Motion of charges in solid helium

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On the basis of representation of the motion of charges in helium crystals as quantum processes of inelastic scattering of delocalized vacancies, an explanation is given of all principal experimental data, including the nonmonotonic dependence of the drift velocity on the electric field and temperature. A symmetry approach is proposed to the question of the structure of charges, for experimental realization of which measurements of the anisotropy of the drift velocity are needed.

The properties of charges in crystals of helium are of interest in view of the possibility of studying the quantum nature of these crystals. A number of theoretical and experimental studies have been devoted to this question (see the review of Dahm[1] and the later work of Golov *et al.*[2]), but up to the present time many basic features of the phenomenon remain unclear.

In analogy with the well studied case of liquid helium it is assumed[3,4] that a negative ion in a helium crystal is an electron located in a cavity. Positive charges apparently are ions of He^+, He_2^+, or even He_3^+ (Ref. 1) located in the center of a region which is highly deformed under the action of electrostrictive forces. Estimates of the size of ion complexes of both signs lead, however, to values of the order of the interatomic distance, and therefore they cannot be considered to be purely macroscopic with neglect of the discreteness of the crystal lattice.

Direct and very accurate measurements of the drift velocity of charges in solid ^4He were made by Keshishev[5] by means of a three-electrode method. The most characteristic properties of the motion of charges are the following. On reduction of the temperature the drift velocities for the most part fall off exponentially, and close agreement is observed of the activation energies of the mobility of positive charges of isotopic admixtures of ^3He (Ref. 6) and vacancies.[7] The latter serve as an important basis for the vacancy mechanism of motion. For negative charges the vacancy mechanism was discussed by Shikin[4] on the basis of macroscopic description of the diffusion-viscous flow of electron density in the crystal. Meĭerovich and one of the present authors[8] proposed a quantum approach to the vacancy mobility of charges of both signs which makes use to a substantial degree of the effect of quantum delocalization of vacancies in crystals of ^4He and their conversion into freely moving quasiparticles.

In strong electric fields two qualitatively different dependences of the drift velocity of charges on the electric field are observed. For positive charges at not too low pressures and for negative charges at all pressures, with increase of the field strength there is a transition from a linear dependence to a cubic dependence of the form $(E + E_0)^3$, where E_0 depends on the temperature and the pressure. The proportionality of the drift velocity in rather strong fields to the cube of the field can be explained if one assumes that in this case the inelastic scattering of vacancies by charges is accompanied by spontaneous emission of photons.[8] Keshishev and Meĭerovich,[9] calculating in strong fields the next term, quadratic in the field, of the form E_0E^2, attempted to estimate E_0, but the nature of the $(E + E_0)^3$ dependence itself remained unclear.

At a low pressure of 25.8 atm Keshishev[5] observed for positive charges a transition from a linear dependence to a weaker dependence of the drift velocity on the field, which was attributed to the saturation found in Ref. 8 of the vacancy phonon-free mobility. The saturation was a direct consequence of the $1/v$ law (v is the velocity of vacancies near the bottom of the band) for the cross section of the inelastic process. The applicability of this law to the present case was questioned by Piradashvili,[10] who obtained a constant cross section instead of $1/v$ for the model of inelastic collisions considered by him. Piradashvili's result, as we shall see, is valid also in the general case. It turns out that instead of saturation one should observe a transition from a linear dependence to a square-root dependence of the drift velocity on the field strength. The analysis carried out below of the results of Keshishev[5] shows that the square-root dependence is in reasonable agreement with the experimental data. In the framework of the quantum approach used, one finds a natural explanation of the features of the motion of charges of both signs discussed above, and also of the anisotropy of the activation energy for motion of charges which was noted by Lau, Dahm, and Jeffers,[11] and of the nonmonotonic nature of the field and temperature dependences of the drift velocity observed by Golov, Efimov, and Mezhov-Deglin.[2] The approach proposed permits quite definite predictions to be made on the behavior of the change of the nature of the motion on further reduction of the temperature. In addition, it turns out to be possible to formulate a symmetry approach to the question of the structure of ionic complexes, for experimental realization of which it is necessary to have direct measurements of the anisotropy of the drift velocity.

1. STRUCTURE OF CHARGES, AND TRANSLATION VECTORS

For analysis of the motion of charges in a crystal the symmetry aspect of their structure is important. We are discussing here the symmetry of the effect produced in the crystal as the result of presence of a charge. The most important manifestation of this symmetry is a set of vectors, translation by which forms the principal mechanism of migration of the charge. We shall make clear the general situation in simple examples.

A negative charge in solid helium is a region of reduced density in which an electron is localized. The decrease of the density of the crystal near the charge is the result of two different processes–the inelastic process of production of some number of vacancies near the charge and the elastic deformation of the lattice. The symmetry of the system can be readily illustrated by assuming the elastic strain to be removed and by representing a crystal with a defect as an

ideal crystal in which the lattice sites that become vacant in the course of formation of a charge complex are marked. In what follows we shall discuss the vacancy structure of negative charges in just this sense. Actually, of course, the number and mutual arrangement of vacancies in a complex are determined by the requirement that the energy be minimal with allowance for the subsequent deformation.

We shall consider first the simplest case in which the number of vacancies is equal to unity, so that a charge complex consists of an electron localized in the free space of an isolated vacancy. This case is completely realistic at least in some interval of not too low pressures. It was discovered previously[8] for crystal lattices with one atom per unit cell. The more interesting case of hexagonal close packed crystals of ^{4}He exhibits substantial anomalies. In hexagonal close packed crystals there are two types of translation-nonequivalent but crystallographically equivalent lattice sites. In view of the latter of their properties, charge complexes corresponding to vacancies in the two sublattices have identical energies. In Fig. 1 we show the configuration of lattice sites of hexagonal close packed crystals. The dots show sites which belong to a single plane perpendicular to a sixfold axis, and the crosses show sites in a plane displaced by half of the period $\mathbf{a}_3$ along the axis perpendicular to the plane of the figure. In Fig. 1 we show also the elementary translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ in the plane perpendicular to C_6. We shall assume that the most probable quantum processes are transfer of charge to states corresponding to vacancies occupying the closest lattice sites. Such transitions correspond to only 18 charge translation vectors $\mathbf{u}_n^{(1)}$ with $n = 1,2,...,6$ and $\mathbf{u}_n^{(2)}$ with $n = 1,2,...,12$. Of these, the vectors

$$\mathbf{u}_1^{(1)}=\mathbf{a}_1, \quad \mathbf{u}_2^{(1)}=\mathbf{a}_1+\mathbf{a}_2, \quad \mathbf{u}_3^{(1)}=\mathbf{a}_2, \quad \mathbf{u}_{4,5,6}^{(1)}=-\mathbf{u}_{1,2,3}^{(1)} \quad (1)$$

correspond to displacements inside the sublattices, while the vectors

$$\mathbf{u}_1^{(2)}=\tfrac{1}{3}(\mathbf{a}_1-\mathbf{a}_2)+\tfrac{1}{2}\mathbf{a}_3, \quad \mathbf{u}_4^{(2)}=\tfrac{1}{3}(\mathbf{a}_1-\mathbf{a}_2)-\tfrac{1}{2}\mathbf{a}_3,$$

$$\mathbf{u}_2^{(2)}=\tfrac{1}{3}(\mathbf{a}_1+2\mathbf{a}_2)+\tfrac{1}{2}\mathbf{a}_3, \quad \mathbf{u}_5^{(2)}=\tfrac{1}{3}(\mathbf{a}_1+2\mathbf{a}_2)-\tfrac{1}{2}\mathbf{a}_3, \quad (2)$$

$$\mathbf{u}_3^{(2)}=-\tfrac{1}{3}(2\mathbf{a}_1+\mathbf{a}_2)+\tfrac{1}{2}\mathbf{a}_3, \quad \mathbf{u}_6^{(2)}=-\tfrac{1}{3}(2\mathbf{a}_1+\mathbf{a}_2)-\tfrac{1}{2}\mathbf{a}_3$$

correspond to transitions from the first sublattice, whose sites are shown by the dots in Fig. 1, to sites marked by crosses. The vectors

$$\mathbf{u}_{7,...,12}^{(2)}=-\mathbf{u}_{1,...,6}^{(2)} \quad (3)$$

correspond to transitions from the second sublattice to the first.

Let n_1 and n_2 be the probabilities of finding a charge respectively in the first or second sublattice, so that $n_1 + n_2 = 1$. We shall denote by w_{1n} and w_{2n} the probabilities of displacement per unit time of a charge by the vectors
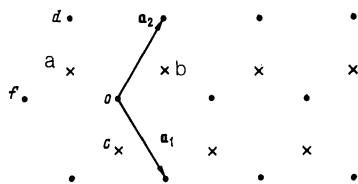

FIG. 1.

$\mathbf{u}_n^{(1)}$ and $\mathbf{u}_n^{(2)}$ respectively. We have

$$\dot{n}_1 = -n_1\sum_{n=1}^{6}w_{2n}+n_2\sum_{n=7}^{12}w_{2n},$$

$$\dot{n}_2 = n_1\sum_{n=1}^{6}w_{2n}-n_2\sum_{n=7}^{12}w_{2n}. \quad (4)$$

Under stationary conditions we obtain

$$n_1 = \left(\sum_{n=7}^{12}w_{2n}\right)\Big/\left(\sum_{n=1}^{12}w_{2n}\right),$$

$$n_2 = \left(\sum_{n=1}^{6}w_{2n}\right)\Big/\left(\sum_{n=1}^{12}w_{2n}\right). \quad (5)$$

The average drift velocity of the charge is determined by the formula

$$\mathbf{v}=n_1\left\{\sum_{n=1}^{6}\mathbf{u}_n^{(1)}w_{1n}+\sum_{n=1}^{6}\mathbf{u}_n^{(2)}w_{2n}\right\}$$

$$+n_2\left\{\sum_{n=1}^{6}\mathbf{u}_n^{(1)}w_{1n}+\sum_{n=7}^{12}\mathbf{u}_n^{(2)}w_{2n}\right\}, \quad (6)$$

which with inclusion of (5) gives

$$\mathbf{v}=\sum_{n=1}^{6}\mathbf{u}_n^{(1)}w_{1n}+\left(\sum_{n=7}^{12}w_{2n}\right)\left(\sum_{n=1}^{12}w_{2n}\right)^{-1}\left(\sum_{n=1}^{6}\mathbf{u}_n^{(2)}w_{2n}\right)$$

$$+\left(\sum_{n=1}^{6}w_{2n}\right)\left(\sum_{n=1}^{12}w_{2n}\right)^{-1}\left(\sum_{n=7}^{12}\mathbf{u}_n^{(2)}w_{2n}\right). \quad (7)$$

Let us consider one more characteristic example. Let the number of vacancies be equal to four. Their most compact relative arrangement in a hexagonal close packed lattice corresponds to the four vertices of a tetrahedron, for example $oabc$ in Fig. 1. In this case there are four translation-nonequivalent states with the same energy. There are two states with the vertex o belonging to the first sublattice, for example, $oabc$ and $o\,\overline{abc}$, where the points $\overline{a}$, $\overline{b}$, and $\overline{c}$ are obtained respectively from a, b, and c by reflection in the plane in which the atoms shown by the dots lie. The two other states are obtained from the first two by permutation of the sublattices. These are, for example, the tetrahedra $aofd$ and $\overline{a}ofd$.

The most probable processes of transition between states of this type, which lead to a shift of the center of gravity of charge complex are displacements of a vertex vacancy by the vectors $\pm \mathbf{a}_3$. Here transitions $1\leftrightarrow2$ and $3\leftrightarrow4$ occur between the states. Here we number the states in the order in which they were listed above. The center of gravity of the charge is displaced alternately by the vectors $\mathbf{u}^{(1)} = (1/4)\mathbf{a}_3$ and $-\mathbf{u}^{(1)}$. It is clear, however, that processes only of this type cannot displace a charge a large distance. It is necessary to take into account some processes which lead to displacement of the complex in the direction of the vertex vacancy. The most probable of these are two-particle processes, a typical representative of which is transition of the tetrahedron $oabc$ into $oafd$ by displacement of the vacanacies c and b respectively to the locations f and d. For states of type 1 this

leads to a displacement of the center of gravity of the charge by the vectors

$$\mathbf{u}_1^{(2)}=\tfrac{1}{3}\mathbf{a}_1+\tfrac{2}{3}\mathbf{a}_2-\tfrac{1}{4}\mathbf{a}_3,\quad \mathbf{u}_2^{(2)}=\tfrac{1}{3}\mathbf{a}_1-\tfrac{1}{3}\mathbf{a}_2-\tfrac{1}{4}\mathbf{a}_3,$$

$$\mathbf{u}_3^{(2)}=-\tfrac{2}{3}\mathbf{a}_1-\tfrac{1}{3}\mathbf{a}_2-\tfrac{1}{4}\mathbf{a}_3$$

with transition to states of type 3; for states of type 2 this leads to displacement by the vectors

$$\mathbf{u}_4^{(2)}=\tfrac{1}{3}\mathbf{a}_1+\tfrac{2}{3}\mathbf{a}_2+\tfrac{1}{4}\mathbf{a}_3,\quad \mathbf{u}_5^{(2)}=\tfrac{1}{3}\mathbf{a}_1-\tfrac{1}{3}\mathbf{a}_2+\tfrac{1}{4}\mathbf{a}_3,$$

$$\mathbf{u}_6^{(2)}=-\tfrac{2}{3}\mathbf{a}_1-\tfrac{1}{3}\mathbf{a}_2+\tfrac{1}{4}\mathbf{a}_3$$

with transition to states of type 4; for states of type 3 this leads to displacement by

$$-\mathbf{u}_1^{(2)},\quad -\mathbf{u}_2^{(2)},\quad -\mathbf{u}_3^{(2)}$$

with transition to states of type 1; for states of type 4 this leads to displacement by

$$-\mathbf{u}_4^{(2)},\quad -\mathbf{u}_5^{(2)},\quad -\mathbf{u}_6^{(2)}$$

with transition to states of type 2.

We shall denote by n_1, n_2, n_3, and n_4 the probabilities of the corresponding states, so that $n_1 + n_2 + n_3 + n_4 = 1$. We then have

$$\dot{n}_1=-n_1\left(w_1^{(+)}+\sum_{n=1}^{3} w_{2n}^{(+)}\right)+n_2 w_1^{(-)}+n_3\sum_{n=1}^{3} w_{2n}^{(-)},$$

$$\dot{n}_2=n_1 w_1^{(+)}-n_2\left(w_1^{(-)}+\sum_{n=4}^{6} w_{2n}^{(+)}\right)+n_4\sum_{n=4}^{6} w_{2n}^{(-)},$$

$$\dot{n}_3=n_1\sum_{n=1}^{3} w_{2n}^{(+)}-n_3\left(w_1^{(-)}+\sum_{n=1}^{3} w_{2n}^{(-)}\right)+n_4 w_1^{(+)},$$

$$\dot{n}_4=n_2\sum_{n=4}^{6} w_{2n}^{(+)}+n_3 w_1^{(-)}-n_4\left(w_1^{(+)}+\sum_{n=4}^{6} w_{2n}^{(-)}\right).\tag{8}$$

Here $w_1^{(+)}$ is the probability of displacement by $\mathbf{u}^{(1)}$ per unit time, $w_1^{(-)}$ is the same for displacement by $-\mathbf{u}^{(1)}$, $w_{2n}^{(+)}$ is for displacement by $\mathbf{u}_n^{(2)}$, and $w_{2n}^{(-)}$ is for displacement by $-\mathbf{u}_n^{(2)}$.

Assuming that all probabilities $w_1^{(\pm)}$ with subscript 1 significantly exceed the probabilities of two-particle processes $w_{2n}^{(\pm)}$, we obtain under stationary conditions from the equations (8)

$$n_1 = \frac{w_1^{(-)}}{w_1^{(+)}+w_1^{(-)}}n_{12},\quad n_2=\frac{w_1^{(+)}}{w_1^{(+)}+w_1^{(-)}}n_{12},$$

$$n_3=\frac{w_1^{(+)}}{w_1^{(+)}+w_1^{(-)}}n_{34},\quad n_4=\frac{w_1^{(-)}}{w_1^{(+)}+w_1^{(-)}}n_{34},$$

where the quantities $n_{12}=n_1+n_2$ and $n_{34}=n_3+n_4$ are given by the equations

$$n_{12}=\left[w_1^{(+)}\sum_{n=1}^{3} w_{2n}^{(-)}+w_1^{(-)}\sum_{n=4}^{6} w_{2n}^{(-)}\right]$$

$$\times\left[w_1^{(+)}\left(\sum_{n=1}^{3} w_{2n}^{(-)}+\sum_{n=4}^{6} w_{2n}^{(+)}\right)+w_1^{(-)}\left(\sum_{n=1}^{3} w_{2n}^{(+)}+\sum_{n=4}^{6} w_{2n}^{(-)}\right)\right]^{-1},$$

$$n_{34}=\left[w_1^{(-)}\sum_{n=1}^{3} w_{2n}^{(+)}+w_1^{(+)}\sum_{n=4}^{6} w_{2n}^{(+)}\right]$$

$$\times\left[w_1^{(+)}\left(\sum_{n=1}^{3} w_{2n}^{(-)}+\sum_{n=4}^{6} w_{2n}^{(+)}\right)+w_1^{(-)}\left(\sum_{n=1}^{3} w_{2n}^{(+)}\sum_{n=4}^{6} w_{2n}^{(-)}\right)\right]^{-1}.$$

The average drift velocity of the charge is equal to

$$\mathbf{v}=n_1\left(\mathbf{u}^{(1)}w_1^{(+)}+\sum_{n=1}^{3}\mathbf{u}_n^{(2)} w_{2n}^{(+)}\right)$$

$$+n_2\left(-\mathbf{u}^{(1)}w_1^{(-)}+\sum_{n=4}^{6}\mathbf{u}_n^{(2)} w_{2n}^{(+)}\right)$$

$$+n_3\left(-\mathbf{u}^{(1)}w_1^{(-)}-\sum_{n=1}^{3}\mathbf{u}_n^{(2)} w_{2n}^{(-)}\right)$$

$$+n_4\left(\mathbf{u}^{(1)}w_1^{(+)}-\sum_{n=4}^{6}\mathbf{u}_n^{(2)} w_{2n}^{(-)}\right).\tag{9}$$

By straightforward manipulations with use of the formulas given above, we obtain from (9)

$$\mathbf{v}=\sum_{n=1}^{3}(\mathbf{u}_n^{(2)}-\mathbf{u}^{(1)})(n_1 w_{2n}^{(+)}-n_3 w_{2n}^{(-)})$$

$$+\sum_{n=4}^{6}(\mathbf{u}_n^{(2)}+\mathbf{u}^{(1)})(n_2 w_{2n}^{(+)}-n_4 w_{2n}^{(-)}).\tag{10}$$

The drift velocity, as should be the case, is proportional to the small probabilities of two-particle processes. We call attention to the coincidence of the vectors $\mathbf{u}_n^{(2)}-\mathbf{u}^{(1)}$ and $\mathbf{u}_n^{(2)}+\mathbf{u}^{(1)}$ in Eq. (10) with the vectors $\mathbf{u}_{4,5,6}^{(2)}$ and $\mathbf{u}_{1,2,3}^{(2)}$ of the preceding example [see Eqs. (2)]. This coincidence is not accidental. In the limiting case considered, in which the frequency of hops of the vertex vacancy is large in comparison with the frequency of two-particle processes, a complex of four vacancies will behave essentially as a five-vacancy complex and will differ from it only in that instead of two vertex vacancies there is one, which, however, is smeared in a quite definite proportion between two possible locations. Furthermore, the complex of five vacancies is equivalent in the sense of its symmetry, obviously, to single vacancies with the additional condition that the probabilities of displacement by the vectors (1) in this case are negligible in comparison with displacements by the vectors (2).

We can now formulate a general approach to the question of the relation between the structure and symmetry of the charges and their drift velocity. In the general case there is some number of translation-nonequivalent but crystallographically equivalent positions of the charge complex. The relative probabilities n_a ($a = 1,2,...,\Sigma n_a = 1$) of their population under stationary conditions are determined by the probabilities $w^{(a)}$ of the most probable transitions between these states and are homogeneous zero-order functions of $w^{(a)}$. The most important characteristics of the structure of a charge is the set $\mathbf{u}_n$, $n = 1,2,...$ of the vectors of displacement of the center of gravity of the charge, which determine the average drift velocity by a relation of the form

$$\mathbf{v}=\sum_{n,a}\mathbf{u}_n n_a w^{(a)}(\mathbf{u}_n).\tag{11}$$

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Below we shall consider specific mechanisms of transitions of charges between different localized states, we shall determine the nature of the dependence of the probabilities $w^{(a)}(\mathbf{u}_n)$ on the temperature and on the magnitude and direction of the electric field, and we shall show that Eq. (11) can be effectively used for finding the directions of the vectors $\mathbf{u}_n$ on the basis of experimental data on the anisotropy of the drift velocity.

We emphasize that the approach set forth is applicable with equal success also to positive charges. Depending on whether the positive charges are ions of He^+, He_2^+, or He_3^+ and on how these ions are distributed in the unit cell of the crystal, the charge complexes are characterized by different numbers and directions of the principal displacement vectors $\mathbf{u}_n$. Determination of these quantities from experimental data is possible by means of the general formula (11).

2. INELASTIC SCATTERING OF VACANCIES BY CHARGES

As in the work of Meĭerovich and one of the present authors,[8] we shall assume that the principal mechanism of transitions of a charge complex between different localized states is inelastic scattering of vacancies by charges. For the cases discussed above of one-vacancy and four-vacancy complexes the nature of the processes which occur is shown respectively in Figs. 2 and 3. In the first case the charge is initially localized at vacancy O. A free vacancy (one without charge inside it), which in helium crystals is a freely moving quasiparticle, can in its motion fall inot one of the points adjacent to O (for example, point A in Fig. 2). The two-vacancy charge complex AO which has been produced should with the passage of time emit one free vacancy. If this is the vacancy coming from the site O, then the process shown in Fig. 2 is accompanied by displacement of charge from O to A (if this is vacancy A, then this process is not of interest to us since it is not accompanied by migration of charge). In Fig. 3 we have shown a two-particle process of transition of a charge vacancy tetrahedron from the state $oabc$ to the state $aofd$. The free vacancy comes from infinity to d, after which it departs from c, arrives at f, and finally goes b to infinity. Since so complicated a trajectory of the vacancy must be accomplished below the barrier, the probability of the process is small. In this connection we note that the characteristic value of the cross section for inelastic scattering of vacancies by charges, as follows from the experiments of Keshishev[5] [see also Ref. 12, page 262, below Eq. (12)], is about 10^2–10^3 times smaller than the characteristic area of the unit cell of the crystal. The appearance of a small factor such as 10^{-2}–10^{-3} is not surprising even for a complex of four vacancies in view of the complexity of the sub-barrier trajectory and of the exponential nature of the corre-
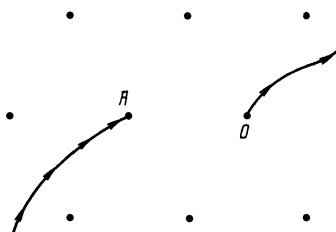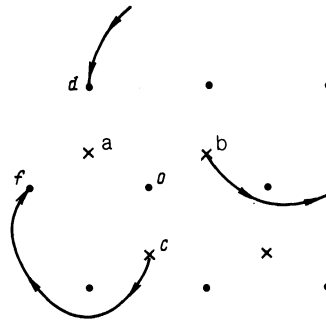

FIG. 3.

sponding smallness. In addition, the not so small observed value of the cross section, in view of its exponential nature, is an argument against a rather large number of vacancies in the charge complex.

We shall write the probability $w^{(a)}(\mathbf{u})$ of the transition, which enters into Eq. (11), in terms of the corresponding differential probabilities $w^{(a)}(\mathbf{u};\mathbf{k},\mathbf{k}')$ of the inelastic process, as a result of which the charge is displaced by the vector $\mathbf{u}$ from the localized state a and the incident vacancy with wave vector $\mathbf{k}$ goes over to a final state with wave vector $\mathbf{k}'$:

$$w^{(a)}(\mathbf{u}) = \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} w^{(a)}(\mathbf{u};\mathbf{k},\mathbf{k}')n(\mathbf{k}), \qquad (12)$$

where $n(\mathbf{k}) = \exp[-\varepsilon(\mathbf{k})/T]$ is the equilibrium distribution function of the vacancies.

In view of the mentioned exponential smallness of the transition probability, we have

$$w^{(a)}(\mathbf{u};\mathbf{k},\mathbf{k}') \propto \exp[-\varphi^{(a)}(\mathbf{u};\mathbf{k},\mathbf{k}')] \qquad (13)$$

with large φ. The principal role in the integral over $\mathbf{k}$ in (12) is played by a small region near the minimum of the expression

$$\varphi^{(a)}(\mathbf{u};\mathbf{k},\mathbf{k}') + \varepsilon(\mathbf{k})/T. \qquad (14)$$

At sufficiently low temperatures ($T \ll \Delta/\varphi$, where Δ is the width of the band of vacancies) the minimum of the expression (14) corresponds to the bottom of the energy band of vacancies. Here if the electric field $\mathbf{E}$ still satisfies the condition $e\mathbf{E}\cdot\mathbf{u} \ll \Delta$ (e is the charge of the complex), then in view of the conservation of energy $\varepsilon(\mathbf{k}') = \varepsilon(\mathbf{k}) + e\mathbf{E}\cdot\mathbf{u}$ the final wave vector also will be close to the position of the bottom of the band. We shall write the probability (12) in the form

$$w^{(a)}(\mathbf{u}) = \int d\varepsilon\, e^{-\varepsilon/T} \int \frac{dS}{(2\pi)^3} \sigma_a(\mathbf{k}), \qquad (15)$$

where dS is the element of area of the equal-energy surface in $\mathbf{k}$-space, $\varepsilon = \varepsilon(\mathbf{k})$, and

$$\sigma_a(\mathbf{k}) = \int \frac{d^3k'}{(2\pi)^3} \frac{1}{v(\mathbf{k})} w^{(a)}(\mathbf{u};\mathbf{k},\mathbf{k}') \qquad (16)$$

is a quantity which has the meaning of the inelastic scattering cross section. Here $\mathbf{v}(\mathbf{k}) = \partial\varepsilon/\partial\mathbf{k}$ is the velocity of the incident vacancy.

Near the bottom of the band the cross section (16) corresponds to inelastic scattering of slow particles. In the work of Meĭerovich and one of the present authors[8] the well known (Ref. 13, Section 140) general law $1/v$ was used for

FIG. 2.

the vacancies. Subsequently Piradashvili,[10] considering the problem of elastic scattering of vacancies by an impurity particle in the Hubbard model, obtained a constant cross section instead of $1/v$. The Piradashvili result can be obtained also in the general case if one notes that in a weak electric field ($eE\cdot u \ll \Delta$) we are discussing not simply the scattering of slow particles [$v(\mathbf{k}) \to 0$] but a process which at the same time is close to the "threshold" of the reaction [$v(\mathbf{k'}) \to 0$]. Here (see Ref. 13, Sections 144 and 141) the inelastic-scattering cross section is inversely proportional to the velocity of the incident vacancy and simultaneously directly proportional to the velocity of the produced vacancy:

$$\sigma_a(\mathbf{k}) \propto \frac{v(\mathbf{k'})}{v(\mathbf{k})} \propto \left[\frac{\varepsilon(\mathbf{k'})-\varepsilon_0}{\varepsilon(\mathbf{k})-\varepsilon_0} \right]^{1/2}. \qquad (17)$$

In the last relation it has been taken into account that near the bottom of the band the energy is a quadratic function of the quasimomentum and that ε_0 is the energy corresponding to the bottom of the band.

For $\mathbf{E} = 0$ we obtain from (17) a constant cross section, i.e., the result of Piradashvili,[10] while for not too small $\mathbf{E}$ we get the $1/v$ law used in Ref. 8. In the general case we have from Eq. (17)

$$\int \frac{dS}{(2\pi)^3} \sigma_a(\mathbf{k}) = \lambda_a[(\varepsilon-\varepsilon_0)(\varepsilon+e\mathbf{E}\cdot\mathbf{u}-\varepsilon_0)]^{1/2}, \qquad (18)$$

where λ_a is a constant.

Substitution of (18) into (15) gives

$$w^{(a)}(\mathbf{u}) = \lambda_a T^2 e^{-\varepsilon_0/T} \Phi\left(\frac{|e\mathbf{E}\cdot\mathbf{u}|}{T} \right) \cdot \begin{cases} 1, & e\mathbf{E}\cdot\mathbf{u}>0, \\ e^{-|e\mathbf{E}\cdot\mathbf{u}|/T}, & e\mathbf{E}\cdot\mathbf{u}<0, \end{cases} \qquad (19)$$

where

$$\Phi(z) = \int_0^\infty e^{-x}[x(x+z)]^{1/2} dx = \begin{cases} 1, & z\ll1, \\ {}^{1}/_{2}(\pi z)^{1/2}, & z\gg1. \end{cases}$$

The probabilities (19) satisfy a number of additional relations which are a consequence of invariance to time reversal. In view of these relations the drift velocities (7), (10), and (11) vanish at $\mathbf{E} = 0$. If on translation by the vector $\mathbf{u}$ the localized configuration a goes into configuration b, then for $\mathbf{E} = 0$ one should have the equality $w^{(a)}(\mathbf{u}) = w^{(b)}(-\mathbf{u})$, from which it follows that $\lambda_a = \lambda_b$. Substitution of the expressions (19) into the formulas (7), (10), and (11) for the drift velocity shows that in weak fields ($eEu \ll T$) the velocity is naturally proportional to the electric field. With increase of the field, in the region $eEu \sim T$ there is a transition from a linear dependence to the weaker dependence $v \propto E^{1/2}$. This behavior of the drift velocity was observed by Keshishev[5] at a low presure 25.8 atm for positive charges. Previously[5] this was associated with the saturation obtained in Ref. 8 of the field dependence of the drift velocity for $eEu \sim T$. The correct square-root dependence is in good agreement with the experimental data. In Fig. 4 the values of drift velocity obtained by Keshishev[5] for various temperatures (1.20, 1.34, and 1.42 K) are plotted as functions of $E^{1/2}$. The temperature-dependent normalization factors in Fig. 4 were chosen so that the results for different temperatures according to Eq. (19) lie on a single curve. The minimal energy of the vacancies occurred with this adjustable parameter. It can be seen that for $\varepsilon_0 = 4.4$ K there is reasona-
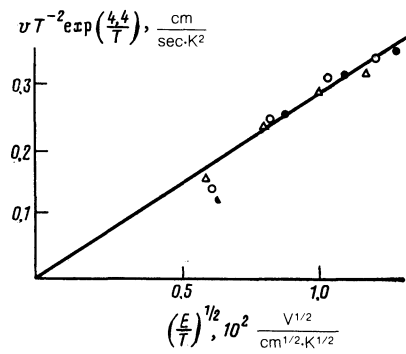

FIG. 4.

ble agreement of Eq. (19) with experiment in the region of strong fields.

3. THRESHOLD BEHAVIOR

In the region of still stronger electric fields such that $eEu \sim \Delta$, the rise of the probabilities of transition processes with increase of the field should be replaced by a falloff. Furthermore, for each of the processes there is a definite threshold value of the field, above which the zero-phonon mechanism considered is completely impossible and the transition probability $w^{(a)}(\mathbf{u})$ is equal to zero. The threshold value of the field is determined by the relation $e\mathbf{E}\cdot\mathbf{u} = \Delta$, which is a direct consequence of the conservation of energy $\varepsilon(\mathbf{k'}) = \varepsilon(\mathbf{k}) + e\mathbf{E}\cdot\mathbf{u}$ and of the definition of the width Δ of the energy band of vacancies $\Delta = \max[\varepsilon(\mathbf{k'}) - \varepsilon(\mathbf{k})]$. We shall consider here $e\mathbf{E}\cdot\mathbf{u} > 0$, since for $eEu \gg T$ the probabilities of the inverse processes accompanied by a decrease of the vacancy energy are exponentially small. We shall explain the behavior of the probabilities of transitions of charges in fields close to threshold.

Near threshold the energy of an incident vacancy $\varepsilon(\mathbf{k})$ is close to the minimal energy ε_0, and the energy of a departing vacancy $\varepsilon(\mathbf{k'})$ is close to the maximal energy ε_m in the band ($\varepsilon_m - \varepsilon_0 = \Delta$). Since near ε_0 and ε_m the energy spectrum is quadratic and the velocities of the two vacancies are small and are proportional respectively to $(\varepsilon - \varepsilon_0)^{1/2}$ and $[\varepsilon_m - \varepsilon(\mathbf{k'})]^{1/2}$, we have in complete analogy with Eq. (17)

$$\sigma_a(\mathbf{k}) \infty \frac{v(\mathbf{k'})}{v(\mathbf{k})} \propto \left[\frac{\varepsilon_m-\varepsilon(\mathbf{k'})}{\varepsilon(\mathbf{k})-\varepsilon_0} \right]^{1/2} = \left[\frac{\Delta-e\mathbf{E}\cdot\mathbf{u}-(\varepsilon-\varepsilon_0)}{\varepsilon-\varepsilon_0} \right]^{1/2}. \qquad (20)$$

Integration over the equal-energy surface $\varepsilon(\mathbf{k}) = \varepsilon$ gives

$$\int \frac{dS}{(2\pi)^3} \sigma_a(\mathbf{k}) = \gamma_a\{(\varepsilon-\varepsilon_0)[(\Delta-e\mathbf{E}\cdot\mathbf{u})-(\varepsilon-\varepsilon_0)]\}^{1/2},$$

where γ_a are constants.

We shall find the transition probability by means of the general formula (15):

$$w^{(a)}(\mathbf{u}) = \gamma_a T^2 e^{-\varepsilon_0/T} \psi\left(\frac{\Delta-e\mathbf{E}\cdot\mathbf{u}}{T} \right). \qquad (21)$$

Here

$$\psi(z) = z^2 \int_0^1 [x(1-x)]^{1/2} e^{-zx} dx = \begin{cases} {}^{1}/_{2}(\pi z)^{1/2}, & z\gg1, \\ {}^{1}/_{8}\pi z^2, & z\ll1. \end{cases}$$

In the region $T \ll \Delta - e\mathbf{E}\cdot\mathbf{u} \ll \Delta$ the transition probabili-

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ty falls off on approach to the threshold in proportion to $(\Delta - e\mathbf{E}\cdot\mathbf{u})^{1/2}$. In a small vicinity of the field threshold, such that $\Delta - e\mathbf{E}\cdot\mathbf{u} \ll T$, this law is replaced by a more rapid falloff proportional to $(\Delta - e\mathbf{E}\cdot\mathbf{u})^2$.

The results of the present section explain naturally the nonmonotonic dependence, observed by Golov et al.,[2] of the charge drift velocity on the electric field at low pressures and temperatures. One can state that the results of Keshishev[5] discussed above show that in the region of low pressures and temperatures the square-root dependence of the drift velocity on the field which is characteristic of phononless processes is observed. In this region on further increase of the field, as is clear from the formulas obtained above, one should observe a falling dependence of the drift velocity on the field, which agrees fully with the results of Golov et al.[2]

4. PHONON PROCESSES

For what follows it is necessary to consider the possibility of emission or absorption of phonons in a quantum transition of a charge under the influence of an incident vacancy. We shall restrict the discussion to one-phonon processes, which is justified if the temperature and $e\mathbf{E}\cdot\mathbf{u}$ are small in comparison with the characteristic energy U of interaction of the atoms in the crystal. In quantum crystals of helium the energy U is of the order of the Debye temperature Θ—the ratio Θ/U is the well known de Boer parameter.[12]

The probability $w^{(a)}(\mathbf{u})$ of a quantum transition of a charge as the result of inelastic scattering of a vacancy from a state $\mathbf{k}$ to a state $\mathbf{k}'$ with emission of a phonon can be written in a form similar to Eq. (12):

$$w^{(a)}(\mathbf{k}) = \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \, w^{(a)}(\mathbf{u}; \mathbf{k}, \mathbf{k}') n(\mathbf{k}) [1+N(\omega)],$$

(22)

where $N(\omega) = (e^{\omega/T} - 1)^{-1}$ is the distribution function of equilibrium phonons; $w^{(a)}(\mathbf{u};\mathbf{k},\mathbf{k}')$ is the differential probability summed over all polarizations and wave vectors of the emitted photon for a given value of its energy ω. The energy ω itself is determined here by conservation of energy if $\varepsilon(\mathbf{k})$, $\varepsilon(\mathbf{k}')$, and the value $e\mathbf{E}\cdot\mathbf{u}$ are given.

The differential probability is exponentially small and satisfies essentially the same formula (13) as above, with the difference that now we permit emission of a phonon and therefore in the absence of an electric field $\varepsilon(\mathbf{k}) > \varepsilon(\mathbf{k}')$. Since the factor in square brackets in (22), which contains the phonon distribution function, acts only on the pre-exponential factor, the main role in the probability (22), as above, is played by a small vicinity of the minimum of the expression (14).

Assume that the temperature satisfies the condition $T \gg \Delta/\varphi$. Then the minimum of expression (14) is the minimum of the function φ and it is realized at certain (temperature-independent) values $\mathbf{k}_0$ and $\mathbf{k}_0'$. Here it is important to note the following. The large value of the function φ is due to the tunnel nature of the process which occurs with a free vacancy that has no charge. Therefore the function $\varphi(\mathbf{u};\mathbf{k},\mathbf{k}')$ will not depend on the electric field, provided that the latter satisfies the condition $e\mathbf{E}\cdot\mathbf{u} \ll U$, which is satisfied since in the region of fields of interest to us we have $e\mathbf{E}\cdot\mathbf{u} \sim \Delta \ll U$. The vectors $\mathbf{k}_0$ and $\mathbf{k}_0'$ therefore also do not depend on the electric field. The energy of the emitted pho-

ton is determined by conservation of energy

$$\omega = \varepsilon(\mathbf{k}_0) - \varepsilon(\mathbf{k}_0') + e\mathbf{E}\mathbf{u}$$

(23)

and will depend on the electric field.

When we recognize that in the region of fields of interest to us the energy of the phonon is small in comparison with the Debye temperature, and therefore the probability of emission of a phonon will depend on the energy ω like ω^3 (Refs. 8 and 9), we find from Eq. (22) the following dependence of the transition probability on temperature and electric field:

$$w^{(a)}(\mathbf{u}) = Ae^{-\varepsilon(\mathbf{k}_0)/T}\omega^3[1+N(\omega)],$$

(24)

where A is a constant and ω is given by Eq. (23).

We shall also give formulas for the probabilities of transition of a charge, accompanied by absorption of the phonon. These formulas are very easy to obtain by using the symmetry with respect to time reversal, like the probabilities of processes which are inverse to those discussed above. As considered above in Section 2, let there be a localized configuration which is obtained from a as the result of transition by the vector $\mathbf{u}$ with probability $w^{(a)}(\mathbf{u})$ given by Eq. (24). Symmetry with respect to time reversal permits us to write immediately the expression for the probability $w^{(b)}(-\mathbf{u})$ of transition of a charge from state b by a vector $-\mathbf{u}$, in which a phonon with energy determined by the previous formula (23) is absorbed, since there is still symmetry of the energy spectrum of vacancies and phonons with respect to space inversion. We have

$$w^{(b)}(-\mathbf{u}) = Ae^{-\varepsilon(\mathbf{k}_0')/T}\omega^3 N(\omega)$$

(25)

with the same constant A as in Eq. (24). For $\mathbf{E} = 0$ the probabilities (24) and (25) are equal to each other, which assures absence of drift of the charge in zero electric field.

At temperatures $T \sim \Delta/\varphi$ the minimum of the expression (14) is accomplished for temperature-dependent $\mathbf{k}_0(T)$ and $\mathbf{k}_0'(T)$. Equations (24) and (25) formally remain valid also in this case, but since in addition to $\mathbf{k}_0$ and $\mathbf{k}_0'$ the quantity A is now also an unknown function of temperature, in essence these formulas determine the dependence of the transition probability only on the electric field.

This dependence is such that it explains the nature of the field dependence, observed by Keshishev,[5] of the drift velocity of charges of the form $(E + E_0)^3$. Actually in weak fields for $e\mathbf{E}\cdot\mathbf{u} \ll T$ substitution of Eqs. (24) and (25) into Eqs. (7), (10), and (11) leads to a linear dependence of the drift velocity on the field. For $e\mathbf{E}\cdot\mathbf{u} \gg T$ only transitions along the field ($e\mathbf{E}\cdot\mathbf{u} > 0$) play a role, and only those transitions among them which are accompanied by emission of phonons. Here in Eq. (24) it is possible to omit the factor which contains the phonon distribution function, and we obtain a dependence of the transition probability on the field of the form

$$w^{(a)}(\mathbf{u}) = a(E+E_0)^3 \cos^3\theta,$$

(26)

where a is a constant and θ is the angle between the translation vector $\mathbf{u}$ and the field $\mathbf{E}$. The quantity E_0 turns out to be equal to

$$E_0 = [\varepsilon(\mathbf{k}_0) - \varepsilon(\mathbf{k}_0')]/eu \cos\theta.$$

(27)

In the general case it depends on the temperature. It is clear
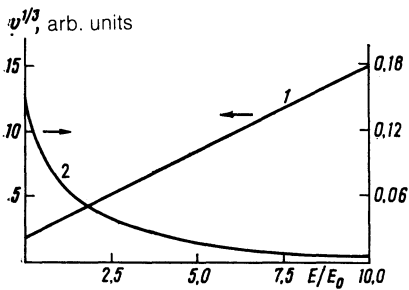
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FIG. 5.

from what has been said above that with reduction of the temperature the energy $\varepsilon(\mathbf{k}_0)$, and with it also $\varepsilon(\mathbf{k}_0')$, which is smaller than $\varepsilon(\mathbf{k}_0)$, appraoches the bottom of the vacancy band ε_0. Here, as can be seen from (27), E_0 falls off. Keshishev[5] actually observed a decrease of E_0 with reduction of the temperature.

Equation (26) actually leads to an $(E + E_0)^3$ law for the drift velocity of a charge only in the case in which in strong fields the main role is played by transitions with any one translation vector $\mathbf{u}$. In the general case, on substitution of the expressions (26) into the linear combinations (7), (10), and (11) of terms with different $\mathbf{u}$, more complicated expressions are obtained as a result of the presence of $\cos\theta$ in Eq. (26) and the expression (27) for E_0. It is interesting, however, that for numerical and geometrical reasons the difference of the exact formulas from an $(E + E_0)^3$ law turns out to be insignificant. We made numerical calculations on the basis of Eq. (7), setting in them

$$w_{1n}=A_1(E\cos\theta_n^{(1)}+E_0)^3, \qquad w_{2n}=A_2(E\cos\theta_n^{(2)}+E_0)^3,$$

if $\cos\theta_n^{(1)} > 0$, $\cos\theta_n^{(2)} > 0$, and $w_{1n} = w_{2n} = 0$ for negative values of $\cos\theta_n^{(1)}$ or of $\cos\theta_n^{(2)}$, respectively. Here A_1, A_2, and E_0 are constants and $\theta_n^{(1,2)}$ are the angles between the directions of the vectors $\mathbf{u}_n^{(1,2)}$ and the direction of the electric field $\mathbf{E}$. For ratios A_1/A_2 from 0.2 to 5 and all directions of the field an extremely insignificant difference of the results from the law $(E + \text{const})^3$ is observed, although the value of const does not necessarily agree with the value of E_0 in the expressions (26). In Fig. 5 we have shown the typical result in the case $A_1/A_2 = 2$ for a field direction along the vector $\mathbf{a}_1$. As abscissa we have plotted the ratio E/E_0, and the left ordinate axis gives the drift velocity (7) to the power 1/3 in arbitrary units. Curve 1, which corresponds to the left ordinate axis, as can be seen from the figure, is very close to the straight line which is the asymptote as $E \to \infty$. Curve 2, which corresponds to the right ordinate axis, gives the difference between curve 1 and its asymptotic straight line. For $E/E_0 \gtrsim 2$ the difference of $v^{1/3}(E)$ from the straight line does not exceed a percent.

5. DISCUSSION OF RESULTS

Let us turn again to a number of features of the experimental data which find a natural explanation in the framework of the approach used. As was noted by Golov et al.,[2] the drift velocity does not have a simple exponential temperature dependence. Generally speaking, it consists of three parts, which can be put in correspondence with the three cases discussed above: $T \gg \Delta/\varphi$, $T \sim \Delta/\varphi$, and $T \ll \Delta/\varphi$. The activation energies at low temperatures (ε_0) and high

temperatures $[\varepsilon(\mathbf{k}_0)]$ do not coincide. The observed nonmonotonic behaviors in the temperature dependence of the drift velocity are easy to explain if one considers its nonmonotonic field dependence found above in Section 3. If the characteristic field values which limit the falling portion in the field dependence of the velocity depend on the temperature, this naturally produces a nonmonotonic behavior in the temperature dependence of the velocity for a given field value.

The anisotropy noted by Lau et al.[11] in the activation energy for the motion of charges can be explained by Eqs. (7) and (11) if one takes into account that the activation energies which enter into the expressions for the probabilities of transitions with different values of $\mathbf{u}$, as we have seen, do not, generally speaking, coincide.

The activation energy observed by Keshishev[5] for positive charges in that region of low pressures in which the field dependence contains the $E^{1/2}$ portion is appreciably smaller than for negative charges, for which a law $(E + E_0)^3$ is observed over the entire range of pressures. This corresponds completely to Eqs. (19) and (24), since $\varepsilon_0 < \varepsilon(\mathbf{k}_0)$.

The main prediction which can be made on the basis of the analysis carried out above is that at a sufficiently low temperature the nature of the field dependence should correspond to Sections 2 and 3, i.e., it should contain an $E^{1/2}$ portion and a falling portion. The fact that up to the present time this type of field dependence has been observed only at low pressures is explained naturally by the rapid dependence on pressure of the limiting characteristic temperature Δ/φ. With increase of the pressure, Δ drops rapidly, and the tunnel argument φ increases.

In our opinion the most interesting experimental problem is determination of the set of translation vectors $\mathbf{u}$ for charges of both signs on the basis of data on the anisotropy of the drift velocity. The equations (11) and the analysis carried out above of the probabilities w show that the anisotropy of the velocity has extremely distinctive features which permit solution of the problem posed. In fact, we have seen that in strong fields $(eEu \gg T)$ only transitions along the field $(e\mathbf{E}\cdot\mathbf{u} > 0)$ play a role. With change of the field direction the drift velocity changes discontinuously when the vector $\mathbf{E}$ passes through the plane perpendicular to one of the vectors $\mathbf{u}$. In the transition region, the angular width of which is of the order T/eEu, the drift velocity changes rapidly both in direction and in absolute value. These features were mentioned previously by Meĭerovich and one of the present authors,[8] but in Ref. 8 it was assumed that the role of the vectors $\mathbf{u}$ is played always by the elementary translation vectors of the crystal lattice. The features about which we are talking would be reflected directly in such a case only by the geometry of the crystal lattice (see also Section 6 of Ref. 12). In reality, as has been shown above, observation and study of these features permits determination of the basic symmetry characteristic of the charge structure–the set of translation vectors $\mathbf{u}$.

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