Binary quasiparticles in quantum crystals

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The behavior of tightly bound pairs of point defects in quantum crystals is investigated. In crystals of solid helium with hexagonal symmetry, such complexes may be distinctive delocalized binary quasiparticles—bidefectons, moving as a whole through the crystal and characterized by a definite quasimomentum and energy spectrum. Among the entire class of such objects there are three-dimensional quasiparticles, moving in any direction, as well as one-and two-dimensional quasiparticles which only move along definte axes or in certain planes of the crystal lattice. A classification of binary quasiparticles is given and the values of their energy spectra are obtained. The influence of these complexes on the diffusion of point defects and on the dissipative properties of quantum crystals is investigated. The vacancion mechanism for the transport of impurity particles, in which the vacancy-impurity complexes which are formed diffuse as a whole, without decaying, with a velocity characteristic for the diffusion of individual vacancions, is found to be particularly effective. The quantum analog of Zener relaxation is also discussed. The energy absorption lines are determined by resonance transitions of bidefectons between different branches of theiry energy spectrum.

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One of the most unusual properties of quantum crystals with zero-point vibrations of large amplitude is that at sufficiently low temperatures the point defects of a crystal lattice are delocalized and transformed into quasiparticles—defectons—which move freely through the crystal.[1] The diffusion properties of these quasiparticles are determined by defecton-phonon scattering[1-5] and by the interaction of the defectons with each other.[6-8] The quantum theory of defects was experimentally confirmed by investigations of the diffusion of He^3 atoms in He^4.[6,7,9]

The present article is devoted to an investigation of "bidefectons"—systems of two point defects tightly bound to each other, together constituting a single binary quasiparticle. It is shown that depending on the distance between the two defects and their mutual orientation, in regard to the nature of their motion such pairs may be three-dimensional as well as one- or two-dimensional quasiparticles that move freely along certain axes or, respectively, in certain planes of the crystal lattice. The question of the influence of "bidefectons" on the physical properties of quantum crystals of solid helium is also discussed.

First of all let us describe what the bound state of two point defects in quantum crystals is. At low temperatures the motion of defects in solid helium is accomplished by means of sub-barrier tunneling transitions to neighboring sites. As a consequence of the possibility of such transitions, the energy levels corresponding to localization of the particles on specific crystal lattice sites become quite broadened. In order of magnitude the width of the broadening is equal to the exchange integral J or, what amounts to the same thing, the width Δ of the delocalized defecton band. Upon a deformation of the crystal, the energy levels corresponding to localization of the defect on different lattice sites are shifted. If the relative displacement of the levels on neighboring sites exceeds the magnitude of the level broadening, a tunneling transition between such crystal lattice sites is impossible.

Thus, a defecton may freely diffuse only in that region of space in which the change of its potential energy $V(\mathbf{r})$, characterized by the deformation of the crystal, is bounded by the condition

$$|\delta V(\mathbf{r})| \leqslant \Delta.$$

The exchange integral J is a very small quantity.[6,7,9,10] On the other hand, the elastic interaction energy of two point defects increases with decreasing distance between them like

$$V(r) \sim V_0(a/r)^3,$$

where a is the interatomic distance, and V_0 is some constant characterizing the scale of the interaction. The inequality

$$V_0 \gg J \tag{1}$$

is usually satisfied with ample margin. This leads to the result that, if two defectons are close to each other, they can only diffuse through the crystal jointly.[11,12]

Moreover, a defecton can tunnel from one crystal lattice site $\mathbf{N}_1$ to a neighboring site $\mathbf{N}_2$ ($|\mathbf{N}_1 - \mathbf{N}_2| = a$) only provided that[1]

$$|(\mathbf{N}_1 - \mathbf{N}_2)\nabla V(\mathbf{r})| \leqslant \Delta.$$

As a consequence of the discreteness of the crystal lattice, only transitions to those lattice sites $\mathbf{N}_2$ for which

$$V(\mathbf{N}_1) = V(\mathbf{N}_2)$$

turn out to be possible for defectons located at a sufficiently small distance from each other.

It is clear from symmetry considerations that this condition can be satisfied for certain pair configurations, but for other configurations—it cannot. In the first case such a double defect can move as a whole through the crystal, where the distance between its constituent particles does not vary during the time of motion; in the second case—both particles are completely localized. Thus, for example, particles C and D in Fig. 1 cannot move, but the pair of particles $\{AB\}$ can freely move as a whole along the x axis by means of sequential tunneling transitions $B \to B_1$, $A \to A_1$, $B_1 \to B_2$, ..., since the interaction energy obviously doesn't change in this connection $V(A, B) = V(AB_1) = V(A_1, B_1) = \dots V(A_n, B_n)$.

Such a mode of motion of the complexes consisting of two point defects is only possible in hexagonal or cubic face-centered crystals (the probability for tunneling

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transitions of the defects to non-nearest neighbor sites of the crystal is exponentially small). The fact that, thanks to the hexagonal symmetry of He^4 crystals, a tunneling movement of pairs of strongly interacting defects (1) located at an arbitrary distance from each other may occur, was noted by Andreev,[12] who showed that the only restriction on the size R of the complex, consisting of two tightly bound defects and moving as a whole, is the condition

$$R \ll R_0, \quad R_0 = a(V_0/\Delta)^{1/3} \gg a.$$

Richards, Smith, and Toft[13] called attention to the fact that a pair of two point defects located at an interatomic distance from each other can move as a whole.

Such objects, moving by means of sequential sub-barrier transitions without energy changes, represent unusual binary quasiparticles—bidefectons, characterized by a definite quasimomentum $\hbar\mathbf{k}$ and by an energy spectrum $\epsilon(\mathbf{k})$. It is shown below that besides the two types already known[12,13] a whole class[1)] (twelve types in all) of such quasiparticles exists, their classification is given, and expressions are obtained for their energy spectra. Pairs, differing by symmetry transformations of the crystal from those investigated in this work, are, of course, not described. An hexagonal close-packed lattice with translation vectors

$$\mathbf{R}_1 = a(1, 0, 0), \quad \mathbf{R}_2 = a(1/2, 3^{1/2}/2, 0),$$
$$\mathbf{R}_3 = a(0, 0, 2^{3/2}/3^{1/2})$$

and having two sublattices, separated by the vector

$$\boldsymbol{\rho} = a(0, -1/3^{1/2}, 2^{1/2}/3^{1/2}).$$

is considered. The following notation has been introduced:

$$f(\mathbf{k}) = [\varepsilon(\mathbf{k}) - \varepsilon_n]/J, \quad \varphi_i = \mathbf{k}\mathbf{R}_i, \quad \varphi = ka,$$

where ϵ_n denotes the pair's energy in the absence of tunneling.

ONE-DIMENSIONAL DEFECTONS

A1. The simplest and at the same time the most common type of bidefectons are pairs analogous to the pair of particles {AB} shown in Fig. 1. To determine the energy spectrum of quasiparticles with a small probability for tunneling in the crystal lattice, it is sufficient to confine our attention to the tight-binding approximation in which the wave functions of the particle are linear combinations of the wave functions in translationally inequivalent states. In the present case there are two such basis states for the pair {AB}: as the basis states one can choose, for example, the position of the pairs {AB} and {AB$_1$}.

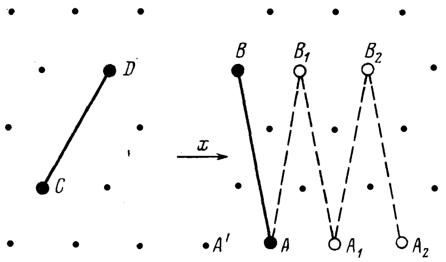

FIG. 1. Particles C and D are completely localized. By means of the sequential tunneling transitions B → B$_1$, A → A$_1$, B$_1$ → B$_2$, etc. the complex {AB} may move along the x axis without a variation of the interaction energy of the particles.

After the usual transformations of the Schrödinger equation, the following secular equation is obtained for the dependence of the energy ϵ on the one-dimensional quasimomentum $\hbar\mathbf{k}$:

$$\operatorname{Det}\{[\varepsilon_n - \varepsilon(\mathbf{k})]\delta_{ik} + a_{ik}\} = 0. \tag{2}$$

In the present case the transition matrix appearing in Eq. (2) is a second rank matrix of the form

$$a_{ik} = \begin{Vmatrix} 0 & J_B + J_A e^{i\varphi} \\ J_B + J_A e^{-i\varphi} & 0 \end{Vmatrix}.$$

The values of the exchange integrals J_A and J_B differ somewhat from their characteristic values for the individual particles {A} and {B}; however, this renormalization is unimportant.

The energy spectrum of such binary defects consists of two branches:

$$\varepsilon(k) = \varepsilon_n \pm (J_A^2 + J_B^2 + 2J_A J_B \cos\varphi)^{1/2}.$$

The tunneling probabilities for particles {A} and {B} may differ significantly from each other: for example, if {A} is a vacancy and {B} is an impurity atom, then $J_A \gg J_B$. In this case the motion of the complete complex takes place at the velocity characteristic of the "slowest" particle {B}:

$$d\varepsilon/dk \approx \mp J_B a \sin\varphi \quad \text{for} \quad J_A \gg J_B.$$

For identical particles

$$\varepsilon(k) = \varepsilon_n \pm J(2 + 2\cos\varphi)^{1/2}.$$

In what follows we shall assume for simplicity that the defects forming the complex are identical. The results are easily generalized to the case of different particles {A} and {B}.

In order for the complex {AB} to be a one-dimensional quasiparticle freely moving along the x axis (Fig. 1), it is necessary that the defect {B} should be on one of the lattice sites which are located in a plane perpendicular to the x axis and passing through the middle of the segment AA$_1$ or A'A.

A2. One-dimensional quasiparticles of the type under consideration are pairs {AB} in which the defect {B} is located in the same sublattice as {A}, on one of the following axes

$$(\mathbf{r}_B - \mathbf{r}_A)/a = (1/2, -3^{1/2}/2, 0) + t(1, 0, 0),$$
$$(\mathbf{r}_B - \mathbf{r}_A)/a = (0, 3^{1/2}, 0) + t(-2^{3/2}/3^{1/2}, 0, 1).$$

In the first case the bidefecton may move along the axis (0, 0, 1); in the second case it may move along the axis (1, 0, 1). In both cases four translationally inequivalent states exist for the pair. Consequently the secular equation (2) is a fourth-order equation, and the spectrum contains four branches:

$$f_{1,2,3,4}(k) = \pm[2 \pm (2 + \cos\varphi)^{1/2}]^{1/2}.$$

A3. In quasiparticles of this type, moving along the axis (1, 0, 0), the defect {B} is found on one of the sites of the same sublattice as the defect {A}, situated on the axis

$$(\mathbf{r}_B - \mathbf{r}_A)/a = (0, -3^{-1/2}, 2^{1/2}/3^{1/2}) + t(0, -2^{3/2}, 1).$$

In the case under consideration the complex can also exist in four translationally inequivalent states. The energy spectrum of the particles is determined from the algebraic equation

$$f^4(k) - 2f^2(k)[3 + 2\cos\varphi] - 4f(k)[1 + \cos\varphi] + 2 - 2\cos\varphi = 0.$$

A4. Complexes with five translationally inequivalent states exist. In such pairs, freely moving along the axis (1, 0, 0), the particle {B} is found—just as in the preceding case—on the axis

$$(\mathbf{r}_B-\mathbf{r}_A)/a=(0,\ -3^{-1/2},\ 2^{1/2}/3^{1/2})+t(0,\ -2^{3/2}.\ 1),$$

but belongs to the other sublattice.

Two branches of the energy spectrum coincide with the spectrum of the type A1 particles:

$$f_{1,2}(k)=\pm(2+2\cos\varphi)^{1/2}.$$

The three remaining branches are determined from the cubic equation

$$f^3(k)-2f(k)(3+\cos\varphi)-4-4\cos\varphi=0.$$

A5. Finally, three types of one-dimensional defectons having six translationally inequivalent states exist. In the first case the defect {B} is found on the axis

$$(\mathbf{r}_B-\mathbf{r}_A)/a=(1/2,\ -3^{1/2}/2,\ 0)+t(0,\ 2^{1/2},\ 1),$$

and the quasiparticle may move along the axis (1, 0, 0). In the energy spectrum, besides the two branches which are identical to the spectrum of the type A1 particles:

$$f_{1,2}(k)=\pm(2+2\cos\varphi)^{1/2},$$

four more branches exist

$$f_{3,4,5,6}(k)=\pm[4+2\cos\varphi\pm4(1+\cos\varphi)^{1/2}]^{1/2}.$$

A6. Defect pairs of the following type can freely move along the axis (1, 0, 0). Particle {B} belongs to the same sublattice as {A}, and is located on the axis

$$(\mathbf{r}_B-\mathbf{r}_A)/a=(1/2,\ 3^{-1/2}/2,\ 2^{1/2}/3^{1/2})+t(0,\ -2^{3/2},\ 1).$$

The six branches of the energy spectrum are given by the roots of the following cubic equation with respect to $f^2(k)$:

$$f^2(k)[f^2(k)-4-2\cos\varphi]^2=4\cos^2\varphi.$$

A7. To the last type of one-dimensional quasiparticles belong pairs, also moving along the axis (1, 0, 0), in which the particle {B} lies on the same axis as in the preceding case, but belongs to the other sublattice. Two degenerate branches, $f_{1,2}(k) = 0$, exist in the spectrum, corresponding to localized states of the pair. The four remaining branches of the spectrum are determined as

$$f_{3,4,5,6}(k)=\pm[3+\cos\varphi\pm(5+6\cos\varphi+\cos^2\varphi)^{1/2}]^{1/2}.$$

TWO-DIMENSIONAL DEFECTONS

B1. The structure of defectons of the present type is shown in Fig. 2a. The defect {A} is located in the plane of the figure, and the second defect {B} lies in any other plane parallel to it; the projection of the defect {B} onto the plane of the figure must coincide with one of the sites nearest to {A}. This complex may move in the plane of the figure. Thus, for example, the pair {AB} may change into the state $\{A_3B_1\}$ through the states $\{A_1B\}$, $\{A_1B_1\}$, and $\{A_2B_1\}$.

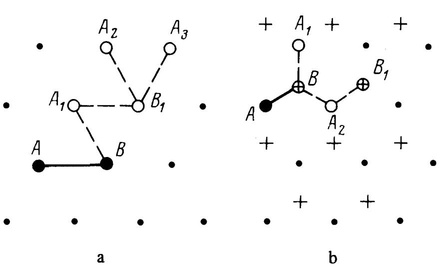

FIG. 2. Two-dimensional quasiparticles: a) type B1, b) type B2. Particle {A} moves in the plane of the figure, and particle {B} moves in another plane parallel to it. The projections of the sites of the second sublattice onto the plane of the figure (x, y, 0) are denoted by crosses.

The spectrum of such two-dimensional quasiparticles was investigated in the article by Andreev.[12] The six branches of the energy spectrum are determined by the roots of the following cubic equation with respect to $f^2(\mathbf{k})$:

$$f^2(\mathbf{k})\left\{f^2(\mathbf{k})-4\left[\cos^2\frac{\varphi_1}{2}+\cos^2\frac{\varphi_2}{2}+\cos^2\frac{\varphi_1-\varphi_2}{2}\right]\right\}^2$$
$$=256\cos^2\frac{\varphi_1}{2}\cos^2\frac{\varphi_2}{2}\cos^2\frac{\varphi_1-\varphi_2}{2}.$$

B2. These particles are shown in Fig. 2b. The projections of the sites of the second sublattice onto the plane of the figure are denoted by crosses. The defecton {B} belongs to the second sublattice and must not be located on a site nearest to {A}. One may select the positions of the pairs {AB}, $\{A_1B\}$, and $\{A_2B\}$ as translationally inequivalent basis states. The quasiparticle moves freely in parallel to the plane of the figure. The energy spectrum is determined from the cubic equation

$$f^3(\mathbf{k})-4f(\mathbf{k})\left\{\cos^2\frac{\varphi_1}{2}+\cos^2\frac{\varphi_2}{2}+\cos^2\frac{\varphi_1-\varphi_2}{2}\right\}$$
$$=4\{1+\cos\varphi_1+\cos\varphi_2+\cos(\varphi_1-\varphi_2)\}.$$

B3. The defect {B} is found on the site $\mathbf{r}_B-\mathbf{r}_A = a(1/2,\ 3^{3/2}/2,\ 0)$. The complex {AB} may move in the plane of the axes (1, 0, 0) and (0, 0, 1). There are eight translationally inequivalent states. Consequently the transition matrix a_{ik}, which determines the energy spectrum (2), is an Hermitian matrix of rank eight.

B4. The pairs {AB} with $\mathbf{r}_B-\mathbf{r}_A = a(3/2,\ -3^{1/2}/2,\ 0)$ belong to the last type of two-dimensional defectons. The spectrum is determined from the secular equation (2) of sixth order. The complex moves in the plane $(x/2,\ 3^{1/2}x/2,\ z)$.

THREE-DIMENSIONAL DEFECTONS

The only case in which a tightly bound pair of point defects constitutes a single three-dimensional binary quasiparticle is that in which the two defects are located on neighboring sites of the crystal lattice. Such a pair has twelve translationally inequivalent positions.

In the case under consideration the state of the complex and its energy spectrum to a large extent depend on the kind of particles forming the pair, since they are located at an interatomic distance from each other, where the exchange interaction between them is substantial. Pairs consisting of two He^3 atoms or of a He^3 atom and a vacancy in a crystal of He^4 are of the greatest interest.

Since the He^3 atom has spin 1/2, the complex consisting of two such impurity atoms may have total spin 0 or 1. The energy levels $\epsilon^{(0)}$ and $\epsilon^{(1)}$ of pairs in these states (in the absence of tunneling through the lattice of the matrix) differ by the value of the exchange integral (J_{33}) of the He^3—He^3 atoms. Owing to the possibility of tunneling transitions and exchange between the He^3 and He^4 atoms (the exchange integral $J_{34} \ll J_{33}$), twelve branches of the energy spectrum $\epsilon_i^{(S)}(\mathbf{k})$ of the binary quasiparticles correspond to each energy level $\epsilon^{(0)}$ and $\epsilon^{(1)}$. The values of the elements a_{ik} of the transition matrix are different for the cases $S = 0$ or $S = 1$, for when the total spin is equal to zero the coordinate part of the wave function is symmetric with respect to interchange of the particles, and at $S = 1$ it is antisymmetric. Examples of numerical solutions of Eq. (2) for different directions of the vector **k** are shown in Fig. 3.

The velocity of motion $\partial\epsilon/\partial\mathbf{k}$ of such pairs is actually equal to the velocity of individual He^3 impuritons and is determined by the quantity J_{34}. In a magnetic field each of the branches of the spectrum for quasiparticles with spin $S = 1$ is split into three lines.

The shape of the spectrum for vacancy-impurity complexes depends substantially on the relationship between the vacancy—matrix atom exchange integral J_{v4} and the vacancy—impurity atom exchange integral J_{v3}. Since $J_{34} \ll J_{v4}, J_{v3}$, He^3—He^4 exchange processes are extremely unlikely in comparison with v—He^3 and v—He^4 exchange processes. The movement of the complex $\{v, He^3\}$ takes place by means of the interchange of positions between the vacancy and the helium atoms, without direct interchanges in the positions of the He^3 and He^4 atoms.

Provided that $J_{v3} \gg J_{v4}$, the spectrum of the $\{v, He^3\}$ pairs if similar to that cited above for the $\{He^3, He^3\}$ pairs and consists of two classes of branches having a characteristic scale J_{v4} at a distance J_{v3} from each other. When the ratio J_{v3}/J_{v4} is decreased these two bands converge and in the limit $J_{v3} \ll J_{v4}$ they go over into a system of twelve slightly separated branches.

In order of magnitude, the average velocity of the quasiparticles $\{v, He^3\}$ coincides with the smallest of the values of the average velocity of individual vacancions in crystals of pure He^3 and He^4 and exceeds by far the velocity of motion of individual impuritons (compare with what was said apropos of type A1 quasiparticles) of He^3 in He^4 crystals. A suitable vacancion mechanism for the transport of ions was investigated earlier[11] by the author.

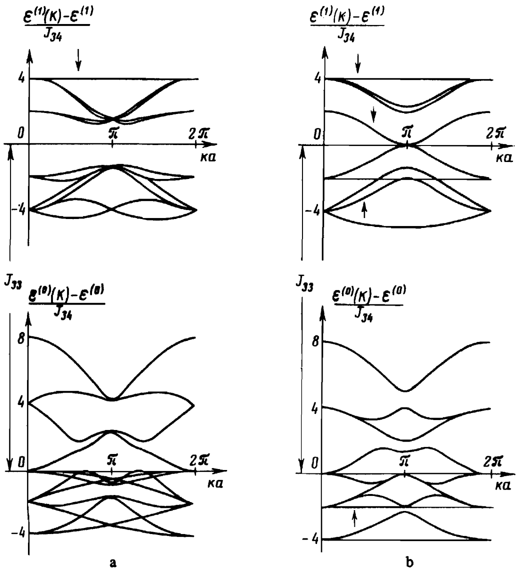

FIG. 3. The energy spectrum of three-dimensional quasiparticles for two directions of the vector k. Degenerate branches are indicated by arrows. The lower bands correspond to spin S = 0, and the upper—to spin S = 1. The vector k is parallel to a) the vector $\mathbf{R}_1 + \mathbf{R}_2 + \mathbf{R}_3$, b) the vector $\mathbf{R}_1$.

In connection with the formation of binary quasiparticles involving the participation of vacancions, it is pertinent to note the following property. The width of the vacancions' energy band is quite large, on the order of a degree. Therefore, it may turn out (this depends on the ratio between the magnitude of the characteristic interaction energy V_0 of the point defects and the value of the exchange integral J_v) that the vacancies participate in tightly bound pairs only at elevated pressures. In any case the maximum size of the bidefectons involving the participation of vacancies is much smaller than the maximum radius of pairs of impurity particles.

INFLUENCE OF BIDEFECTONS ON THE PROPERTIES OF A CRYSTAL

It is necessary to discuss the question of how binary defectons influence the properties of helium crystals. The treatment of a collection of point defects in quantum crystals as a collection of individual defectons can only be valid in the gas approximation, in which the concentration c of defects is assumed to be small:

$$cN \ll 1,$$

where N is the number of lattice sites in a sphere of radius $R_0 = N_0 a$ (R_0 is the maximum distance between the two defects, at which they can form a tightly bound pair).

To a considerable degree the role of the bi-defectons in various physical processes is determined by their concentration. In the gas approximation, the concentration of pairs is of second-order smallness with respect to the particle density c.

Thus,

$$c_\alpha = c^2 N_\alpha, \tag{3}$$

where N_α (N_0) denotes the number of type α binary quasiparticles in which a defect located at a fixed lattice site may participate, and c_α denotes the concentration of the corresponding pairs.

Since the concentration of the complexes which the impurity atoms participate in is small, but their velocity of motion agrees in order of magnitude with the velocity of the individual impuritons, in investigations of the diffusion of impurities one can neglect the presence of practically all kinds of binary particles. The only exceptions (but very important ones) are pairs of impurity atoms and vacancies located on neighboring sites of the crystal lattice. As was indicated above, the velocity of motion of such pairs considerably exceeds the velocity of ordinary impuritons. The movement of impurity atoms with the aid of bound pairs $\{i, v\}$ is an unusual vacancion mechanism of diffusion. Such a mechanism may prove to be the most effective method for the transport of impurity particles in quantum crystals at not too low temperatures T, when the vacancy concentration c_v is not very small.

The concentration of vacancy-impurity complexes is given by

$$c_{(i,v)} = 12 c_i c_v \exp\{(E-E')/T\}.$$

The presence of the exponential factor takes account of the difference between the energy E′ of pair formation and the activation energy E of vacancies far from an impurity. The diffusion coefficient of the impurity atoms, determined by the motion of the pairs $\{i, v\}$, is given by

$$D \sim \frac{c_{(i,v)}}{c_i} \frac{\Delta_v a}{\hbar} l,$$

where Δ_V is the width of the vacancion energy band. At comparatively high temperatures the mean free path l of the pairs is determined by their interaction with phonons and increases with a reduction of the temperature. In this connection, if the possibility of disintegration of the complex associated with phonon scattering is not taken into account, the quantity l—in the same way as for ordinary defectons [1]—is determined by the relationship

$$l \sim \frac{\Delta_v a}{\Theta}\left(\frac{\Theta}{T}\right)^9,$$

where Θ is the Debye temperature.

At lower temperatures it may turn out that the concentration of pairs $\{i, v\}$ is still appreciable, but owing to the reduction in the number of phonons their scattering primarily takes place on impurity particles ($c_i \gg c_{\{i, v\}}$). In this case the mean free path of the pairs is inversely proportional to their cross section σ for scattering by impurity atoms and to the impurity concentration c_i:

$$D \sim \frac{c_{\{i,v\}}}{c_i}\frac{\Delta_v a^4}{\hbar\sigma c_i}$$

Perhaps the experimentally observed [14] dependence of the diffusion coefficient on the impurity atom concentration associated with the vacancion mechanism for the transport of impurities is due to the influence of precisely such a method for the movement of the impurity particles.

The motion of impurity atoms through a He^4 crystal may be realized simultaneously with the aid of the mechanism under consideration as well as with the aid of the general vacancion mechanism for the transport of impurity particles investigated earlier. [8] If the width of the vacancion band is large, $\Delta_V \gg V_0$, then—as noted at the end of the first part of the present article—bound pairs $\{i, v\}$ do not exist and the transport of He^3 atoms is accomplished in accordance with the theory [8]. With an increase of the pressure the width Δ_V of the band decreases, and provided that $V_0 \gg \Delta_V \gg T$ both vacancion mechanisms act in parallel. The influence of the transport mechanism [8] is strong only if the characteristic wavelength of the vacancions is sufficiently large, which corresponds to the following condition on the temperature:

$$T \ll \Delta_v(\Delta_v/V_0)^{2/3}.$$

In this connection the contribution of the pairs $\{i, v\}$ to the diffusion process is predominant at small concentrations of the impurity particles (compare with [8])

$$c_i \ll \frac{a^2}{\sigma}\left(\frac{\Delta_v}{T}\right)^{3/2}\exp\left\{\frac{E-E'}{T}\right\}$$

The difference between the energy E′ and the activation energy E of the vacancies leads to an indirect effect of the concentration on the exponential factor in the dependence of the diffusion coefficient on the temperature.

The role of the complexes is also important in another circle of phenomena which are associated with energy dissipation in quantum crystals, for example, with internal friction. As is well known, the scattering of elastic energy by individual vacancies and by substitutional impurities takes place only upon a spatially inhomogeneous deformation of the crystal. The corresponding computation of the energy absorption coefficient under the conditions of the Gorskiĭ effect was carried out earlier. [15] However, the recently published results of measurements of the internal friction in quantum crystals [16,17] indicate that the dissipation processes are possibly more complex.

The presence of pairs of point defects leads to energy dissipation even for a homogeneous deformation of the crystal. The absorption maxima are related to processes involving reorientation of different types of pairs. Reorientations of the pairs in ordinary crystals correspond in quantum crystals to resonance transitions of the bidefectons between the branches of their energy spectrum. In the present case the subject of discussion is actually the quantum analog of Zener relaxation. Notwithstanding the fact that, at high frequencies energy scattering also takes place on individual defects, the lines of dissipation on bidefectons should be clearly distinguishable due to their clearly expressed resonance character. We shall discuss this question in somewhat more detail.

The absorption peaks are smeared out at not too low temperatures due to relaxation processes. The shape of the absorption line is characterized by the usual Debye maximum of the form

$$\omega\tau/(1+\omega^2\tau^2)$$

at a frequency $\omega\tau \sim 1$, and differs from the line shape in ordinary crystals only by having a different temperature dependence of the relaxation time τ.

The time required to establish the equilibrium distribution function of the bidefectons is determined by the collisions with phonons. In the present case relaxation processes involving different relaxation times τ are possible. In the first place, an equilibrium distribution of the particles with respect to the different branches of their energy spectrum must be established for each type of bidefecton. Such an equilibrium is established by inelastic scattering of the phonons, in which their energy changes by an amount of order J during a time interval [4]

$$\frac{1}{\tau} \sim \frac{\Theta}{\hbar}\left(\frac{T}{\Theta}\right)^7. \tag{4}$$

The equilibrium distribution of the complexes with respect to their energies may also be established by means of collisions with phonons involving the transformation of different kinds of pairs into each other. The branch systems of the energy spectrum for the different kinds of pairs are separated from one another by gaps of the order of magnitude of the characteristic interaction energy of two point defects at close spacing, $V_0 \gg J$. The inequality $V_0 \gg T$ is usually valid over a wide range of temperatures and, since we are interested in the region of rather low frequencies, $V_0 \gg \hbar\omega \sim J$, such relaxation processes can be neglected. However, for certain kinds of defects [10] and for a large distance between them, the interaction energy V of the elements of a pair may turn out to be small, $T \gg V \gg J$. In this case the relaxation time is determined by annihilation and creation processes for different kinds of bidefectons and also increases with decreasing temperature according to formula (4). Just as for all defectons, the momentum relaxation time is proportional to T^{-9}.

The case of low temperatures, $\hbar/\tau \ll J$, $\hbar\omega$, is physically more interesting. In this connection sharp resonance absorption peaks should be observed for each kind of bidefectons at the frequencies of transitions between different branches of their energy spectrum. Complexes having different values of the quasimomentum **k** participate in the transitions; just as for any quasiparticles in a crystal the absorption maxima correspond to extremal points of the energy spectrum, near which the density of states is largest. At these points the absorbed power (neglecting relaxation processes) tends to infinity. The peaks differ from δ-shaped peaks to the extent that the density of states differs from zero for the nonextremal frequencies. Outside the immediate neighborhood of the resonance point, the shape of the peak is practically independent of the relaxation processes. The width of the resonance peaks is determined by the width of the bidefecton band, and in order of magnitude it is equal to the exchange integral J.

If relaxation processes are neglected, i.e., the collision integral in the kinetic equation, the amount of power W absorbed per unit volume under the influence of the perturbing potential (homogeneous deformation) $\hat{H}\cos\omega t$ is calculated with the aid of the well known formula of perturbation theory:

$$W_\alpha=\frac{1}{2}\pi c_\alpha\frac{\hbar\omega^2}{T}\int\frac{d^3k}{(2\pi)^3}\frac{d^3k'}{(2\pi)^3}\sum_{\nu'>\nu}|H^{\nu\nu'}_{\mathbf{kk}'}|^2[\delta(\varepsilon-\varepsilon'-\hbar\omega)+\delta(\varepsilon-\varepsilon'+\hbar\omega)]. \tag{5}$$

In this expression the indices α and ν determine, respectively, the type of quasiparticles and the label on the branches of their energy spectrum, $\epsilon=\epsilon_\nu(\mathbf{k})$, $\epsilon'=\epsilon_{\nu'}(\mathbf{k}')$. Furthermore, it is considered that, due to the smallness of the defecton exchange integral $J \ll T$, the following relationship is valid for the equilibrium distribution function $n(\epsilon)$ of the particles with respect to their energies:

$$n(\varepsilon)-n(\varepsilon')=c_\alpha(\varepsilon'-\varepsilon)/T.$$

For the determination of the matrix element $H^{\nu\nu'}_{\mathbf{kk}'}$, we note that the wave function Ψ_ν of each of the states ν is a linear combination of the wave functions Φ_n of the basis (translationally inequivalent) states of the pair

$$\Psi_\nu=e^{i\mathbf{kr}}\sum_n z_{\nu,n}(\mathbf{k})\Phi_n, \tag{6}$$

where each of the sets of coefficients $z_\nu=\{z_{\nu,n}\}$ is an eigenvector of the matrix (2). The vectors z_ν are orthonormalized

$$\sum_n z^*_{\nu',n}z_{\nu,n}=\delta_{\nu\nu'}.$$

One can easily determine the matrix element of the perturbation operator with the aid of the wave functions (6)

$$H^{\nu\nu'}_{\mathbf{kk}'}=\sum_n z^*_{\nu',n}z_{\nu,n}\lambda_n\delta(\mathbf{k}-\mathbf{k}'), \tag{7}$$

where λ_n denotes the change in the energy of a pair of point defects having the n-th orientation under the action of the corresponding tensile stress. The quantities λ_n are determined from the usual theory of elasticity.[18]

Formulas (5) and (7) and the spectra obtained in the first part of this article describe Zener relaxation in quantum crystals. As an example, we present the value of the absorption coefficient for quasiparticles of type A1. Complexes of this type give the greatest contribution to the dissipation since their concentration exceeds the concentration of complexes of any other kind. Only the concentration of type A1 pairs is proportional to the square of the interaction radius $R_0 = N_0a$ (see formula (3)):

$$c_{A1}=c^2N_{A1},\qquad N_{A1}(N_0\to\infty)\to3\pi N_0^2/2^{3/2}.$$

The value of the absorbed power is given by

$$W_{A1}=\frac{c_{A1}}{8\pi a^3}\frac{\lambda^2}{T}\frac{\hbar\omega^2}{J(1-\hbar^2\omega^2/16J^2)^{1/2}}$$
$$W_{A1}(\hbar\omega>4J)=0,$$

where $\lambda=\lambda_1-\lambda_2$ is the relative change of the pair's energy in the two basis states (the states $\{AB\}$ and $\{AB_1\}$ for the pair of point defects shown in Fig. 1) under the influence of the perturbing field.

Transitions between the bands $\epsilon^{(0)}_i(\mathbf{k})$ and $\epsilon^{(1)}_j(\mathbf{k})$ are impossible for three-dimensional binary quasiparticles in the absence of an electromagnetic field because of spin selection rules. In connection with the effect on a He^4 crystal of a spatially inhomogeneous magnetic field which is oscillating in time, the energy absorption should take place with a maximum at the frequency $\hbar\omega \sim J_{33}$.

In conclusion the following fact should be mentioned. Besides the completely localized pairs and the pairs which move freely through the crystal, tightly bound pairs exist which, although they are not able to move, are still able to reorientate themselves. Such complexes, corresponding to objects having several energy levels, do not participate in the diffusion motion, but do contribute to the scattering of energy in the crystal.

Delocalized quasiparticles—defectons consisting of more than two point defects—may also exist in the crystal. For example, the complex of three defects $\{ABC\}$, as shown in Fig. 4, may freely travel along the x axis. However, the concentration of such complexes is insignificantly small.

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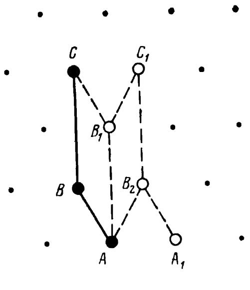

FIG. 4. The complex of three particles {A, B, C} may pass through the positions {A, B_1C}, {AB_1C_1}, {AB_2C_1} into the position {$A_1B_2C_1$} without a change in the energy of its constituent defects. The complex constitutes a one-dimensional quasiparticle, freely traveling along the axis AA_1.

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[1] It was recently noted (W. J. Mullin, R. A. Guyer, and H. A. Goldberg) that the anisotropy of the interaction energy of the defects with respect to the two lattices of an hexagonal close-packed crystal may turn out to be large in comparison with the width Δ of the band. For those point defects for which this property holds, the types of bidefections differ somewhat from those described in this article. However, this case is easily investigated by the method used in this work, and moreover the basic physical results are retained without changes.

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