

# Vacancion mobility of ions in quantum crystals

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Vacancion transfer of ions in quantum crystals of solid helium is determined by scattering of long-wave vacancions by ions<sup>[1,2]</sup>. It is shown that the presence of an external electric field significantly affects of the cross section for vacancion scattering by ions. Discrete negative energy levels of bound states appear in the vacancion energy spectrum after a certain threshold value of the electric field strength is attained. The level system has a condensation point at zero energy. At low temperatures and in strong fields vacancion transfer of ions is determined precisely by such vacancies localized near the ions. The motion of an ion-vacancy complex may be accompanied by spontaneous emission of photons. The dependence of ion mobility on the temperature and on the external field strength is determined.

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In ref. 1 we investigated the motion of charges and impurity atoms in solid-helium quantum crystals. We determined there the dependence of the ion mobility on the temperature  $T$  and on the external electric field  $E$  without resorting to model representations of the ion structure. It was shown that at not too low temperatures the ion transport is via inelastic scattering of long-wave vacancions by ions, a scattering accompanied by transition of the ions to neighboring sites of the crystal lattice. We used there the concepts of quantum theory of delocalized point defects (defectons.<sup>[2,3]</sup> It has turned out that the character of the dependence of the mobility on the temperature and on the external field is determined by the relations between the following quantities: the temperature  $T$ , the width  $\Delta$  of the delocalized-vacancion energy band, and the quantity  $eEa$  ( $e$  is the ion charge and  $a$  is the interatomic distance).

A significant fact in the determination of the vacancion mobility of the ions is that the width  $\Delta$  of the vacancion band is large, of the order of several degrees, and that the following inequality holds at not too high pressures and temperatures:

$$T \ll \Delta. \quad (1)$$

Unusual results were obtained in the region

$$T \ll eEa \ll \Delta, \quad (2)$$

where the ion drift velocity was practically independent of  $E$ .

In this paper, on the basis of ideas developed earlier,<sup>[1]</sup> we study in greater detail the dependence of the vacancion mobility of the ions on the external electric field. It is noted that a significant dependence of the mobility on the field appears in the temperature dependence of the ion drift velocity, in the case of the vacancion motion mechanism, in the vicinity of the point  $T = 0$  even in the weak fields (2). It is shown in this connection how the corresponding formulas of ref. 1 should be modified to make them suitable in the region (2) not only for finite temperatures but as  $T \rightarrow 0$ . We have also investigated the ion mobility in strong fields

$$eEa \gg \Delta. \quad (3)$$

It is shown in the second part of the paper that, when a sufficiently strong electric field acts on the ion, a system of an infinite number of discrete negative energy levels appears in the energy spectrum of the vacancions, and this system corresponds to bound states of the vacancions in the vicinity of the ion, and has as its condensation point the zero-energy level. This makes possible a new motion mechanism that can turn out to be

significant in strong electric fields  $eEa \gg \Delta$  and at low temperatures.

The calculations in the present paper are based on the following circumstance: The vacancion ion-transport mechanism is determined by the inelastic scattering of the vacancions by the ions. The condition (1)  $T \ll \Delta$  means that the vacancions are close to the bottom of the band, where their velocity is low, and the energy depends quadratically on the quasimomentum  $\hbar k$ . The probability of the inelastic process is proportional to the square of the modulus of the vacancion wave function  $\Psi$  in the "reaction zone ( $r \sim a$ ). For slow particles ( $k \rightarrow 0$ ) this means in fact that the asymptotic form of the dependence of the scattering cross section  $\sigma$  on  $k$  as  $k \rightarrow 0$  (but not of the constant in this dependence) is determined by that part of the potential  $V(\mathbf{r})$  which falls off most slowly with distance as  $r \rightarrow \infty$  (see, e.g., ref. 4). The potential  $V$  in which the vacancions move is determined by the crystal strain tensor  $u_{ijk}$ . In the absence of an electric field, the crystal becomes deformed around the ion, as it does around any dilatation center ( $V \sim u_{ijk} \sim 1/r^3$ ,<sup>[5]</sup>), and also as a result of the polarization produced in the medium by the ion charge ( $u_{ijk} \sim 1/r^4$ ).

The presence of an electric field in the crystal produced additional stresses of the dipole type, due to deformation of the lattice by the ion acted upon by the force  $eE$ . The corresponding value of the potential  $V(\mathbf{r})$ , as will be shown below, is proportional to  $1/r^2$ . So slow a decrease of the potential causes<sup>[4]</sup> the function  $\sigma(k)$  to differ in general from known expression  $\sigma \sim 1/k$  for inelastic scattering of slow particles, an expression used earlier in ref. 1. In weak electric fields (2), however,  $eEa \ll \Delta$ , the difference between the true function  $\sigma(k)$  and the relation  $\sigma \sim 1/k$  is negligible at not too small  $k$ . This causes the results of the first part of the present paper to differ from our results<sup>[1]</sup> for weak external fields only in a small vicinity of the point  $T = 0$ . In the first part of the paper we present briefly calculations of the scattering cross section  $\sigma$ , together with the calculation of the ion drift velocity  $u$ .

## 1. INTERACTION OF VACANCIONS WITH IONS IN THE PRESENCE OF AN ELECTRIC FIELD. ION MOBILITY

The potential of the forces acting on the vacancies is<sup>[5]</sup>

$$V(\mathbf{r}) = -K\Omega_{ij}u_{ij}, \quad (4)$$

where  $K^{-1}$  is the coefficient of hydrostatic compress-

sion,  $\Omega_{ik}$  is a tensor characterized by the lattice symmetry and determines the change of the crystal volume when vacancies are introduced in the crystal:  $\Omega_{ll} \sim a^3$ . The deformation due to the action of the force  $eE$  on a point defect (ion) is given by the Green's tensor  $G_{ik}$  of the crystal, since we are in fact dealing with the action of a  $\delta$ -like force on the medium:

$$u_{ik} = \frac{1}{2} eE_i \left\{ \frac{\partial G_{ik}}{\partial x_k} + \frac{\partial G_{ki}}{\partial x_i} \right\}. \quad (5)$$

I. Lifshitz and Rozentsveĭg<sup>[6]</sup> have described a procedure for constructing the Green's tensor for a crystal of any symmetry from the elastic tensor  $\lambda_{iklm}$ , and have shown that for an arbitrary anisotropic medium  $G_{ik}$  is a homogeneous function of the coordinates, in the form  $G_{ik} = r^{-1} \Phi_{ik}(\mathbf{n})$ , where the functions  $\Phi_{ik}$  depend only on the components  $n_i$  of the unit vector  $\mathbf{n} = \mathbf{r}/r$ . Thus,  $V(\mathbf{r})$  is of the form

$$V(\mathbf{r}) = eEa \frac{a^2}{r^2} g(\mathbf{n}), \quad (6)$$

with the function  $g(\mathbf{n})$  expressed in terms of  $\Phi_{ik}$  with the aid of formulas (4) and (5).

The Schrödinger equation for the vacancion wave function  $\Psi(\mathbf{r})$  can be written in the form

$$\nabla^2 \Psi + \left[ k^2 - \frac{eEa}{\Delta} \frac{g(\mathbf{n})}{r^2} \right] \Psi = 0. \quad (7)$$

A few words concerning the limits of validity of (7). It is clear that this equation is meaningful only at sufficiently large distances from the ion where, first, the function  $V(\mathbf{r})$  (6), which tends slowly to zero with increasing  $r$ , is the principal part of the scattering potential, and second,  $|V(\mathbf{r})| \ll \Delta$ . The last condition is necessary in order that the kinetic-energy operator depend quadratically on the quasimomentum operator  $\hbar\mathbf{k} = -i\hbar\partial/\partial\mathbf{r}$ , and is determined by the usual formula  $-\hbar^2\nabla^2/2M$  (the effective mass  $M$  is connected with the width of the band by the relation  $M = \hbar^2/2a^2\Delta$ ). As the vacancion moves away from the ion, the vacancion energy lies, subject to condition (1) ( $T \ll \Delta$ ), near the bottom of the band, where the spectrum is quadratic; to the contrary, in the region of space where  $|V(\mathbf{r})| \sim \Delta$ , the particle is not near the bottom of the band and the Schrödinger equation should contain, as the kinetic-energy operator, not a Laplacian but another function of the operator  $\hat{\mathbf{k}} = -i\nabla$ , which has a rather complicated form and takes into account the band character of the energy spectrum of the vacancions.<sup>[2,7,8]</sup>

Since Eq. (7) is valid only when the distance  $r$  from the ion exceeds a certain value  $r_0 > a$ , to solve the scattering problem we must know the boundary condition for the wave function  $\Psi$  at  $r \sim r_0$ . It is known<sup>[4]</sup> that this boundary condition can be formulated in quite general form, independent of the form of the potential at  $r < r_0$ , only for slow particles for which  $kr_0 \ll 1$ . In weak electric fields  $eEa \ll \Delta$ , the inequality  $kr_0 \ll 1$  is satisfied if  $T \ll \Delta$ , since the inequality  $|V(\mathbf{r})| \ll \Delta$  is valid in such electric fields for the potential  $V(\mathbf{r})$  (6) all the way to interatomic distances. To the contrary, for a strong external field  $eEa \gtrsim \Delta$ , the use of the formulas derived below imposes on the temperature a more stringent limitation than (1):

$$T \ll \Delta^2/eEa.$$

Let us turn to an investigation of Eq. (7). This equation is separable in the spherical coordinate system  $(r, \theta, \varphi)$ . The equation for the radial part  $R(r)$  of the wave function  $\Psi(\mathbf{r}) = R(r)Y(\theta, \varphi)$  takes the form

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \left[ k^2 - \frac{z_n}{r^2} \right] R = 0. \quad (8)$$

The separation constants  $z_n$  in (8) are eigenvalues of the angular part of the wave function

$$[\hat{l}^2 - eEag(\theta, \varphi)/\Delta] Y(\theta, \varphi) = z_n Y(\theta, \varphi), \quad (9)$$

where  $\hat{l}$  is the angular-momentum operator.

The solutions of (8) are cylindrical functions of order  $p_n = (1/4 + z_n)^{1/2}$ . By using the known procedures<sup>[4]</sup> we can determine from the asymptotic forms of the wave function the dependence of the inelastic-scattering cross section on the wave vector  $k$ :

$$\sigma_n \sim k^{2p_n-2}.$$

To determine the cross section  $\sigma$  in this case it suffices to confine oneself, as always in the study of the scattering of slow particles, to the smallest eigenvalue  $z_0$  of the equation for the angle-dependent part of the wave function

$$\sigma \sim k^{2p_0-2}.$$

The integration with respect to the vacancion variables is carried out in the same way as before.<sup>[1]</sup> As a result, the scattering cross section  $\sigma$  yields the ion drift velocity  $u$ :

$$u = u_0 \left( \frac{T}{\Delta} \right)^{p_0-1/2} \frac{\Gamma(1+p_0)}{\Gamma(3/2)}, \quad (10)$$

where  $u_0$  is the drift velocity calculated in ref. 1, and  $\Gamma(x)$  is the gamma function.

We must now determine the constant  $z_0$ . In weak electric fields this problem can be solved analytically, with condition (2) ensuring the possibility of applying perturbation theory to Eq. (9). The smallest eigenvalue of (9) is determined as a correction to the smallest eigenvalue of the operator of the squared angular momentum  $\hat{l}^2$ , i.e., to  $l(l+1) = 0$ . In first order of perturbation theory we have

$$z_0^{(1)} = - \frac{eEa}{4\pi\Delta} \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta g(\theta, \varphi). \quad (11)$$

Owing to certain symmetry properties of the Green's tensor  $G_{ik}$ , the integral (11) can vanish. This is precisely the situation for cubic and hexagonal crystals, and also in the isotropic-medium approximation. This is seen even from the fact that it follows for these substances, from the equation for the Green's tensor, that the latter is not altered by the inversion transformation  $\mathbf{r} \rightarrow -\mathbf{r}$  (this can be verified also directly with the aid of the tensors  $G_{ik}$  obtained by I. Lifshitz and Rozentsveĭg<sup>[6]</sup>). The fact that the Green's tensor is even,  $G_{ik}(\mathbf{r}) = G_{ik}(-\mathbf{r})$ , leads according to (4)–(6) to parity of the function  $g(\theta, \varphi) = -g(\pi - \theta, \pi + \varphi)$ , and consequently to vanishing of the integral (11).

Thus the quantity  $z_0$  is determined for all crystal-line modifications of solids (bcc, fcc, and hcp) by the second perturbation-theory approximation

$$z_0 = - \frac{1}{4\pi} \left( \frac{eEa}{\Delta} \right)^2 \sum_{l,m} \frac{1}{l(l+1)} \left| \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta Y_{l,m}(\theta, \varphi) g(\theta, \varphi) \right|^2, \quad (12)$$

where  $Y_{l,m}$  are orthonormal spherical functions corresponding to the total angular momentum  $l$  and to its projection  $m$  (it is taken into account in (11) and (12) that  $Y_{00} = (4\pi)^{-1/2}$ ).

By way of example we present the value of  $z_0$  for an isotropic medium. In this case

$$G_{ik} = \frac{1}{r} \frac{1+\nu}{8\pi\mathcal{E}(1-\nu)} \times [(3-4\nu)\delta_{ik} + n_i n_k],$$

where  $\mathcal{E}$  is Young's modulus,  $\nu$  is the Poisson coefficient, and  $n_i$  are the components of the unit tensor  $\mathbf{n} = \mathbf{r}/r$ .<sup>[9]</sup> In addition, for an isotropic medium we have  $\Omega_{ik} = \Omega_0 \delta_{ik}$ . Consequently

$$V(r) = \xi \Delta \cos \theta a^2/r^2, \\ \xi = \frac{1}{12\pi} \frac{eEa}{\Delta} \frac{\Omega_0}{a^3} \frac{1+\nu}{1-\nu}.$$

As a result we obtain for  $z_0$

$$z_0 = -1/\xi \xi^2. \quad (13)$$

In strong fields (3), the determination of  $z_0$ , i.e., of the smallest eigenvalue of the operator  $\hat{p}^2 + eEa g(\theta, \varphi)/\Delta$ , can be solved by a variational method. In this case it is convenient to carry out the minimization with respect to the coefficients of the expansion  $A_n$  of the trial function in the eigenfunctions of the operator  $\hat{p}^2$ , which are Legendre polynomials. Thus, for an isotropic medium we have

$$z_0 = \min_{\{A_n\}} \sum_n \left\{ n(n+1) A_n^2 - \xi \frac{n A_n A_{n-1}}{(2n-1)(2n+1)^{1/2}} - \xi \frac{(n+1) A_n A_{n+1}}{(2n+1)(2n+3)^{1/2}} \right\} / \sum_n A_n^2. \quad (14)$$

An analysis of (14) shows that  $z_0$  is a negative function of  $\xi^2$  and tends monotonically to  $(-\infty)$  as  $\xi^2 \rightarrow \infty$  ( $z_0(\xi) = z_0(-\xi)$ ). The plot of  $z_0(\xi)$  obtained by numerical calculation is shown in the figure. In practice, up to  $\xi = 2$ , formula (13) determines  $z_0$  with perfectly satisfactory accuracy.

In conclusion, a few words concerning Eq. (10). It is obvious that this equation is valid only when  $z_0 \leq -1/4$ . The mobility of the ions in stronger fields, at  $z_0 < -1/4$ , is discussed in the next part of the paper. The boundary value  $z_0 = -1/4$  corresponds, according to a numerical colcation, to an electric field given by

$$\frac{1}{12\pi} \frac{eEa}{\Delta} \frac{\Omega_0}{a^3} \frac{1+\nu}{1-\nu} \approx 1.28.$$

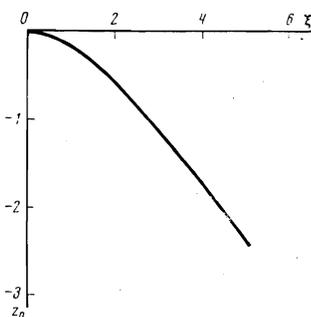
In weak electric fields  $eEa \ll \Delta$  we have according to (11) and (12)  $|z_0| \ll 1$ . The last factor in (10) then determines a small correction, linear in  $z_0$ , to  $u_0$

$$\Gamma(1+p_0)/\Gamma(3/2) = 1 + z_0 \Gamma'(3/2)/\Gamma(3/2) = 1 + 0.037 z_0.$$

At not too low temperatures,  $T/\Delta \gg \exp\{-1/|z_0|\}$ , in weak fields, the factor  $(T/\Delta)^{p_0} - 1/2$  also gives rise to a small correction to  $u_0$ :

$$(T/\Delta)^{p_0-1/2} = 1 + z_0 \ln(T/\Delta).$$

At lower temperatures this factor differs significantly from unity, and the value of  $u$  [Eq. (10)] differs ap-



Plot of  $z_0(\xi)$  for an isotropic medium, obtained by numerical calculation. The function  $z_0(\xi)$  is even:  $z_0(\xi) = z_0(-\xi)$ .

preciably from  $u_0$  even in the weak electric field (2). Since  $z_0$  is always negative, the inequality  $|u| > |u_0|$  is satisfied, and in strong fields we have  $|u| \gg |u_0|$  as  $T \rightarrow 0$ .

## 2. BOUND STATES OF VACANCIONS IN THE VICINITY OF IONS

At  $z_0 < -1/4$ , the formulas for the scattering cross section and for the ion drift velocity (10), derived in the preceding section of the paper, become meaningless. The physical meaning is the following: The  $S$  vacancies ( $l = 0$ ) located far from the ion are effectively attracted to the latter in an electric field ( $z_0 < 0$ ), and the corresponding potential tends to zero with increasing  $r$  like  $\Delta z_0 a^2/r^2$ . In such an attraction field there can exist discrete negative energy levels corresponding to bound states of vacancies near the ion. At  $z_0 > -1/4$ ,<sup>[4]</sup> the number of such levels can be only finite, and their contribution to the partition functions should not be large, so that the question of the very existence of these levels is resolved by starting from the form of the potential at small  $r$ ; if as  $r \rightarrow 0$  the vacancies are, say, repelled from the ion, then there are no negative energy levels.

The situation is different at  $z_0 < -1/4$ . In this case the energy spectrum of the vacancies changes strongly and an infinite system of discrete negative energy levels  $\epsilon_n < 0$  is produced and has the level  $\epsilon = 0$  as its condensation point. Such a spectrum of bound states of vacancies exists at  $z_0 < -1/4$  regardless of the behavior crystal deformation potential at short distances from the ion, although the energies  $\epsilon_n$  of the discrete-spectrum states are of course strongly dependent on the form of the potential as  $r \rightarrow 0$ . However, the requirement that the wave functions of states with different energies  $\epsilon_n$  be orthogonal makes it possible to express all values of  $\epsilon_n$  near the limiting value  $\epsilon = 0$  in terms of only one constant, without making any assumptions about the form of the potential  $V(r)$  near the ion.

This is done mathematically as follows: Far from the ion, the radial part of the wave function of the vacancies is determined by Eq. (8), which takes in the case of negative energy eigenvalues  $\epsilon_n = -\Delta(\kappa_n a)^2$  the form

$$\frac{1}{r} \frac{d^2}{dr^2} (r R_n) + [-\kappa_n r - z_0/r^2] R_n = 0. \quad (15)$$

This equation has a solution, finite as  $r \rightarrow \infty$ , in the form of a spherical Hankel function of imaginary order  $i\mu = i(-1/4 - z_0)^{1/2}$  (we recall that  $z_0 < -1/4$ )

$$R_n = h_{\mu, \nu}^{(1)}(i\kappa_n r)$$

with asymptotic behavior

$$\frac{1}{i\kappa_n r} \exp\left[-\kappa_n r + \frac{\pi}{2}(\mu - i/2)\right], \quad \kappa_n r \rightarrow \infty, \\ \left(\frac{2i\pi}{\kappa_n r}\right)^{1/2} \frac{e^{\mu\pi/2}}{|\Gamma(1+i\mu)| \text{sh}(\mu\pi)} \sin\left[\mu \ln\left(\frac{\kappa_n r}{2}\right) - \Phi_\mu\right], \quad \kappa_n r \rightarrow 0; \quad (16) \\ \Gamma(1+i\mu) = |\Gamma(1+i\mu)| \exp(i\Phi_\mu).$$

The wave functions corresponding to various values of  $\kappa_n$  should be orthogonal to one another. For shallow levels,  $\kappa_n a \ll 1$ , the main contribution to all the spatial integrals is made by the region of large  $r \sim 1/\kappa_n$ . When writing down the orthogonality condition it is therefore possible to neglect the contribution from the region  $r \sim a$ , and to use as the radial wave function the solution (16) of Eq. (15).

With the aid of (15), the condition of the orthogonality of the wave function of the  $n$ th energy level  $R_n$  to the function of  $m$ th level  $R_m$  can be expressed in the form

$$(\kappa_n^2 - \kappa_m^2) \int_0^\infty R_n R_m r^2 dr = \left[ r R_m \frac{d(r R_n)}{dr} - r R_n \frac{d(r R_m)}{dr} \right]_0^\infty = 0.$$

As a result, formulas (16) lead to the following quantization condition for shallow levels of the discrete energy spectrum

$$\varepsilon_n = -\Delta (\kappa_0 a)^2 e^{-2\pi n/\mu}, \quad n=0; 1; \dots \quad (17)$$

where  $\kappa_0$  is a certain constant.

The questions of the existence of levels with lower energy and of the determination of  $\kappa_0$  remain open. It should be noted that in very strong electric fields there can exist bound states that differ from those described above and are analogous to those investigated earlier.<sup>[8]</sup> Indeed, assume that at the initial instant of time the vacancion is located at a point  $r_0$  such that  $|V(\mathbf{r}_0)| > \Delta$ . The total vacancion energy, which is the sum of the potential and kinetic energies, is conserved, while the kinetic energy, owing to the band character of the vacancion energy spectrum, can vary only within the limits of the band, i.e., by an amount not larger than  $\Delta$ . Therefore the vacancion motion is localized inside the region  $|V(\mathbf{r}) - V(\mathbf{r}_0)| \leq \Delta$ , and since the potential energy  $V(\mathbf{r}) \rightarrow 0$  as  $r \rightarrow \infty$ , this region of space is bounded. In quantum mechanics, classically finite motion corresponds to energy levels of a discrete bound-state spectrum. A detailed analysis of such spectra, however, is beyond the scope of the present paper.

Thus, without resorting to model representations concerning the crystal structure near the ion, it is possible to describe the system of shallow ( $|\varepsilon_n| \ll \Delta$ ) energy levels (17). Nonetheless, with the aid of the spectrum (17) we can hope to obtain a rather complete description of the system consisting of an ion and vacancies, for as  $r \rightarrow 0$ , for any realistic boundary condition corresponding to repulsion of the vacancion from the ion at short distances, there cannot be many levels deeper than (17), and we therefore neglect their contributions in all the partition functions.

Let us determine first the number, per unit volume, of the vacancies that are in a state bound to the ion. This number is

$$N_{cb} = e^{-W} \sum_n \frac{\exp(-\varepsilon_n/T)}{\rho_n},$$

where  $W$  is the activation energy of the vacancies, and  $\rho_n = 1/\kappa_n$  is the dimension of the  $n$ th bound state. Going over from summation to integration over the spectrum (17), we get

$$N_{cb} = e^{-W} \int_{-\Delta(\kappa_0 a)^2}^0 d\varepsilon \frac{\mu}{2\pi\varepsilon} e^{-\varepsilon/T} \left( -\frac{\varepsilon}{\Delta} \right)^{\gamma} \frac{1}{a^2} \\ = \frac{\mu}{2\pi a^2} e^{-W} \left( \frac{T}{\Delta} \right)^{\gamma} \gamma\left( \frac{3}{2}, -\frac{\Delta \kappa_0^2 a^2}{T} \right),$$

where  $\gamma(3/2, x)$  is the incomplete gamma function.

Comparison of the number of bound vacancions with the volume concentration of the positive-energy vacancions

$$N = \frac{1}{4\pi^2 a^3} \Gamma\left( \frac{3}{2} \right) e^{-W/T} \left( \frac{T}{\Delta} \right)^{3/2}$$

shows that at high temperatures  $T \gg \Delta(\kappa_0 a)^2$  the contribution of the bound particles to all the partition

functions is small, as expected. Let us dwell in greater detail on a case of greater physical interest,  $T \ll \Delta(\kappa_0 a)^2$ , in which the ion mobility is determined precisely by the bound vacancions. In this case the ion mobility can be calculated in the following manner: The probability of an inelastic process that causes an ion to tunnel to the location of the vacancion bound to it and to be displaced thereby through a vector  $\mathbf{a}$ , and wherein the vacancion acquires an energy  $eEa$  and goes over into a state belonging to the continuous positive-energy spectrum, is proportional to the square of the modulus of the vacancion wave function  $\Psi_n$  in the "reaction zone," i.e., in the region  $r \sim a$ . It is obvious that

$$|\Psi_n(a)|^2 \sim (a/\rho_n)^2.$$

Proceeding from summation over  $n$  to integration, we obtain in this motion mechanism for the ion drift velocity

$$\mathbf{u} = \mathbf{u}_0 2\pi\mu\gamma(3/2, -\Delta\kappa_0^2 a^2/T) / \Gamma(3/2) \quad (18)$$

where, as above,  $\mathbf{u}_0$  is the previously calculated<sup>[1]</sup> drift velocity. We see that at low temperatures  $T \ll \Delta(\kappa_0 a)^2$  the ion drift velocity  $\mathbf{u}$  is exponentially larger than  $\mathbf{u}_0$ : at  $x \gg 1$  the function

$$\gamma(3/2, -x) = \int_0^{\infty} z^2 e^{-z} dz$$

increases like  $x^{1/2} e^x$  and we have asymptotically

$$u \approx u_0 4\pi^2 \mu (\kappa_0 a) (\Delta/T)^{3/2} \exp\{\Delta(\kappa_0 a)^2/T\}. \quad (19)$$

Such a motion mechanism, however, is impossible in very strong fields. The vacancion energy, owing to the band character of the energy spectrum, cannot change by an amount larger than the width  $\Delta$  of the band. Therefore, owing to the energy conservation law, the ion cannot, when it changes places with the vacancion, be displaced through a vector  $\mathbf{a}$  such that  $eE \cdot \mathbf{a} > \Delta$ , since the vacancion cannot absorb the energy  $eE \cdot \mathbf{a}$  released in this case. Thus, in electric fields having a magnitude and orientation such that  $|e\mathbf{E} \cdot \mathbf{a}_k| > \Delta$ , another vacancion ion transport mechanism is realized for all the lattice translation vectors  $\mathbf{a}_k$ ; in this mechanism the tunneling of the ion to the vacancion that forms with the ion a bound state is accompanied by spontaneous emission of phonons of frequency  $e\mathbf{a}_k \cdot \mathbf{E}/\hbar$ .

The rate at which the phonons are spontaneously produced is proportional to the cube of the frequency and to the square of the overlap integral of the wave functions of the initial and final states of the ion-vacancy complex. The latter quantity is proportional to the square of some effective width of the band of this complex, and for the  $n$ -th bound state this width is

$$\Delta_n \sim \Delta (a/\rho_n)^2.$$

As a result, the ion drift velocity is defined as

$$u \sim \left( \frac{eEa}{\Theta} \right)^2 \frac{\Delta^2 a}{\hbar\Theta} e^{-W/T} \sum_n \exp\left( -\frac{\varepsilon_n}{T} \right) \left( \frac{a}{\rho_n} \right)^6,$$

where  $\Theta$  is the Debye temperature,

After changing from summation over the states of the discrete spectrum (17) to integration, we obtain for the drift velocity at  $T \ll \Delta(\kappa_0 a)^2$  the asymptotic value

$$u \sim \left( \frac{eEa}{\Theta} \right)^2 \mu \frac{\Delta^2 a}{\hbar\Theta} \left( \frac{T}{\Delta} \right)^3 \left[ \frac{\Delta(\kappa_0 a)^2}{T} \right]^2 \exp\left\{ -\left( W - \Delta\kappa_0^2 a^2 \right) \frac{1}{T} \right\}. \quad (20)$$

We note that in this ion transport mechanism the vacancion remains in the same energy state, and the

vacancy-ion complex moves as a unit without disintegrating.

In principle, analogous ion-transport processes are possible, accompanied by scattering rather than spontaneous emission of phonons. But the probability of such processes in fields  $eEa \gg T$  is much lower than for spontaneous emission of phonons, and is proportional to  $T^4$ .

In conclusion, a few words concerning the possible experimental consequences of Eqs. (18)–(20) for the ion drift velocity. According to the indicated formulas, the drift velocity  $u$  depends exponentially on the temperature, but in contrast to the equations previously obtained for the mobility in ref. 1 and in the first part of the present paper (it should be recalled that  $u_0 \sim e^{-W/T}$ ), the argument of the exponential differs from  $-W/T$  in our case. In addition, since the constant  $\kappa_0$  is determined by the crystal-deformation field near the ion, the value of  $\kappa_0$ , and hence of the arguments of the exponentials in the function  $u(T, E)$ , can be different for positive and negative ions.

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