

# Diffusion in quantum crystals

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The contemporary theoretical ideas on quantum diffusion of impurity particles and point defects in crystals of solid helium are reviewed. Results are given of experimental studies on diffusion of isotopic impurities and ions in solid helium in which quantum diffusion was actually found. The energy spectrum of a quantum crystal in the presence of impurities or point defects is discussed. Owing to the specific dynamics of impurity particles, excitations of the crystal exist that behave like one- or two-dimensional quasiparticles within the volume of the three-dimensional crystal. Experimental nuclear magnetic resonance data in solid solutions of helium isotopes confirm the existence of two-dimensional quasiparticles. The features of behavior of dislocations in quantum crystals are elucidated. Experiments are discussed in which these features should be manifested.

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## 1. INTRODUCTION

The ordinary "quantum" theory of solids is based on assuming a quasiclassical crystal lattice. On the one hand, the quantum effects in this theory play an important role for the phonons of the crystal (namely, at temperatures below the Debye temperature). On the other hand, the particles that form the crystal are viewed as being localized near definite equilibrium positions. The latter property is purely classical. Actually, the mutually identical particles that form the crystal prove here to be individualized by belonging to definite lattice sites. Yet, in quantum mechanics identical particles must be indistinguishable. Although the quasiclassical picture of a crystal is therefore approximate, its accuracy for the vast majority of crystals is very high, and it considerably exceeds the possibilities of experiment.

However, there is a small group of so-called quantum crystals in which the deviations from the usual picture are quite appreciable. The most clearly marked quantum crystals are those of the isotopes of helium ( $^3\text{He}$ ,  $^4\text{He}$ , and their solutions). This is evident even from simply examining their phase diagrams. As we know, the picture of quantum-mechanically indistinguishable particles plays the decisive role at low temperatures in the properties of liquid helium (a quantum liquid). Liquid helium crystallizes upon a slight increase in pressure (25–30 atm) with a relatively small change in density (~5%). Evidently the crystals that arise here must to a substantial degree retain their quantum nature.

This article aims to review the set of phenomena involved with the behavior of impurities and defects in solid helium. As will be evident below, it is precisely these phenomena that manifest most clearly the quantum nature of helium crystals, which gives rise to qualitatively new effects such as quantum diffusion.

## 2. QUANTUM CRYSTALS

Let us examine the problem of quantitatively characterizing the region of applicability of the ordinary quasiclassical theory, and that of the cases in which one can expect the maximum deviations from this theory. In order to do this, we must elucidate the relationship between two types of quantum effects in crystals, of which certain ones are taken into account in the quasiclassical theory, while others give deviations from this theory, i.e., a quantum type of crystal. Let us study the temperature dependence of the mean-square amplitude  $\bar{u}^2$  of the vibrations of an atom of the crystal about an equilibrium position. At temperature  $T$  considerably above the Debye temperature  $\Theta$ , the classical linear relation  $\bar{u}^2 \sim a^2 T/U$  holds. Here  $a$  is the interatomic distance, and  $U$  is the interaction energy of adjacent atoms in the crystal. The ordinary quantum effects, which are accounted for in the quasiclassical theory, have the effect that the  $\bar{u}^2(T)$  curve reaches a plateau at temperatures  $T \sim \Theta$  that determines the amplitude  $\bar{u}_0^2$  of the zero-point vibrations of the atom. Evidently the quantity  $\bar{u}_0^2$  can be found from the classical formula for  $\bar{u}^2(T)$  by the substitution  $T \sim \Theta$ . That is,  $\bar{u}_0^2 \sim a^2 \Theta/U$ . The restricted applicability of the quasiclassical theory involves the possible delocalization of an atom by its

migration to an adjacent crystal lattice site, or in other words, it involves the probability  $w(a)$  of finding an atom at the distance  $u \sim a$  from the equilibrium position. At low temperatures where the zero-point vibrations play the major role, the probabilities  $w(u)$  of different values of  $u$  are determined by the square of the modulus of the wave function of the ground state of the oscillator, and they obey a Gaussian law:  $w(u) \propto \exp(-u^2/2\bar{u}_0^2)$ . Hence the probability  $w(a)$  of quantum tunneling of an atom to an adjacent lattice site is  $w(a) \propto \exp(-1/\Lambda)$ , where  $\Lambda \sim \Theta/U$ . The condition for applicability of the quasiclassical theory is that  $w(a)$  should be small, as happens with small values of the dimensionless parameter  $\Lambda$ . However, an essential point is that the ordinary quantum effects in a crystal involve the finiteness of the Debye temperature, which is proportional to  $\Lambda$ :  $\Theta \sim \Lambda U$ . Hence these effects are governed by the same parameter  $\Lambda$ . The difference between the ordinary quantum theory of crystals and the theory of quantum crystals consists in the idea that the former takes account only of the quantum effects that are proportional to some power of the parameter  $\Lambda$ , while it neglects the exponentially small effect of delocalization of particles. The parameter  $\Lambda$  is very small for most crystals (it is equal to the ratio of the Debye temperature to the temperature  $T \sim U$  at which strong anharmonicity of the vibrations of the crystal sets in), and the quasiclassical theory is highly accurate. In quantum crystals,  $\Lambda \sim 1$ , and the effect of delocalization of particles is quite considerable. We stress that even the zero-point vibrations of quantum crystals are strongly anharmonic.

We can easily express the parameter  $\Lambda$  in terms of the characteristics of the atoms of the crystal. Upon taking account of the fact that  $\Theta \sim \hbar\omega$ , where  $\omega \sim \sqrt{\kappa/m}$  is the characteristic vibration frequency of the atoms,  $m$  is their mass, and  $\kappa \sim U/a^2$  is the stiffness of the "spring" that holds the atoms in the equilibrium positions, we find that  $\Lambda \sim (\hbar/a)(mU)^{-1/2}$ . In this form, the parameter  $\Lambda$  is known as the quantum parameter of de Boer. Its value is greatest for crystals consisting of the lightest and most weakly interacting atoms. The highest values of  $\Lambda$  are attained by  $^3\text{He}$  ( $\Lambda = 0.49$ ), by  $^4\text{He}$  ( $\Lambda = 0.43$ ), by hydrogen  $\text{H}_2$  ( $\Lambda = 0.28$ ), and by neon ( $\Lambda = 0.07$ ). The parameter  $\Lambda$  is infinitesimally small in all other pure substances. There are other important cases in which the delocalization effect is important for a fraction, rather than all of the constituent particles of a crystal. For example, this pertains to admixtures of hydrogen in the lattices of certain metals (niobium, zirconium). Owing to their small mass and relatively weak interaction with the atoms of the matrix, the hydrogen atoms can be delocalized in the crystal, while the atoms of the matrix themselves behave quite classically.

Now let us turn our attention to the following situation. The interaction energy  $U$  of adjacent atoms depends on the distance  $a$  between them. The interatomic distance  $a$  decreases with increasing pressure, while the interaction energy  $U$  increases. Here the quantum parameter  $\Lambda$  declines or increases, depending on whether the product  $Ua^2$  increases or decreases. Inasmuch as the interaction energy of neutral atoms

changes with varying distance considerably faster than  $1/a^2$ , the parameter  $\Lambda$  declines rather quickly with increasing pressure. Thus the most characteristic quantum crystal is solid helium at minimal pressures.

### 3. DIFFUSION IN AN IMPURITON GAS

There is the following very simple way of detecting the effect of delocalization of particles in a crystal. Let us consider a helium crystal containing one impurity atom, e.g., a  $^3\text{He}$  impurity in a crystal of  $^4\text{He}$ . Even at absolute zero, this impurity atom can migrate in the crystal by the above-mentioned quantum tunneling, in which it changes places with an adjacent atom of the matrix. Owing to the periodic potential in which the impurity atom moves, the good quantum number in this case is not the coordinate, but the quasimomentum  $p$ . The energy of the system is some periodic function  $E(p)$  of the quasimomentum. The situation here is quite analogous to the well-known case of electrons in a metal. The impurity atoms behave like quasiparticles that freely migrate through the crystal with constant velocity. These quasiparticles were introduced by I. M. Lifshitz and me<sup>[1]</sup> and by Guyer and Zane,<sup>[2]</sup> and are called impuritons or mass-fluctuation waves. [Translator's note: The currently-accepted term in English is "impuriton" and is due to<sup>[3]</sup>, whereas the Russian authors use the term "primeson."] Their most important characteristics are the width  $\Delta$  of the energy band (or the tunneling frequency  $J \sim \Delta/\hbar$ ) and the velocity of motion  $v = \partial E/\partial p \sim aJ$ . Typical values for a  $^3\text{He}$  impurity in a  $^4\text{He}$  lattice are:  $\Delta \leq 10^{-4}$  °K,  $J \leq 1$  MHz,  $v \leq 10^{-1}$  cm/sec. Significantly, the band width  $\Delta$  is considerably smaller than all the other energies that characterize the helium crystal. We shall see below that the dynamics of impuritons is thereby very distinctive.

If the concentration of the impurities is small enough, then they constitute a rarefied impuriton gas. Thus the simple arguments given above imply a very important conclusion on the nature of the diffusion of impurities in quantum crystals.<sup>[1]</sup> Namely, a so-called quantum diffusion must take place that has the same characteristic features as for diffusion of particles in a gas. We can use the ordinary formula  $D \sim vl$  of gas-kinetic theory to calculate the diffusion coefficient, where  $l$  is the free flight path of the impurities. We can neglect phonons at low temperatures, and the scattering of impuritons by one another plays the major role. The free flight path is  $l \sim (n\sigma)^{-1} \sim a^3/\sigma x$ . Here  $n$  is the number of impurities per unit volume,  $x$  is the concentration, and  $\sigma$  is the scattering cross-section of an impuriton by an impuriton. The diffusion coefficient

$$D \sim \frac{Ja^4}{\sigma x} \quad (1)$$

is inversely proportional to the concentration, and it does not depend on the temperature.<sup>[3-14]</sup>

Quantum diffusion has been detected experimentally by Richards, Pope, and Widom<sup>[3]</sup> and by Grigor'ev, Esel'son, Mikheev, and Shul'man.<sup>[5-7]</sup> Figure 1 shows the concentration dependence of the diffusion coefficient of  $^3\text{He}$  impurities in an h.c.p. crystal of  $^4\text{He}$  with a molar

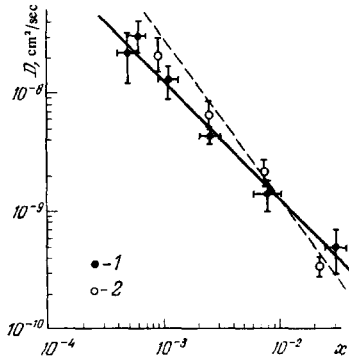


FIG. 1. The concentration dependence of the diffusion coefficient of  $^3\text{He}$  impurities in an h.c.p. crystal of  $^4\text{He}$  at a molar volume of  $21 \text{ cm}^3$  at  $T < 1.2 \text{ K}$ . 1—data of [13], 2—data of [5].

volume of  $21 \text{ cm}^3$ , as obtained by NMR. The experimental data fit well the solid straight line corresponding to the law  $Dx = 1.2 \times 10^{-11} \text{ cm}^2/\text{sec}$ . Moreover, Grigor'ev *et al.* [5-7] have studied in detail the temperature dependence of diffusion, and they showed it to be temperature-independent in the low-temperature region. We find by comparing Eq. (1) with the experimental data for  $J \sim 1 \text{ MHz}$  the scattering cross-section  $\sigma \sim 100 \text{ \AA}^2$ . Such a large cross section amazes at first glance, yet it can be easily explained by the features of the dynamics of impuritons that arise from their very narrow energy band. Indeed, let us examine the mutual interaction of two impuritons. The total energy of the system is

$$E_{12} = E(\mathbf{p}_1) + E(\mathbf{p}_2) + U(\mathbf{r}_{12}). \quad (2)$$

Here  $\mathbf{p}_1$  and  $\mathbf{p}_2$  are the quasimomenta of the impuritons,  $E(\mathbf{p})$  is the energy of an isolated impuriton as a function of its quasimomentum,  $U(\mathbf{r}_{12})$  is the interaction energy, and  $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ , where  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are the coordinates of the impuritons. The sum of kinetic energies  $E(\mathbf{p}_1) + E(\mathbf{p}_2)$  cannot vary by an amount greater than  $2\Delta$ , since  $\Delta$  is the total width of the energy band. Since the total energy is conserved, the potential energy  $U(\mathbf{r}_{12})$  also cannot vary by more than  $2\Delta$ . Hence the colliding impuritons cannot approach to a distance less than the interaction radius that is defined by the relationship  $U(R_0) \sim \Delta$ . Since  $\Delta$  is small in comparison with all the other characteristic energies,  $R_0$  considerably exceeds the interatomic distance. At large distances, the interaction of impuritons arises mainly from elastic interaction. An impuriton creates a lattice deformation about it, with which another impuriton interacts. Elasticity theory [15] gives the following expression for the elastic-interaction energy of any sort of point defects:

$$U(\mathbf{r}_{12}) = V_0(n) \left( \frac{a}{r_{12}} \right)^3. \quad (3)$$

Here  $V_0$  is a certain characteristic energy that depends on the mutual orientation of the defects, with  $n = \mathbf{r}_{12} / |\mathbf{r}_{12}|$ . Thus we find the interaction radius  $R_0 \sim a(V_0/\Delta)^{1/3}$  and the impuriton-impuriton scattering cross section

$$\sigma \sim R_0^2 \sim a^2 \left( \frac{V_0}{\Delta} \right)^{2/3}.$$

The experimental value of the cross-section  $\sigma \sim 100 \text{ \AA}^2$  makes it possible to determine a characteristic interaction energy  $V_0 \sim 10^3 \Delta$ , which agrees with the result of direct calculation [16] based on the formulas of elasticity theory.

Thus the experimental data completely fit a description of the impurities as being a gas of impuritons. Yet the following question arises. The region of applicability of the gas model is determined by the requirement that the mean distance between the impuritons is large in comparison with the interaction radius. That is,  $a/x^{1/3} \gg R_0$ , or  $x \ll \Delta/V_0 \sim 10^{-3}$ . Moreover, experiment shows (see Fig. 1) that the diffusion coefficient is approximately inversely proportional to the concentration in the broader concentration range  $10^{-4} < x < 10^{-2}$ . Hence we must consider the region of higher concentrations  $10^{-3} < x < 10^{-2}$ , in which the mean distance between impurity atoms is less than  $R_0$ , and the system of impuritons is not a gas.

#### 4. DIFFUSION OF STRONGLY-INTERACTING IMPURITONS

Let two impurity atoms lie at a mutual distance less than the interaction radius. That is,  $r_{12} < R_0$ . Let us find the distance range  $r_{12}$  in which these atoms can be treated as interacting impuritons with a total energy defined by Eq. (2). This formula holds whenever the change in the interaction energy

$$\delta U(r_{12}) = U(r_{12} + a) - U(r_{12}) \sim a \frac{\partial U}{\partial r_{12}}, \quad (4)$$

that arises in the tunnel transition of one of the atoms to an adjacent lattice site is small in comparison with the band width  $\Delta$ . This condition is more than satisfied at  $r_{12} \sim R_0$ , since

$$\delta U(R_0) \sim V_0 \frac{a^4}{R_0^3} \sim \left( \frac{a}{R_0} \right) \Delta \sim 10^{-1} \Delta.$$

It breaks down in the distance range  $r_{12} < R_1$ , when  $R_1 \sim a(V_0/\Delta)^{1/4}$ . Thus, in the intermediate range  $R_1 < r_{12} < R_0$ , the interaction between the impurity atoms is already strong, but these atoms still behave like interacting impuritons.

The concentration range in which the picture of strongly-interacting impuritons is valid is determined by the requirement that the mean distance between the  $^3\text{He}$  atoms is smaller than  $R_0$  but larger than  $R_1$ . That is,

$$\frac{V_0}{\Delta} < x < \left( \frac{V_0}{\Delta} \right)^{3/4} \quad \text{or} \quad 10^{-3} < x < 10^{-2}.$$

This is precisely the region that we must treat in order to explain the experimental data. In order to elucidate the nature of the motion of the strongly interacting impuritons, it is convenient to treat first the simplified problem of the motion of an isolated impuriton when acted on by the constant force  $\mathbf{F}$ . We find from the ordinary equation of motion  $\dot{\mathbf{p}} = \mathbf{F}$  the time-dependence of the quasimomentum  $\mathbf{p} = \mathbf{p}_0 + \mathbf{F}t$ , where  $\mathbf{p}_0$  is the initial value of the quasimomentum. If  $\mathbf{F}$  lies along one of the crystallographic axes, then the energy  $E(\mathbf{p})$  and the ve-

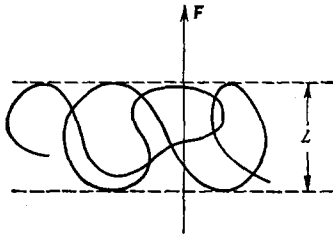


FIG. 2. Trajectory of movement of an impuriton when acted on by a constant force.

locity  $\mathbf{v} = \partial E / \partial \mathbf{p}$  vary periodically with varying  $\mathbf{p}$  with a period of the order of  $\hbar/a$ . Since  $\mathbf{p}$  is a linear function of the time,  $E$  and  $\mathbf{v}$  are periodic functions of the time with a period of the order of  $\hbar/aF$ . Here the mean velocity is zero. Thus, when acted on by a constant force, an impuriton oscillates about some mean position with a frequency of the order of  $aF/\hbar$  and an amplitude of the order of  $v/(aF/\hbar) \sim \Delta/F$ . Yet there is a substantial difference between the special case discussed here and the general case in which the direction of the force is arbitrary. Since there is no periodicity in momentum space along an arbitrary direction, all three components of the velocity of the impuriton in the general case vary in time in a rather random way. The trajectory of the impuriton is a random curve like that shown in Fig. 2. Since the potential energy  $-F \cdot r$  cannot vary by more than  $\Delta$ , the trajectory is confined within a layer perpendicular to the direction of the force having a thickness of the order of  $L \sim \Delta/F$ . The characteristic radius of curvature of the trajectory matches in order of magnitude the thickness  $L$  of the layer. The impuriton moves along the trajectory with a velocity of the order of  $\omega J$ . Hence it diffuses in a plane perpendicular to the direction of the force. In order of magnitude, the diffusion coefficient is  $D \sim vL$ , or

$$D \sim \frac{\hbar J^2 a}{F}. \quad (5)$$

In principle, such a pattern of motion has been known for a long time in the theory of electrons in metals. However, the discussed diffusional movement is unobservable for electrons, owing to the vast width of their energy band, whereby the characteristic distance  $L$  always considerably exceeds the free flight path.

The arguments given here clarify the nature of the movement of strongly interacting impuritons. The force  $F$  caused by their interaction is

$$F \sim \frac{\partial U}{\partial r_{12}} \sim V_0 \frac{a^2}{r_{12}^3}. \quad (6)$$

When acted on by this force, each of the impuritons diffuses with a diffusion coefficient determined by Eqs. (5) and (6):

$$D \sim \frac{\hbar J^2}{a^2 V_0} r_{12}^3. \quad (7)$$

In order to calculate the diffusion coefficient of a  $^3\text{He}$ - $^4\text{He}$  solution in the concentration range  $10^{-3} < x < 10^{-2}$ , it suffices to substitute for  $r_{12}$  in Eq. (7) the mean distance between the  $^3\text{He}$  atoms, i.e.,  $r_{12} \sim a/x^{1/3}$ . Consequently we find

$$D \sim \frac{\hbar J^2 a^2}{V_0} x^{-4/3}. \quad (8)$$

This formula agrees with the experimental data, since it gives the same result when  $x \sim \Delta/V_0 \sim 10^{-3}$  as Eq. (1) does, while the experimental accuracy is not great enough in the range  $10^{-3} < x < 10^{-2}$  to distinguish the similar  $x^{-1}$  and  $x^{-4/3}$  laws. The dotted straight line in Fig. 1 corresponds to the  $x^{-4/3}$  law. Thus the experimental data in the region of substantial concentrations are explained naturally by the specifics of the diffusion of impuritons when acted on by the interaction force.<sup>[17]</sup>

Landesman and Winter<sup>[8]</sup> and Huang *et al.*<sup>[14]</sup> have treated the problem of diffusion of impurities in the region of substantial concentrations. Although these authors have especially stressed that their approach is an alternative to the description using the impuriton concept, Eq. (8) agrees with the result of Landesman and Winter. Hung *et al.* got a numerically similar result. We should note that in<sup>[8]</sup> they gave the inequality  $x \gg (\Delta/V_0)^2 \sim 10^{-6}$  as the region of applicability of Eq. (8), from which the authors concluded that one can't observe impuritons in the experimentally studied concentration range.

## 5. TEMPERATURE DEPENDENCE OF DIFFUSION

Thus far we have been studying the region of low enough temperatures in which quantum diffusion is governed by the mutual interaction of impuritons. With increasing temperature, the interaction of impuritons with phonons also begins to play an important role. This diminishes the free flight path. Thus the diffusion coefficient of the impuritons must decline with increasing temperature. However, for this reason, thermally activated diffusion, which rises exponentially with increasing temperature, must begin to play a more substantial role than quantum diffusion at a high enough temperature. Hence there are three characteristic temperature ranges (Fig. 3). In region I, diffusion is limited by impuriton-impuriton scattering, and it is independent of the temperature. In region II, diffusion is limited by scattering of impuritons by phonons, and it declines with increasing temperature. Finally, in region III, the thermally activated diffusion mechanism plays the major role. Since evidently diffusion is concentration-dependent only in region I, increasing concentration will narrow region II, and finally make it vanish completely. The dotted curves in Fig. 3 demonstrate the changing nature of the temperature de-

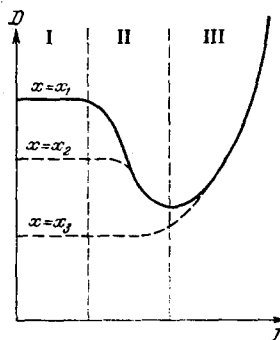


FIG. 3. Temperature dependence of the diffusion coefficient of impurities.

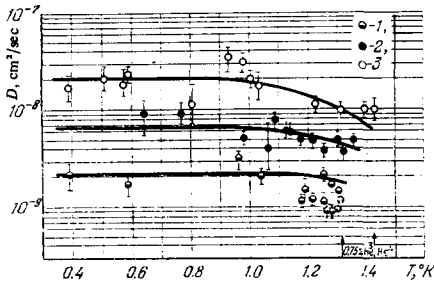


FIG. 4. Temperature dependence of the diffusion coefficient of  $^3\text{He}$  impurities in an h.c.p. crystal of  $^4\text{He}$  at a molar volume of  $21 \text{ cm}^3$  [6] at different concentrations. 1—0.75%; 2—0.25%; 3—0.092%. The vertical arrows indicate the transition temperature to the b.c.c. phase for pure  $^4\text{He}$  and for a solution of concentration 0.75%  $^3\text{He}$ .

pendence with larger concentrations, with  $x_3 > x_2 > x_1$ .

Let us examine the phonon region II in greater detail. The time between collisions of an impuriton with phonons is  $\tau \sim (Nc\sigma_{\text{ph}})^{-1}$ , where  $N \sim (T/\Theta a)^3$  is the number of phonons per unit volume,  $c$  is the velocity of sound, and  $\sigma_{\text{ph}}$  is the scattering cross section of a phonon by an impuriton. If the temperature is small in comparison with the Debye temperature, then long-wavelength acoustic phonons play the major role. As we know, their cross section for scattering by point defects is proportional to the fourth power of the wave vector of the phonons  $q \sim T/\Theta a$ . Thus,  $\sigma_{\text{ph}} \sim a^2(qa)^4 \sim a^2(T/\Theta)^4$ , and the time between collisions proves to be  $\tau \sim (a/c)(\Theta/T)^7 \sim (\hbar/\Theta)(\Theta/T)^7$ . However, rather than  $\tau$ , it is the transport time between collisions, which strongly differs from  $\tau$ , that enters into the expression for the diffusion coefficient of impuritons  $D \sim v^2\tau_{\text{tr}}$ . The point is that the width of the impuriton energy band is smaller than the temperature at all attainable temperatures. Hence the quasimomenta of the impuritons are equal in order of magnitude of  $\hbar/a$ . However, the momenta of the phonons are considerably smaller. In this case, as usual, the transport time differs from  $\tau$  by the additional factor  $(\Theta/T)^2$ . The diffusion coefficient

$$D \sim \frac{\hbar a^2 J^2}{\Theta} \left(\frac{\Theta}{T}\right)^9 \quad (9)$$

is therefore inversely proportional to the ninth power of the temperature in the phonon region. [1]

The problem of the region of applicability of Eq. (9) is of interest. The free flight path of an impuriton is  $l \sim v\tau \sim a(\Delta/\Theta)(\Theta/T)^7$ .

At temperatures  $T \ll T_0$ , where  $T_0 \sim \Theta(\Delta/\Theta)^{1/7}$ , the free flight path is large in comparison with the interatomic distance, and the derivation given above for Eq. (9) gives no grounds for doubt. Yet, interestingly as Kagan and Maksimov [11] and Kagan and Klinger [12] have shown, Eq. (9) holds without any changes over a considerably larger temperature range up to temperatures of the order of the Debye temperature. One can get this result most simply with the following arguments that show likewise that the impuriton concept keeps its meaning to a substantial degree, even under conditions in which their free flight path is much smaller than the

interatomic distance. [17]

The problem is that of the motion of quasiparticles that interact with phonons, and which have the spectrum

$$E(p) = E_0 + e(p).$$

Here  $E_0$  is a constant, and  $e(p)$  is a function of the quasimomentum that is equal to  $\Delta$  in order of magnitude. Hence it is small in comparison with the temperature. The kinetic equation for the classical distribution function of the quasiparticle  $f(\mathbf{r}, \mathbf{p}, t)$  has the following form:

$$\frac{\partial f}{\partial t} + \frac{\partial e}{\partial \mathbf{p}} \frac{\partial f}{\partial \mathbf{r}} + \mathbf{F} \frac{\partial f}{\partial \mathbf{p}} = I, \quad (10)$$

where  $\mathbf{F}$  is the external force acting on the impuriton, and  $I$  is the collision integral with phonons:

$$I = - \int d^3p' \int d^3q d^3q' W(\mathbf{q}, \mathbf{q}') \{n(\mathbf{q}) [1 + n(\mathbf{q}')] f(\mathbf{p}) - n(\mathbf{q}') [1 + n(\mathbf{q})] f(\mathbf{p}')\} \delta(\mathbf{q} + \mathbf{p} - \mathbf{q}' - \mathbf{p}') \delta[\omega(\mathbf{q}) - \omega(\mathbf{q}')]. \quad (11)$$

Here  $n(\mathbf{q})$  is the distribution function of the phonons,  $\omega(\mathbf{q})$  is their energy spectrum, and  $W$  is the probability of collision of the impuriton with a phonon. We have neglected the quantity  $e(p)$  in the argument of the  $\delta$ -function that expresses the law of conservation of energy as compared with the phonon energy, since the latter coincides in order of magnitude with the temperature.

We can easily see that the kinetic equation in this form holds whenever  $\hbar/\tau \ll T$ . We don't require the more rigid condition  $\hbar/\tau \ll \Delta$ , which is equivalent to saying that the interatomic distance should be small in comparison with the free flight path of an impuriton. Actually, if  $f$  and  $\mathbf{F}$  vary slowly in space and in time and the force  $\mathbf{F}$  is small enough, then Eq. (10) holds also in the general quantum case, although generally the quantity  $I$  that describes the collisions is not even expressed in terms of the distribution function. Yet if we neglect  $e(p)$  in the expression for the impuriton spectrum, then the condition that  $\hbar/\tau \ll \omega \sim T$  guarantees the possibility of using Eq. (11), since the energy uncertainty  $\hbar/\tau$  is small in comparison with the energy of the phonons. Here the energy  $e(p) \sim \Delta$  does not figure at all in the problem. The difference between the cases  $\hbar/\tau \ll \Delta$  (or  $l \gg a$ ) and  $\hbar/\tau \gg \Delta$  (or  $l \ll a$ ) consists only in the fact that one would be able to take account of  $e(p)$  in the former case in the argument of the  $\delta$ -function in (11), while in the latter it would be an exaggeration of the accuracy. In both cases, we should use the gas-kinetic equations (10) and (11) to determine the diffusion coefficient, whence we get Eq. (9). Here the condition  $\hbar/\tau \ll T$  is evidently equivalent to the inequality  $T \ll \Theta$ . However, we should emphasize that the cited arguments do not prove the applicability of Eq. (9) for  $T \ll \Theta$  for the actually observable diffusion coefficient. The discussions have assumed tacitly that we should neglect the thermally activated mechanism of diffusion. Yet it can become the fundamental mechanism of diffusion at temperatures considerably below the Debye temperature. This is just what actually happens in solutions of the helium isotopes.

Figure 4 shows the experimental data of Grigor'ev *et*

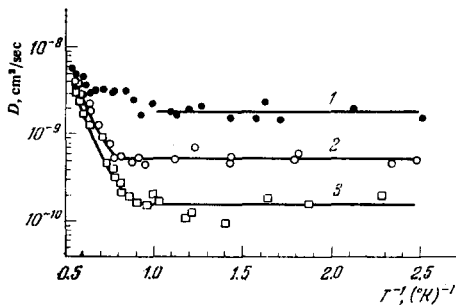


FIG. 5. Relationship of the diffusion coefficient of  $^3\text{He}$  impurities in an h.c.p. crystal of  $^4\text{He}$  at a molar volume of  $20.7 \text{ cm}^3$  to the reciprocal of the temperature. 1—concentration 0.25%; 2—0.75%; 3—2.17%.<sup>[7]</sup>

*al.*<sup>[6]</sup> on the temperature-dependence of the diffusion coefficient of admixtures of  $^3\text{He}$  in an h.c.p. crystal of  $^4\text{He}$  at different concentrations. Here we can see the temperature region I and the beginning of the region II. One cannot make measurements at higher temperatures, since a phase transition occurs at  $1.3\text{--}1.4^\circ\text{K}$  to a b.c.c. crystalline modification. The solid curves in Fig. 4 have been drawn according to the formula  $D^{-1} = 6.2 \times 10^{10} x + 4.6 \times 10^6 T^9$ , which corresponds to taking account simultaneously of scattering of impuritons by one another and by phonons.

Figure 5 shows the experimental data of Grigor'ev *et al.*<sup>[7]</sup> for the molar volume  $20.7 \text{ cm}^3$  and the concentrations  $x = 0.25\%$ ,  $0.75\%$ , and  $2.17\%$ . We can see the temperature regions I and III here. The intermediate phonon region II is absent.

## 6. DIFFUSION INDUCED BY VACANCIONS

Let us study the temperature region III. Two mechanisms of movement of an impurity can occur in it. First, there is the classical thermally activated diffusion in which the impurity atom migrates to an adjacent lattice site by overcoming some energy barrier. Second, there is diffusion caused by the presence of thermally activated vacancies. In the former case, the activation energy that characterizes the temperature-dependence of diffusion equals the height of the energy barrier. In the latter case, it is the energy of formation of a vacancy. The movement of the impurity here results from the following process (Fig. 6). While moving in the crystal, a vacancy can occupy a lattice site nearest to the impurity atom (see Fig. 6a). Then the vacancy can migrate to a site that is occupied either by an atom of the matrix (see Fig. 6b) or an impurity atom (see Fig. 6c). Then the vacancy travels away from the site of the impurity. In the case of Fig. 6c, the process involves displacing the impurity.

Diffusion of impurities induced by vacancies is of especial interest to us. The point is that vacancies are transformed into delocalized quasiparticles in quantum crystals, which are the so-called vacancions or vacancy waves. They are considerably more mobile than impuritons. According to the calculations of Hetherington,<sup>[18]</sup> who first treated this problem, and those of other authors,<sup>[9, 16, 19–21]</sup> the width of the energy

band of a vacancion  $\Delta_v$  is of the order of  $1^\circ\text{K}$ . That is, it considerably exceeds the width of an impuriton band. Hence we can neglect the intrinsic tunneling of the impurity, and treat the process depicted in Fig. 6 as the quantum-mechanical scattering of a delocalized vacancion by a localized impurity atom.<sup>[13]</sup> The process shown in Fig. 6b corresponds to elastic scattering, since here the final state of the target (i.e., the impurity atom) coincides with the initial state. The case of Fig. 6c corresponds to inelastic scattering accompanied by a displacement of the impurity atom. Hence diffusion induced by vacancies is determined by the probability of inelastic scattering. The diffusion coefficient is  $D \sim a^2 \nu$ , where  $\nu$  is the frequency of inelastic-scattering events, as determined by the relationship  $\nu \sim N_v v \sigma_{in}$ . Here  $\sigma_{in}$  is the cross-section for inelastic scattering of a vacancion by an impurity,  $N_v$  is the number of vacancies per unit volume, and  $v$  is their velocity. At high temperatures where  $T \gtrsim \Delta_v$ , we have

$$N_v \sim \frac{1}{a^3} e^{-\epsilon_0/T}, \quad v \sim \frac{a \Delta_v}{\hbar}.$$

Here  $\epsilon_0$  is the energy of formation of a vacancy. Hence we find

$$D \sim \frac{\Delta_v \sigma_{in}}{\hbar} e^{-\epsilon_0/T}. \quad (12)$$

In order to answer what is the nature of the thermally activated diffusion of the  $^3\text{He}$  impurities, we must compare the diffusion coefficients of the  $^3\text{He}$  atoms and of any other impurities in the very same crystal. If the activation energies match, then this will be a strong argument in favor of the vacancion mechanism of diffusion. Apart from isotopic admixtures, one can introduce in a controllable way and study only ions in helium crystals. We can easily calculate the diffusion coefficient of the ions from the experimentally measurable mobility in an external electric field. These measurements have been made by Shal'nikov<sup>[22]</sup> and then by a set of other authors.<sup>[23–27]</sup> Figure 7 shows the temperature-dependence of the diffusion coefficient of positive ions in solid  $^4\text{He}$  at a molar volume of  $20.7 \text{ cm}^3$  as found by Keshishev and Shal'nikov.<sup>[26]</sup> The same diagram shows the corresponding data of Grigor'ev *et al.*<sup>[7]</sup> for the diffusion of isotopic impurities. In the temperature range III where diffusion is thermally activated, not only the activation energy but also the absolute value of the diffusion of  $^3\text{He}$  atoms coincide with the corresponding values for the positive charges.<sup>[27]</sup> The experimental data are described by the equation  $D = 6.6 \times 10^{-7} \exp(-9.5/T)$ . This corresponds to the straight line drawn in Fig. 7. If we assume that  $\Delta_v \sim 1^\circ\text{K}$ , and compare the experimental data with Eq. (12), we get  $\epsilon_0 = 9.5^\circ\text{K}$  and  $\sigma_{in} \sim 5 \times 10^{-3} a^2$ . We can qualitatively explain such a small inelastic scattering cross-section

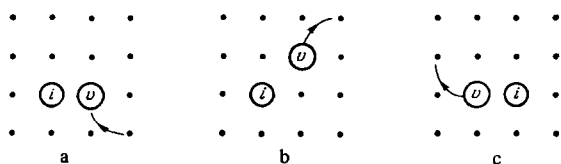


FIG. 6. Interaction of a vacancy with an impurity atom.

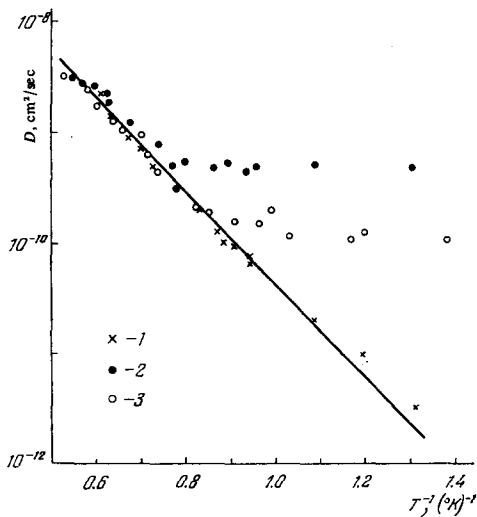


FIG. 7. Temperature dependence of the diffusion coefficient of impurities in an h.c.p. crystal of  ${}^4\text{He}$  at a molar volume of  $20.7 \text{ cm}^3$ . 1—positive ions<sup>[26]</sup>; 2—0.75%  ${}^3\text{He}$ , 3—2.17%  ${}^3\text{He}$ .<sup>[7]</sup>

tion as follows. The situation here is analogous with the case that we treated above of impuriton-impuriton scattering. The interaction energy of a vacancy with an impurity has the analogous form  $U(r) \sim V(a/r)^3$ , where  $V$  is some characteristic interaction energy. If  $V > \Delta_v$ , then the vacancy cannot penetrate into the region  $r < a(V/\Delta_v)^{1/3}$ . More exactly, the probability of such a penetration is very small. As we have seen above, this leads to a large total scattering cross section. However, the inelastic process can occur only whenever the vacancy and the impurity are nearest neighbors in the lattice. Thus, when  $V > \Delta_v$ , the inelastic scattering cross-section is less than  $a^2$  while the total cross section considerably exceeds  $a^2$ . Yet it is essential to note that the interactions of a vacancy with a  ${}^3\text{He}$  impurity and with an ion differ. There is no reason why the inelastic cross sections must agree when they are both considerably smaller than  $a^2$ . Only more detailed simultaneous measurements of diffusion of  ${}^3\text{He}$  and of ion mobility might help in clearing up this question.

The above-presented approach to the problem of vacancy diffusion of ions (or of the equivalent quantity of the ion mobility) permits one to elucidate the relation of the mobility to the temperature and the electric field for low enough temperatures in general form without going into the details of the concrete structure of the ions.<sup>[13]</sup> Let  $\sigma_n(\mathbf{p})$  be the inelastic cross section for scattering of a vacancy having the quasimomentum  $\mathbf{p}$  that involves displacement of the ion by the vector  $\mathbf{a}_n$  that joins the original lattice site to its  $n$ -th nearest neighbor. The energy of the ion, and hence that of the vacancy, varies here by the amount  $e\mathbf{E} \cdot \mathbf{a}_n$ , where  $e$  is the charge of the ion, and  $\mathbf{E}$  is the applied electric field. The mean drift velocity of the ion is expressed in terms of the cross-section by the formula

$$\mathbf{u} = \sum_n \mathbf{a}_n \int \frac{d^3p}{(2\pi\hbar)^3} \sigma_n(\mathbf{p}) v(\mathbf{p}) [n(\epsilon) - n(\epsilon + e\mathbf{E} \cdot \mathbf{a}_n)]. \quad (13)$$

Here  $v(\mathbf{p})$  is the velocity of the vacancy, and  $n(\epsilon)$  is

the equilibrium energy distribution function of the vacancies  $\epsilon = \epsilon(\mathbf{p})$ . Here and hereinafter, the summation over  $n$  is performed over those nearest neighbors  $\mathbf{a}_n$  for which  $e\mathbf{E} \cdot \mathbf{a}_n > 0$ . The displacements of the ions by the vectors  $(-\mathbf{a}_n)$  are accounted for in Eq. (13) as backward processes.

We can write the expression (13) in the form

$$\mathbf{u} = \sum_n \mathbf{a}_n \int \frac{d\epsilon}{(2\pi\hbar)^3} [n(\epsilon) - n(\epsilon + e\mathbf{E} \cdot \mathbf{a}_n)] \int \sigma_n(\mathbf{p}) dS,$$

where the last integral is taken over a constant-energy surface. In the simplest case in which all the vectors  $\mathbf{a}_n$  are crystallographically equivalent (in the b.c.c. but not the h.c.p. crystal of helium), this integral is independent of the index  $n$ , owing to lattice symmetry. Let the temperature be small in comparison with the width of the energy band of the vacancies. Then they will practically all lie near the bottom of the band, where their spectrum is quadratic, while their velocity of movement is small. According to a well-known result of quantum mechanics, the inelastic scattering cross-section of slow particles is inversely proportional to their velocity. Hence,

$$\int \sigma_n dS = \alpha \sqrt{\epsilon - \epsilon_0},$$

where  $\epsilon_0$  is the energy at the bottom of the vacancy band, and  $\alpha$  is some constant.

We can consider the distribution function  $n(\epsilon)$  to be a Boltzmann distribution, since as we have seen above,  $\epsilon_0$  is about  $10^\circ\text{K}$ , and hence, it is much larger than the temperature.

Finally we obtain

$$\mathbf{u} = \frac{\alpha}{16\pi^2\hbar^3} \left(\frac{T}{\pi}\right)^{3/2} e^{-\epsilon_0/T} \sum_n \mathbf{a}_n \left[1 - \exp\left(-\frac{e\mathbf{E} \cdot \mathbf{a}_n}{T}\right)\right]. \quad (14)$$

In weak fields where  $eEa \ll T$ , the drift velocity is proportional to the field:

$$u_i = eB_{ik}E_k,$$

where the mobility tensor  $B_{ik}$  according to (14) is equal to

$$B_{ik} = \frac{\alpha}{16\pi^2\hbar^3} \left(\frac{T}{\pi}\right)^{1/2} e^{-\epsilon_0/T} \sum_n a_{ni} a_{nk}.$$

A peculiar situation arises in strong fields where  $eEa \gg T$ . In practically all field directions, the drift velocity reaches saturation, and it does not depend on  $|E|$ :

$$\mathbf{u} = \frac{\alpha}{16\pi^2\hbar^3} \left(\frac{T}{\pi}\right)^{3/2} e^{-\epsilon_0/T} \sum_n \mathbf{a}_n. \quad (15)$$

However, it is essential to sum here only over the values of  $n$  for which  $e\mathbf{E} \cdot \mathbf{a}_n > 0$ . Therefore, as one varies the field direction, the direction of the velocity varies almost jumpwise when the vector  $\mathbf{E}$  passes through a plane perpendicular to one of the vectors  $\mathbf{a}_n$ . The angular width of the transition region is of the order of  $T/eEa \ll 1$ . In such a transition region, the velocity varies not only in direction, but also in absolute magnitude. For illustration, Fig. 8 shows the relationship

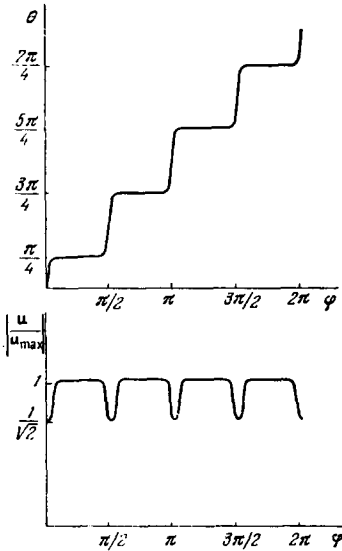


FIG. 8. Relationship of the absolute value and of the direction of the drift velocity of ions to the orientation of the electric field.  $\theta$ —angle between  $u$  and  $a_1$ ;  $\phi$ —angle between  $E$  and  $a_1$ .

of the absolute value of the velocity and its direction to the orientation of the vector  $E$  in a plane square lattice that has two elementary translation vectors  $a_1$  and  $a_2$  that are perpendicular and equal in absolute magnitude. In this case, the maximum drift velocity  $u_{\max}$  is, according to (15):

$$u_{\max} = \frac{\sqrt{2}\alpha}{16\pi^{1/2}} \left(\frac{r}{\pi}\right)^{3/2} e^{-r_0/T} |a_1|.$$

The angular dependence of the drift velocity directly reflects the geometry of the crystal lattice.

## 7. TWO- AND ONE-DIMENSIONAL QUASIPARTICLES

Each of the quasiparticles treated above (impuritons, vacancies) is a direct quantum analog of a corresponding point defect or impurity in a classical crystal. Yet it turns out that the energy spectrum of a quantum crystal is by no means exhausted by these simplest quasiparticles. We shall show below that a quantum crystal must contain peculiar secondary quasiparticles that arise when several impurities or defects of some particular type are simultaneously present. A unique feature of these quasiparticles is that they move freely, but only along certain definite planes or axes of the crystal lattice. That is, they are two- or one-dimensional quasiparticles within the volume of the three-dimensional crystal. We have seen above that two impurity atoms lying at a mutual distance  $r_{12}$  smaller than the interaction radius  $R_0 \sim a(V_0/\Delta)^{1/3}$  but larger than  $R_1 \sim a(V_0/\Delta)^{1/4}$  diffuse under the action of the interaction force. In particular, their coefficient of diffusion characterizes the movement of the pair of impurities as a unit, as defined by Eq. (7). Since the interaction energy is larger than  $2\Delta$  when  $r_{12} < R_0$ , the impurities cannot henceforth separate to an infinite distance. Hence they will behave as though bound by their interaction potential, and this conclusion will hold regardless of the sign of the interaction (attractive or repulsive).

It is interesting to trace the varying nature of the possible types of movement of two impurities upon further decrease in the relative distance  $r_{12}$ .<sup>[17]</sup> When  $r_{12} < R_1$ , tunneling of one of the impurity atoms across an interatomic distance is accompanied by a change in the interaction energy  $\delta U$  (see (4)) that exceeds the width  $\Delta$  of the band. Under these conditions, the probability of tunneling is proportional to  $\Delta^2$ . That is, it is negligibly small. The probability of simultaneous tunneling of both atoms with conservation of energy is just as small. Thus, the possibility of movement of the impurities practically vanishes. Yet there are important exceptions to this result. Let us assume that the straight line joining the impurity atoms is almost parallel to a crystallographic axis of high enough order. The hexagonal axis in an h. c. p. helium crystal is an example. The function  $V_0(\mathbf{n})$  that defines the interaction energy according to Eq. (3) evidently has an extremum for  $\mathbf{n}$  parallel to the hexagonal axis. Hence, displacement of one of the impurity atoms by a small distance  $\rho$  in a direction perpendicular to  $\mathbf{n}$  alters the interaction energy by an amount of the order of

$$\delta U_\rho \sim V_0 \left(\frac{a}{r_{12}}\right)^3 \left(\frac{\rho}{r_{12}}\right)^2. \quad (16)$$

If  $r_{12} > R_2$ , where  $R_2 \sim a(V_0/\Delta)^{1/5}$ , then when  $\rho \sim a$ ,  $\delta U_\rho$  is smaller than the band width  $\Delta$ . Thus, under the studied conditions, motion of the impurities along  $\mathbf{n}$  is practically impossible, but a situation arises for motion in a plane perpendicular to  $\mathbf{n}$  that is analogous to that treated above in Sec. 4. The trajectories of the impurity atoms are random curves that lie in planes perpendicular to the hexagonal axis. The radius of curvature of the trajectories  $\bar{\rho}$  is determined by the condition that  $\delta U_\rho \sim \Delta$  when  $\rho \sim \bar{\rho}$ . That is,  $\bar{\rho} \sim a(\Delta/U_0)^{1/2} (r_{12}/a)^{5/2}$ . Therefore, two impurity atoms lying at a distance  $r_{12}$  such that  $R_1 > r_{12} > R_2$  in a direction  $\mathbf{n}$  near the hexagonal axis will perform a peculiar two-dimensional movement in a hexagonal plane of the crystal. The diffusion coefficient is equal in order of magnitude to

$$D \sim v\bar{\rho} \sim \sqrt{\frac{\Delta^3 r_{12}^3}{h^2 \Gamma_0 a}}.$$

We stress that an extremum of the function  $V_0(\mathbf{n})$  does not suffice to permit such a movement. It is also necessary that the crystal should be periodic in the perpendicular plane.

Finally, let  $r_{12} < R_2$ . Then a displacement of one of the impurity atoms to an adjacent lattice site, even in a direction perpendicular to the hexagonal axis, will generally change the interaction energy by more than  $\Delta$ . However, there are important exceptions here also. Let one of the impurity atoms lie at a certain point  $A$  (Fig. 9) in the hexagonal plane  $\Pi_1$ . The h. c. p. crystal is built of a family of parallel hexagonal planes ( $\Pi_1, \Pi_2, \Pi_3$  in Fig. 9). Let us assume that the second impurity atom lies at some point  $B$  of another, generally speaking, hexagonal plane ( $\Pi_3$  in Fig. 9), but in such a way that its projection  $C$  on the plane  $\Pi_1$  is a nearest neighbor of the point  $A$ . Figure 9 shows the plane  $\Pi_1$  separately, along with the points  $A$  and  $C$ . Displacement of the second atom in its own hexagonal plane from



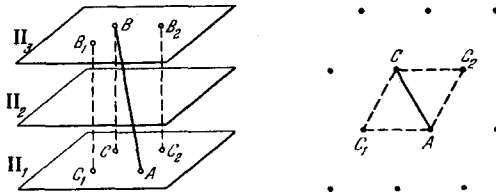


FIG. 9. A two-dimensional quasiparticle consisting of two impurity atoms.

the point  $B$  to the point  $B_1$  or  $B_2$ , whose projections on the plane  $\Pi_1$  are the points  $C_1$  and  $C_2$ , respectively, is generally not accompanied by a change in the interaction energy, since the pairs of points  $AB$ ,  $AB_1$ , and  $AB_2$  are crystallographically equivalent. The same is true for displacement of the first atom in the plane  $\Pi_1$  from  $A$  to  $C_1$  to  $C_2$ . We can easily understand that this type of system can move as a whole over the entire hexagonal plane by displacements of this type. Since the studied displacements do not alter the interaction energy, the motion here is fully coherent. The pair of impurity atoms behaves like a single peculiar two-dimensional quasiparticle that moves as a free particle, but only in a hexagonal plane of the crystal.<sup>[17]</sup> Since a given coordinate of one of the atoms involves six possible positions of the other atom, the energy spectrum of these quasiparticles contains six branches.

Meierovich<sup>[28]</sup> has carried out a detailed analysis of all the possible types of such binary quasiparticles. In particular, he showed that one-dimensional quasiparticles also exist in addition to the two-dimensional ones. Figure 10 shows a configuration of two impurity atoms that can move one-dimensionally. The point  $A$  is the position of the first impurity atom, and the point  $C$  is the projection of the second on the same hexagonal plane. Here the first atom can tunnel without change of interaction energy from  $A$  to  $A_1$ . Then the second atom can tunnel in its own hexagonal plane from a position projected at  $C$  to a position projected at  $C_1$ , etc. The pair of impurity atoms behaves like a one-dimensional quasiparticle that freely moves along a straight line parallel to the direction  $AA_1$ . The energy spectrum of these quasiparticles contains two branches.

Figure 11 shows an interesting example of a complex of three impurity atoms that constitutes a one-dimensional quasiparticle.<sup>[28]</sup> By a displacement each time of one of the atoms to an adjacent lattice site, the initial configuration  $ABC$  can be transformed via the equivalent

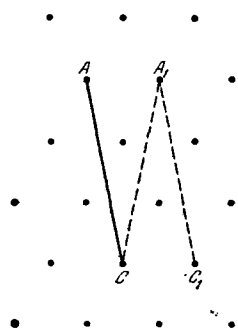


FIG. 10. A one-dimensional quasiparticle consisting of two impurity atoms.

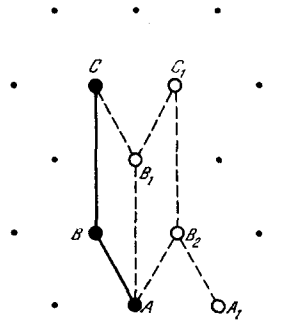


FIG. 11. A one-dimensional quasiparticle consisting of three impurity atoms.

configurations  $AB_1C$ ,  $AB_1C_1$ ,  $AB_2C_1$  to the configuration  $A_1B_2C_1$ , that differs from the original configuration by a translation along a straight line parallel to  $AA_1$ .

Prior to the studies<sup>[17,28]</sup>, Richards *et al.*<sup>[29]</sup> had advanced the idea of possible coherent motion of impurity atoms that form a pair of nearest neighbors. They did this in connection with the experimental data obtained in<sup>[29]</sup> on the dependence of the spin-lattice relaxation time  $T_1$  on the nuclear magnetic resonance frequency for  $^3\text{He}$  impurities in h. c. p. crystals of  $^4\text{He}$ . The most interesting feature of these data is the presence of sharply marked resonance anomalies at frequencies near 1.5 and 3.0 MHz. Later Mullin *et al.*<sup>[30]</sup> found that pairs of impurity atoms that are nearest neighbors behave like two-dimensional quasiparticles. There are two types of such pairs. The first type is a special case of Fig. 9, and it corresponds to the situation in which the two atoms lie in a single hexagonal plane (the point  $B$  coincides with the point  $C$ ). The second type is shown in Fig. 12. In this case the impurity atoms lie in adjacent hexagonal planes. The dots in Fig. 12 correspond to lattice sites lying in one of these planes, and the crosses to the projections of the sites of the second upon the first hexagonal plane. The point  $A$  is the position of the first atom, and the point  $C$  is the projection of the second one. Here the first atom can tunnel without change of energy to  $A_1$  and  $A_2$ , and the second to a state with the projections  $C_1$  and  $C_2$ . Mullin *et al.*<sup>[30]</sup> calculated the contribution of the two-dimensional quasiparticles to the relaxation rate  $T_1^{-1}$ . The calculations indicate resonance features whose nature and position agree with the experimental data.<sup>[29]</sup> Thus experiment<sup>[29]</sup> confirms the existence of two-dimensional quasiparticles.

One might get a more direct confirmation by studying the fine structure of the wings of the nuclear magnetic resonance line. As we know,<sup>[31]</sup> dipole-dipole interaction causes a system of two spins to have resonance frequencies  $\omega$  that are somewhat shifted with respect to the frequency  $\gamma H$  ( $\gamma$  is the gyromagnetic ratio, and  $H$  is

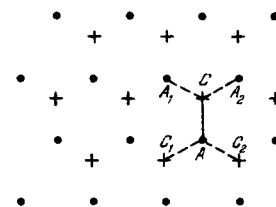


FIG. 12. A two-dimensional quasiparticle consisting of two atoms that are nearest neighbors.

the external magnetic field) of the resonance for an isolated spin:

$$\omega = \gamma H \pm \frac{3}{4} \frac{\hbar \gamma^2}{r_{12}^3} (1 - 3 \cos^2 \theta), \quad (17)$$

Here  $\theta$  is the angle between the magnetic field and the axis joining the nuclei. A dilute solution contains such pairs of atoms as well as isolated  $^3\text{He}$  atoms. We can neglect complexes of a large number of impurities. As we can see from (17), the pairs having  $r_{12} \sim a$  give the greatest frequency shift. These pairs can be of three types: immobile pairs (Eq. (17) is literally applicable to them), and pairs that amount to two- and one-dimensional quasiparticles. In the latter two cases, the state of the system is defined by assigning the quasimomentum  $\mathbf{p}$  (two- or one-dimensional) and the number  $\nu$  of the energy band. Such a state is a superposition of all possible localized states, which we shall number with the index  $i$ , and which possess certain coefficients  $A_i^\nu(\mathbf{p})$ . Generally the resonance frequencies depend on  $\mathbf{p}$  and  $\nu$ , and they are equal to

$$\omega_\nu(\mathbf{p}) = \gamma H \pm \frac{3}{4} \frac{\hbar \gamma^2}{r_{12}^3} (1 - 3 \langle \cos^2 \theta \rangle), \quad (18)$$

where

$$\langle \cos^2 \theta \rangle = \sum_i |A_i^\nu(\mathbf{p})|^2 \cos^2 \theta_i. \quad (19)$$

Here  $\theta_i$  is the angle between the magnetic field and the straight line joining the atoms in the localized state  $i$ . The coefficients  $A_i^\nu(\mathbf{p})$  satisfy the normalization condition

$$\sum_i |A_i^\nu(\mathbf{p})|^2 = 1. \quad (20)$$

Pairs of atoms that are nearest neighbors give the largest frequency shift. They behave like two-dimensional quasiparticles, and as we have seen, they can exist in two types that correspond to Fig. 9 and Fig. 12. In both cases, the index  $i$  takes on three values, since the two pairs have three orientations (which correspond to the configurations  $AC$ ,  $AC_1$ , and  $AC_2$  in Fig. 9 and Fig. 12). Let the magnetic field lie along the hexagonal axis. Then  $\cos \theta_i = 0$  for all  $i$  for pairs of the first type, and  $\cos \theta_i = \sqrt{2/3}$  for pairs of the second type. Then, owing to the condition (20), the expressions in parentheses in Eq. (18) for the two types of pairs are equal in absolute magnitude and opposite in sign, so that the frequency spectrum is discrete, and it consists of only two lines

$$\omega_{1,2} = \gamma H \pm \frac{3\hbar\gamma^2}{4r_{12}^3}$$

of equal intensity. We would have obtained the same result in a rigid lattice as well, but in this case the quasiparticles easily move in the hexagonal plane, and hence they react to the magnetic field gradient, though only to the gradient parallel to the hexagonal plane. An essential point is that the frequency shift considerably exceeds the line width. The size of the shift is of the order of  $\hbar\gamma^2/a^3 \sim 10^4 \text{ sec}^{-1}$ . Yet the relaxation time  $T_2$  observed experimentally<sup>[3,32]</sup> in dilute solutions of  $^3\text{He}$  in solid  $^4\text{He}$  attains values of  $10^{-1}$ – $1 \text{ sec}$ . If the magnetic field lies at an angle to the hexagonal axis, then the

frequencies depend on the quasimomentum, and the spectrum becomes continuous. However, the form of the spectrum can be exactly calculated, since the coefficients  $A_i^\nu(\mathbf{p})$  satisfy a simple system of linear algebraic equations.

For one-dimensional quasiparticles, the spectrum is discrete for any direction of the magnetic field, since here there are only two different orientations of a pair, and the equality holds for any value of the quasimomentum that  $|A_1^\nu(\mathbf{p})| = |A_2^\nu(\mathbf{p})|$ . Each of the one-dimensional particles gives two lines

$$\omega_{1,2} = \gamma H \pm \frac{3\hbar\gamma^2}{4r_{12}^3} \left[ 1 - \frac{3}{2} (\cos \theta_1 + \cos \theta_2) \right].$$

We emphasize that a discrete fine structure of the wings of the NMR lines can be observed only in monocrystalline specimens.

Finally let us discuss the processes that make possible the movement of impurity atoms under conditions in which tunneling of one of them across an interatomic distance involves a change in interaction energy considerably exceeding the band width  $\Delta$ . In particular, the probability  $w$  of these processes (per unit time) is determined by the lifetime of the above-discussed binary quasiparticles. The simplest example here is thermally activated diffusion. However, the corresponding probability  $w$  declines exponentially with falling temperature. Therefore, the fundamental role is played in the low-temperature region by processes of quantum tunneling involving phonons that permit energy balance as the impurity migrates to the adjacent lattice site. Two types of such processes can occur. The first of them is tunneling of an impurity accompanied by scattering of a phonon. We can easily estimate the probability  $w_1$  of this process by using the results of<sup>[11,12]</sup>.

$$w_1 \sim \frac{\Delta^2}{\hbar\Theta} \left( \frac{T}{\Theta} \right)^7.$$

The second process is tunneling of an impurity with simultaneous spontaneous emission of a phonon.<sup>[13]</sup> The energy of the phonon  $\hbar\omega$  equals the change in interaction energy  $\hbar\omega \sim \delta U \sim Fa \sim V_0(a/r_{12})^4$ . As usual, the probability  $w_2$  of spontaneous emission is proportional to the cube of the phonon frequency and to the square of the overlap integral of the wave functions of impurities at adjacent sites, i.e., to the square of the band width  $\Delta$ :

$$w_2 \sim \frac{\Delta^2}{\hbar\Theta} \left( \frac{\hbar\omega}{\Theta} \right)^3 \sim \frac{\Delta^2}{\hbar\Theta} \left( \frac{V_0}{\Theta} \right)^3 \left( \frac{a}{r_{12}} \right)^{12}.$$

For the most important case of quasiparticles having  $r_{12} \sim a$ , the second process becomes predominant at  $T < V_0(\Theta/V_0)^{4/7}$ . In this low-temperature region, the lifetime of most of the quasiparticles does not depend on the temperature.

## 8. DISLOCATIONS IN QUANTUM CRYSTALS

Let us study a linear dislocation in a quantum crystal that lies in a slip plane at some angle to the crystallographic directions.<sup>[17]</sup> As we know, the dislocation line is not a straight line here. It consists of individual rectilinear regions that lie along a direction in which

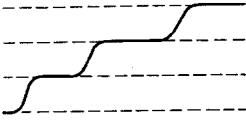


FIG. 13. A dislocation with kinks.

the energy of the dislocation is minimal (this direction coincides with one of the crystallographic axes), and of a certain number of kinks in whose vicinity the dislocation passes from one valley to another (Fig. 13). We can treat each such kink as being a point defect on the dislocation. Since the crystal is periodic along the crystallographic axis, such a point defect in a quantum crystal is converted into a quasiparticle whose state is classified in terms of values of the one-dimensional quasimomentum. Let one kink exist on the dislocation that has a definite quasimomentum. Then the kink lies at all points of the dislocation with equal probability, and this means that the dislocation is uniformly distributed between two adjacent valleys. When there are a large number of kinks, the dislocation is distributed over a large number of valleys. Thus the quantum-mechanical delocalization of kinks leads to delocalization of the dislocation in the slip plane.

If the width of the energy band of the kinks is small, i.e., the probability  $J$  is small of its quantum sub-barrier jumping by one lattice period  $a$  in the direction of the dislocation, then we can apply the well-known close-coupling approximation to calculate the energy spectrum. Consequently we get the following relationship of the energy  $E$  of a kink to the quasimomentum  $p$ :

$$E(p) = E_0 + 2hJ \cos\left(\frac{pa}{\hbar}\right),$$

where  $E_0$  is the energy of a localized kink in the classical limit.

Let  $n$  be the number of kinks per unit length of the dislocation. If the mean distance  $n^{-1}$  between them is large in comparison with the interaction radius  $r_0$ , then the kinks can be treated as a rarefied gas of quasiparticles. The radius of interaction is determined by the condition  $U(r_0) \sim \hbar J$ , where  $U(r) \sim \beta/r$  is the interaction energy of two kinks, which is inversely proportional<sup>[33]</sup> to the first power of the distance  $r$  between them. Here  $\beta$  is a certain constant which is equal in order of magnitude to  $\beta \sim \mu a^4$ , where  $\mu$  is the shear modulus.

An important, experimentally-observable characteristic of a gas of kinks is their diffusion coefficient. In the high-temperature region, it is determined by collisions of kinks with phonons and by oscillations of the dislocation. With falling temperature, the number of phonons and oscillations declines, and the diffusion coefficient rapidly rises until it reaches a limiting value that is determined by the mutual collisions between kinks. It is important to note the following situation in estimating this limiting value. In the one-dimensional case, the momenta acquired by the quasiparticles owing to pair collision are unequivocally determined by the conservation laws. There are two unknown momenta and two equations to determine them (the laws of conservation of energy and momentum). The only solution here is the

trivial one that corresponds to exchange of momenta by the quasiparticles owing to collision. The momentum distribution function of the quasiparticles is not altered here at all. In other words the pair collision integral is zero, and all the kinetic phenomena are determined by triple collisions. The corresponding free flight path  $l_3$  differs from the free flight path  $l_2 \sim n^{-1}$  that characterizes pair collisions by the large factor  $(nr_0)^{-1}$ . Thus the diffusion coefficient is

$$D \sim \frac{\partial E}{\partial p} l_3 \sim \frac{\hbar J^2 a}{\beta n^2}.$$

That is, instead of the usual  $D \propto n^{-1}$  law, one should observe here an inverse proportionality of the diffusion to the square of the density of quasiparticles.

Movement of the kinks existing on a dislocation cannot bring about continuous motion of the dislocation itself when acted on by an external force. Such a motion results from creation of pairs of oppositely-directed kinks, whereby part of the dislocation line migrates to an adjacent valley. In ordinary crystals, this process is thermally activated, and it corresponds to classical super-barrier migration to the next valley. The mean velocity of a dislocation when acted on by a given force declines exponentially with decreasing temperature. Petukhov and Pokrovskii<sup>[34]</sup> have shown that in quantum crystals the creation of pairs of kinks is a quantum-mechanical tunneling process whose probability does not depend on the temperature.

Apparently the most convenient method that permits observing the discussed features of the behavior of dislocations is to measure the internal friction. These measurements make it possible to study the diffusion of defects that cannot be observed by other methods. There are additional possibilities here in quantum crystals.<sup>[35]</sup> Recently performed experiments on internal friction in solid helium<sup>[36]</sup> and in niobium containing a hydrogen impurity<sup>[37]</sup> have demonstrated the quantum nature of the relaxation processes responsible for internal friction. Further development of these experiments can lead to observing the features of the dynamics of dislocations in quantum crystals.

## 9. CONCLUSION

Thus we can consider it now firmly established that at low temperatures impurity atoms in quantum crystals behave like delocalized quasiparticles (impuritons) that move freely through the crystal. This must hold all the more for vacancies (and generally for any sort of point defects in the crystal), which are considerably more mobile than impurity atoms. Although this fact has not yet been directly confirmed experimentally for vacancies, owing to the substantial experimental difficulties of observing vacancies, we can hardly doubt it. In this regard, it is important to note that there is a theoretical possibility in quantum crystals for the existence of the so-called zero-point vacancies,<sup>[1]</sup> i.e., quasiparticles corresponding to vacancies that exist in a crystal at absolute zero like zero-point vibrations. A crystal that contains zero-point vacancies must constitute a unique object.<sup>[1]</sup> It is not in general a solid. It can have two types of motion, one of which

has the properties of motion in a solid, and the other, that in a liquid. Interestingly, indications have recently appeared<sup>[38,39]</sup> that zero-point vacancies exist in solid helium-3. A final elucidation of this problem would be of substantial theoretical interest.

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