodic. The fact of discreteness is taken into account here if one employs the exact scattering wave functions derived in Sec. 1 in going over to the momentum representation:

$$\overline{U}_k^i = \sum_{k'} U^i(k, k') \sigma_{k'}^{\overline{z}}, \tag{3.10}$$

$$U^i(k, k') = \sum_{R, R'} U_{RR'}^i \varphi(R, R'). \tag{3.11}$$

This procedure yields equations that reflect the joint participation of all the lattice quasiparticles in creating the self-consistent field.[58] The quantities A_R and B_R in the Hamiltonian of (3.6) correspond to the dispersion laws of the quasiparticles in going over to the momentum representation:

$$A_R = \sum_k \varepsilon_1(k) \exp(ik\cdot R),$$
$$B_R = \sum_k \varepsilon_2(k) \exp(ik\cdot R). \tag{3.12}$$

The representation of the creation and annihilation operators in terms of the spin operators also allows one to introduce the order parameter η:

$$\overline{\sigma^z} = \eta. \tag{3.13}$$

This implies that one can expand the free energy of the solution corresponding to the Hamiltonian of (3.6) in powers of the quantity η according to the Landau theory of second-order phase transitions. As a result, upon equating the coefficient of η^2 to zero, we obtain the phase-transition temperature.

Figure 7 shows the dependence obtained in this way of the phase-separation temperature on the concentration of Fermi quasiparticles. When $T \ll T_{p.s.}$, the phases are almost fully separated.[58] Separation does not occur throughout the volume, as in a liquid, but yields a mixture of small clusters of each phase. The dimensions of these clusters depend on the concentration of vacancions. The asymmetry of the phase-separation curve indicates the differing behavior of the vacancions at different concentrations of Fermi quasiparticles in the solution, which is also indicated by the experimental facts.[59,61]
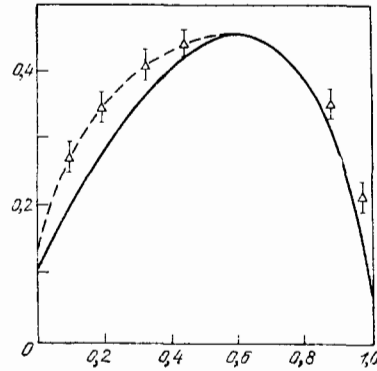

FIG. 7. State diagram of a ^{3}He–^{4}He solution. Solid line—theory[58]; dotted line—experiment.[59,61]

c) On the structure of vacancies in a ^{3}He–^{4}He solution

As was shown in the last subsection, a ^{3}He–^{4}He solution separates into two phases at temperatures $T < T_c$ ($T_c = 0.4$ K) and at concentrations $0 < c < 1$. Separation at such low temperatures indicates that quasiparticles having a specific behavior exist in this crystal.

For example, the behavior of vacancions is highly sensitive to the system of nuclear spins of ^{3}He.[3,33] Therefore, in the presence of vacancions the solution has completely different magnetic properties, depending on which branch of the phase-separation curve is being studied, the branch where $c \ll 1$ or the one where $c \sim 1$.[48]

Let us study the rather broad temperature region defined by the condition:

$$\varepsilon; \ J \ll T \ll \Delta. \tag{3.14}$$

Here J is the magnitude of the exchange interaction ($J \sim 10^{-4}$ K), Δ is the width of the vacancion band ($\Delta \sim 10$ K), and ε is the characteristic interaction energy of ^{4}He atoms with one another.

In this temperature region a vacancion on the former branch of the phase-separation curve behaves as follows. It expels ^{4}He atoms from a region of radius R and fully polarizes the nuclear spins in this region. This occurs at concentrations $10^{-4} \ll c < 1$. On the other branch of the phase-separation curve at concentrations $c \ll 1$, the vacancion expels ^{3}He atoms and is delocalized in the region R_1.

The appearance of ordered macroscopic regions arises from the fact that the formation of a vacancion requires ideal periodicity of the lattice. This is attained by expulsion of either ^{4}He or ^{3}He atoms, depending on the relative concentration.

The minimal work necessary for expelling atoms, e.g., of ^{4}He, is[56]

$$\delta R = \Phi(n) - \Phi(0). \tag{3.15}$$

Here we have

$$\Phi(n) = n\mu_0 + Tn \ln \frac{en}{N} + \psi(p, T), \tag{3.16}$$

$$\Phi(0) = n\mu_0 + n\mu'. \tag{3.17}$$

Also, μ' is the chemical potential of the dissolved material:

$$\mu' = T \ln \frac{n}{N} + \psi(p, T). \tag{3.18}$$

Analogously one can state that the minimal energy for expelling ^{3}He atoms is

$$\delta R = c n_4 T. \tag{3.19}$$

Here c is the concentration of ^{3}He atoms. Then an ordered state arises in the region of a sphere of radius R, with an energy equal to

$$F = \varepsilon \; + \frac{\pi^2 \hbar^2}{2MR^2} + \frac{4\pi}{3} R^3 n_3 T \ln 2 + c \cdot \frac{4\pi}{3} R^3 n_3 T. \tag{3.20}$$

Here ε_0 is the energy of the vacancion band, the third term in this expression corresponds to the energy of the ordered nuclear spins of the ^{3}He atoms, and the last term is the energy of expulsion of N_4 ^{4}He atoms from the region of radius R. On the other branch of the phase-separation curve, i.e., the branch on which the concentration is $c \ll 1$, the energy of the region of radius R_1 will be

$$F_1 = \varepsilon_0 + \frac{\pi^2 \hbar^2}{2MR_1^2} + c \cdot \frac{4\pi}{3} R_1^3 n_4 T. \tag{3.21}$$

We find the radii of the corresponding regions (Fig. 8) from the condition that the expressions (3.20) and (3.21) should be minimal.

$$R = \left(\frac{\pi \Delta}{4T (\ln 2 + c)} \right)^{1/5} a, \tag{3.22}$$

$$R_1 = \left(\frac{\pi \Delta}{4Tc} \right)^{1/5} a. \tag{3.23}$$

We shall find the range of concentrations necessary for manifestation of the stated phenomenon from the condition that the radius of the sphere must be large enough in comparison with the distance between the atoms subject to expulsion:

$$R \gg a c^{-1/3}. \tag{3.24}$$

We can easily see from Eqs. (3.22)–(3.24) that

$$\left(\frac{T}{\Delta} \right)^{2/3} \ll c \ll 1 \tag{3.25}$$

on the initial branch of the phase-separation curve, and

$$\left(\frac{T}{\Delta} \right)^{3/5} \ll c \ll 1 \tag{3.26}$$

on the other branch of this curve, corresponding to the temperature $T \approx 0.4$ K.

The onset of order in macroscopic regions of radii R and R_1 leads to appreciable changes in the magnetic and thermodynamic properties of the ^{3}He-^{4}He solid solution.

d) Absorption of sound by vacancies

Let the solution contain vacancies in concentration c. Under the action of a sound wave with energy $E_0^2 < \Delta$ and
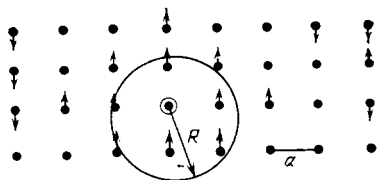

FIG. 8. Macroscopic region of radius R in a ^{3}He-^{4}He solution.

wavelength $2\pi/k > R$, a vacancy begins to oscillate and scatter energy upon interacting with the lattice.

In the field of a sound wave of frequency ω and wave vector $\mathbf{k}$ lying along the x axis, the force $F = F_0 \cos(\omega t - \mathbf{k} \cdot \mathbf{r})$ acts, where $\mathbf{r}$ is the x coordinate of the vacancy.

The energy absorbed per unit time by the vacancy is determined by the mean value $\overline{Fx} = A$ (where $\dot{x}$ is the velocity of the vacancy). Upon taking account of the fact that the mobility of a vacancy is determined by the formula[39] $v^{-1} \sim (a^2/\hbar)(T/\Delta)^{2/5}$, we have the following expression[48] for the absorbed energy:

$$A \sim N_3 \frac{k^2 \Delta^2 E_0^2}{\hbar^3} a^4 \left(\frac{T}{\Delta} \right)^{2/5}. \tag{3.27}$$

The absorption coefficient has the following form:

$$\alpha \sim \left(\frac{\Delta}{\hbar} \right)^3 \frac{a^2 \omega}{\hbar} \left(\frac{T}{\Delta} \right)^{2/5}. \tag{3.28}$$

It is of definite interest to measure these quantities in sound-absorption experiments.

As Andreev, Marchenko, and Meĭerovich[38] showed, the experimentally observed increase in the temperature of magnetic ordering with increase in the applied magnetic field incicates the onset of ferromagnetically ordered macroscopic regions around vacancions.

CONCLUSION

Thus the concept of quasiparticles that Andreev and Lifshitz proposed describes perfectly the physical picture corresponding to quantum crystals. The description in the language of quasiparticles proves so fruitful precisely because at low temperatures one has not too large a number of types of motion to deal with, and hence, not too large a number of quasiparticles. This has enabled us to treat a quantum crystal as a rarefied gas of quasiparticles in the discrete space of the crystal lattice and to apply the method of I. M. Lifshitz to study the scattering process. The discreteness of the space leaves a distinctive imprint on the physical picture as a whole. Quasiparticles after being scattered by one another are a superposition of several waves, whose number depends on the form of the isoenergetic surface. An elucidation of this problem in experiments, e.g., on quantum diffusion, would be of substantial interest.

A quantum crystal containing zero-point vacancions is a unique object.[1,3] Two superfluid motions can occur in it, involving the flow of quasiparticles and the displacement of the lattice nodes. At low enough temperatures such a crystal possesses specific thermodynamic and hydrodynamic properties.

Vacancions in ^{3}He-^{4}He solid solutions have a distinctive behavior. Macroscopic regions appear on the phase-separation curve that lead to a change in the thermodynamic and magnetic state of the material.[48] New phase transitions can occur in such systems.

I express deep gratitude to A. F. Andreev and L. P. Pitaevskiĭ for repeated useful discussions and valuable remarks.

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