MICROSCOPIC QUANTUM THEORY OF DEFECTS AT LOW TEMPERATURES

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Submitted June 3, 1970

Zh. Eksp. Teor. Fiz. 59, 1755–1764 (November, 1970)

Point defects are transformed into quasiparticles (defectons) at low temperatures. The main characteristics of defecton excitations are obtained on the basis of a microscopic model. The scattering of defectons by phonons and electrons is considered. The temperature dependence of the defecton mean free path is found. Defecton-defecton scattering is considered.

At low temperatures, in view of the translational symmetry of the crystal lattice, point defects (vacancies, impurities, interstitial atoms) cannot be regarded as localized at definite points of the crystal. They are transformed into quasiparticles—defectons—with quasimomentum $\mathbf{p}$ and dispersion $\epsilon(\mathbf{p})$. A semiphenomenological theory of defectons was constructed by Andreev and I. Lifshitz[1]. In this article we find the main characteristics of defectons within the framework of a microscopic model.

DISPERSION LAW

We consider a primitive cubic lattice with one point defect. If it is assumed that it is localized at the site $\mathbf{r}$, then the Hamiltonian of such a system is given in the harmonic approximation by

$$H_{\mathbf{r}}=\frac{1}{2}\sum_{\mathbf{R}} m_{\mathbf{R}}\,\dot{u}_{\mathbf{R}}^{2}+\frac{1}{2}\sum_{\mathbf{R}\mathbf{R}'\sigma\sigma'}\Phi_{\mathbf{R}\mathbf{R}'}^{\sigma\sigma'}(\mathbf{r})\,(u_{\mathbf{R}}^{\sigma}-u_{\mathbf{R}}^{0\sigma}(\mathbf{r}))\,(u_{\mathbf{R}'}^{\sigma'}-u_{\mathbf{R}'}^{0\sigma'}(\mathbf{r})), \tag{1}$$

where $u_{\mathbf{R}}^{\sigma}$ is the σ-component of the radius vector of the atom numbered $\mathbf{R}$, $u_{\mathbf{R}}^{0\sigma}(\mathbf{r})$ are the coordinates of the equilibrium position of the same atom, σ = x, y, z, and $\Phi_{\mathbf{R}\mathbf{R}'}^{\sigma\sigma'}(\mathbf{r})$ is the elastic-coefficient matrix.

If we introduce 3N-dimensional vectors $\mathbf{x}$ and $\mathbf{P}$ with components

$$x_i\equiv x_{\mathbf{R}}^{\sigma}=m_{\mathbf{R}}^{1/2}u_{\mathbf{R}}^{\sigma},\quad P_i=m_{\mathbf{R}}^{1/2}\dot{u}_{\mathbf{R}}^{\sigma},\quad i=(\mathbf{R},\sigma), \tag{2}$$

then (1) assumes the more convenient form

$$H_{\mathbf{r}}=\tfrac{1}{2}(\mathbf{P},\mathbf{P})+U_{\mathbf{r}}=\tfrac{1}{2}(\mathbf{x}-\mathbf{x}^{0},\hat{\omega}_{0}^{2}(\mathbf{r})\,(\mathbf{x}-\mathbf{x}^{0})).$$

Here $(\mathbf{a},\mathbf{b})$ denotes the scalar product of the vectors $\mathbf{a}$ and $\mathbf{b}$, and the matrix elements $\hat{\omega}^2$ are connected with the elastic constants by the relation

$$(\hat{\omega}_{0}^{2}(\mathbf{r}))_{\mathbf{R}\mathbf{R}'}^{\sigma\sigma'}=m_{\mathbf{R}}^{-1/2}\Phi_{\mathbf{R}\mathbf{R}'}^{\sigma\sigma'}(\mathbf{r})\,m_{\mathbf{R}'}^{-1/2}.$$

The eigenfunction of the ground state of the crystal can then be written in the form

$$\psi_{\mathbf{r}}(x)=\frac{(\det\hat{\omega}_{0})^{1/4}}{(\pi\hbar)^{3N/4}}\exp\left\{-\frac{1}{2\hbar}(\mathbf{x}-\mathbf{x}^{0},\hat{\omega}_{0}(\mathbf{r})\,(\mathbf{x}-\mathbf{x}^{0}))\right\} \tag{3}$$

(N is the number of atoms), and the energy of the ground state is

$$E_{0}=\tfrac{1}{2}\hbar\,\mathrm{Sp}\,\hat{\omega}_{0}(\mathbf{r}).$$

The ambiguity in the extraction of the square root of the matrix $\hat{\omega}^2$ is eliminated by the requirement that the quadratic form $(\mathbf{x}-\mathbf{x}^0,\omega_0(\mathbf{r})(\mathbf{x}-\mathbf{x}^0))$ be positive definite.

In view of the identity of the lattice sites, the crystal energy does not depend on the location of the defect. Consequently, the correct wave function should have, in the zeroth approximation, the form of a superposition

$$\Psi_{\mathbf{k}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{r}}e^{i\mathbf{k}\mathbf{r}}\psi_{\mathbf{r}}.$$

We consider further the Schrödinger equation

$$\tfrac{1}{2}\hbar^{2}\tilde{\Delta}\Psi+(E-U)\Psi=0,\quad \tilde{\Delta}\equiv\sum_{i}\partial^{2}/\partial x_{i}^{2}. \tag{4}$$

The potential U in this equation is in general a complicated function of the coordinates of all the atoms and takes into account the possibility of the transition of the defect from one site to another. U coincides with $U_{\mathbf{r}}$ in the configuration-space region corresponding to "good localization" of the defect at the site $\mathbf{r}$. In this region $\psi_{\mathbf{r}}$ differs appreciably from zero, and all the $\psi_{\mathbf{r}'}(\mathbf{r}'\neq\mathbf{r})$ are vanishingly small. We therefore have there in first approximation

$$\tfrac{1}{2}\hbar^{2}\tilde{\Delta}\psi_{\mathbf{r}}+(E_{0}-U)\psi_{\mathbf{r}}=0. \tag{5}$$

In the model chosen by us, we shall assume that U coincides at any point of configuration space with one of the functions $U_{\mathbf{r}}$. Therefore, with equal accuracy, we can replace Ψ in (4) by $\Psi_{\mathbf{k}}$. We then multiply (4) from the left by $\Psi_{\mathbf{r}}$, and (5) by $\Psi_{\mathbf{k}}$, subtract one equation from the other, and integrate over the volume in which $\psi_{\mathbf{r}}$ is defined. We transform the resultant expression by means of the Gauss theorem and take into account the fact that the particle flux vanishes at infinity; we then obtain

$$(E-E_{0})\int\psi_{\mathbf{r}}\Psi_{\mathbf{k}}\,dx=\frac{\hbar^{2}}{2}\sum_{i}\int_{S}\left(\psi_{\mathbf{r}}\frac{\partial}{\partial x_{i}}\Psi_{\mathbf{k}}-\Psi_{\mathbf{k}}\frac{\partial}{\partial x_{i}}\psi_{\mathbf{r}}\right)d^{i}x, \tag{6}$$

where $d^{i}x = dx_1\ldots dx_{i-1}\,dx_{i+1}\ldots dx_{3N}$, and S is the surface bounding the region of variation of the defect coordinates. Recognizing that the contribution to the flux is made mostly by the atoms closest to the defects, we get

$$E-E_{0}=\frac{\hbar^{2}}{2}\sum_{\delta}e^{i\mathbf{k}\delta}\int_{S}\left(\psi_{\mathbf{r}}\frac{\partial}{\partial x_{\delta}}\psi_{\mathbf{r}+\delta}-\psi_{\mathbf{r}+\delta}\frac{\partial}{\partial x_{\delta}}\psi_{\mathbf{r}}\right)d^{\delta}x. \tag{7}$$

Here δ runs through the values over the nearest places to which the defect can move, and x_δ is the coordinate of the actually moving atom and relates $\mathbf{r}$ with $\mathbf{r}+\delta$. Thus, for example, in the case of an impurity this is the coordinate of the defect itself, and in

the case of a vacancy it is the coordinate of the atom that goes over to its place.

For a primitive cubic crystal, the integral in the right-hand side of (7) is independent of δ. Thus,

$$\varepsilon(\mathbf{k}) \equiv E - E_0 = A(\cos k_x a + \cos k_y a + \cos k_z a), \quad A = \hbar^2 \int \left(\psi_r \frac{\partial}{\partial x_0} \psi_{r+\delta} - \psi_{r+\delta} \frac{\partial}{\partial x_0} \psi_r \right) d^0 x, \tag{8}$$

where we have put $x_0 \equiv x_\delta$ and a is the lattice constant.

Expression (8) gives the defecton dispersion law, and the width of the defecton band is $\epsilon = 6A$. At small values of the wave vector ($ka \ll 1$) the dispersion is quadratic and the quasiparticle behaves like an ordinary particle with mass $m^* = -\hbar^2/Aa^2$ and velocity $v = kAa/\hbar$.

We see that the main characteristics of the defecton are expressed in simple manner via the probability amplitude of the transition of the defect to the neighboring cell. To calculate this amplitude we choose a coordinate system with origin halfway between the old and new positions of the defect, and with the x_0 axis directed along the straight line joining them. The subscripts plus and minus pertain to the defect location in the half-spaces $x_0 > 0$ and $x_0 < 0$, respectively. The equilibrium positions of the defect will be designated accordingly by l_0 and $-l_0$. Then

$$A = \frac{(\det \hat{\omega}^+)^{1/2}}{(\pi\hbar)^{3N/2}} \hbar \int_{-\infty}^{+\infty} \left[(\hat{\omega}_{00}^+ + \hat{\omega}_{00}^-) l_0 - \sum_{n \neq 0} (\hat{\omega}_{0n}^+ (x_n - x_n^+) - \hat{\omega}_{0n}^- (x_n - x_n^-)) \right] \exp\left\{ -\frac{1}{2\hbar} f(x) \right\} d^0 x, \tag{9}$$

where

$$f(x) = (\hat{\omega}_{00}^+ + \hat{\omega}_{00}^-) l_0^2 - 2l_0 \sum_{n \neq 0} [\hat{\omega}_{0n}^+ (x_n - x_n^+) - \hat{\omega}_{0n}^- (x_n - x_n^-)] + \sum_{n \neq 0,\, m \neq 0} [\hat{\omega}_{mn}^+ (x_m - x_m^+)(x_n - x_n^+) + \hat{\omega}_{mn}^- (x_m - x_m^-)(x_n - x_n^-)], \tag{10}$$

$$l_0 = a\sqrt{m}/2.$$

To simplify the notation we put $\alpha_{mn}^{\pm} = \hat{\omega}_{mn}^{\pm}$ with $m \neq 0$ and $n \neq 0$, and imply summation over repeated indices. Expanding $f(x)$ about the minimum point x^0, we can transform (10) into

$$f(x) = f(x^0) + 2\alpha_{mn}(x_m - x_m^0)(x_n - x_n^0), \tag{11}$$

$$x_m^0 = x_m^+ + l_0 \left[(\alpha^{-1})_{mn} \left(\frac{\hat{\omega}^+ - \hat{\omega}^-}{2} \right)_{n0} - (\alpha^{-1}\alpha^-)_{mn} \Delta_n \right] = x_m^- + l_0 \left[(\alpha^{-1})_{mn} \left(\frac{\hat{\omega}^+ - \hat{\omega}^-}{2} \right)_{n0} + (\alpha^{-1}\alpha^+)_{mn} \Delta_n \right], \tag{12}$$

where $\alpha = (\alpha^+ + \alpha^-)/2$, $\Delta_n = (x_n^+ - x_n^-)/2l_0$ are the relative displacements of the equilibrium positions of the atoms when the defect goes from one cell to the other, and $f(x^0)$ is given by

$$f(x^0) = {}^1/_2 ma^2 [\hat{\omega}_{00} - \hat{\Omega}_{00} + (\hat{\omega}^+ - \hat{\omega}^-)_{0n}\Delta_n - (\hat{\omega}\alpha^{-1}(\alpha^+ - \alpha^-))_{0n}\Delta_n + (\Delta\alpha^-, \alpha^{-1}\alpha^+\Delta)], \quad \hat{\omega} = \frac{\hat{\omega}^+ + \hat{\omega}^-}{2}, \quad \hat{\Omega} = \frac{\hat{\omega}^+ - \hat{\omega}^-}{2} \alpha^{-1} \frac{\hat{\omega}^+ - \hat{\omega}^-}{2}. \tag{13}$$

Substituting (11) in (9) and integrating, we obtain

$$A = \sqrt{\frac{\det \hat{\omega}^+}{\det \alpha} \frac{ma^2}{\pi\hbar}}\, \hbar [\hat{\omega}_{0n}\Delta_n - \hat{\Omega}_{0n}\Lambda_n] \exp\left\{ -\frac{1}{2\hbar} f(x^0) \right\}.$$

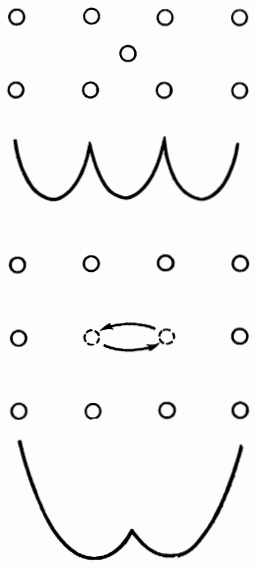

FIG. 1. Effective shape of potential in which interstitial atom is situated.

FIG. 2. Effective shape of potential well for a single event of ejection of a vacancy into the neighboring site.

We see therefore that the transition probability amplitude depends in a very complicated manner on the elastic coefficients and on the displacements of the equilibrium positions of the atoms. We shall therefore consider a simplified model, the form of which is suggested by (8). In this expression, the coordinate along which the defect moves is well pronounced. We therefore assume that the defect has only one degree of freedom and is in a potential well made up of the remaining atoms of the crystal. Depending on the character of the defect, it can have different forms. Thus, for example, in the case of an interstitial atom, it can be represented in the form of an infinite periodic potential well (Fig. 1), whereas in the case of a vacancy it can be assumed for each individual transition that the atom closest to the vacancy is in a double symmetrical potential well (Fig. 2). The vibrations of the remaining lattice atoms will be represented by a single "most dangerous" vibration in the direction of the Y axis, which is perpendicular to X.

The potential energy of the system with the vacancy then takes the form

$$U = \begin{cases} U^+ = \omega^2(X - l_0)^2 + \Omega^2 Y^2 + 2\omega_1^2 (X - l_0) Y, & X > 0, \\ U^- = \omega^2(X + l_0)^2 + \Omega^2 Y^2 - 2\omega_1^2 (X + l_0) Y, & X < 0 \end{cases}$$

$$\hat{\omega}^{\pm} = \frac{1}{2} \begin{pmatrix} \lambda_1 \left(1 - \frac{\varphi}{D}\right) + \lambda_2 \left(1 + \frac{\varphi}{D}\right) & (\lambda_1 \mp \lambda_2) \sqrt{1 - \frac{\varphi^2}{D^2}} \\ (\lambda_1 \mp \lambda_2) \sqrt{1 - \frac{\varphi^2}{D^2}} & \lambda_1 \left(1 + \frac{\varphi}{D}\right) + \lambda_2 \left(1 - \frac{\varphi}{D}\right) \end{pmatrix},$$

$\alpha = {}^1/_2[\lambda_1(1 + \varphi/D) + \lambda_2(1 - \varphi/D)]$, where the eigenvalues λ_1 and λ_2 of the matrices $\hat{\omega}^+$ and $\hat{\omega}^-$ are respectively equal to

$$\lambda_{1,2} = \left[\frac{\Omega^2 + \omega^2}{2} \pm \frac{D}{2} \right]^{1/2}, \quad D = \sqrt{\varphi^2 + 4\omega_1^4}, \quad \varphi = \Omega^2 - \omega^2.$$

The fact that U is positive definite, $\Omega^2\omega^2 > \omega_1^4$, ensures that λ_1 and λ_2 are real. Then

$$f(x^0) = ma^2 \frac{\lambda_1\lambda_2}{\lambda_1(1 + \varphi/D) + \lambda_2(1 - \varphi/D)}.$$

If the energy of the interaction between the oscillators is low, i.e., $2\omega_1^2 \ll |\varphi|$ or $2\omega_1^2 \gg |\varphi|$, but $\omega_1^2 \ll \omega\Omega$, then we obtain the obvious result

$$f(\mathbf{x}^0) \approx m\omega a^2/2.$$

If, however, the interaction energy is of the order of the energy of the oscillators themselves, i.e., $\omega_1^2 \sim \omega\Omega$, then the transition probability increases greatly with increasing ω_1^2:

$$f(\mathbf{x}^0) \approx ma^2\sqrt{\omega\Omega - \omega_1^2}.$$

SCATTERING OF PHONONS AND ELECTRONS BY A DEFECTON

At zero temperature, the defecton moves through the crystal without dissipation. In view of its low velocity compared with that of sound, the "gas" of zero phonons present in the crystal has time to adapt itself to the defecton, which moves together with an adiabatically adapted phonon "cloud" that strongly influences the defecton mass; in the case of a vacancion, this cloud determines the mass completely. With rising temperature, scattering of thermal phonons by the defecton sets in. Since the defecton mass is large and its lifetime much longer than the relaxation time of the phonon gas, the scattering is the same as by a force center. Therefore the cross section for scattering by a defecton can be replaced by the cross section for scattering by an immobile defect.

If the elastic-coefficient matrix $\Phi_{RR'}^{\sigma\sigma'}$ is written in the form of the sum of the matrix of the ideal crystal $L_{R-R'}^{\sigma\sigma'}$ and the perturbation matrix $\Lambda_{RR'}^{\sigma\sigma'}$, then, as is well known[2], the wave function of the scattered phonon is given by

$$\chi_{\mathbf{jk}}^{\sigma}(\boldsymbol{R}) = \frac{V}{(2\pi)^3}\sum_i \frac{1}{m}\int \frac{\lambda_{\mathbf{kx}}^{ji} q_i^{\sigma}(\varkappa)\, e^{i\varkappa R}}{\omega^2 - \mu_i(\varkappa) + i0}\, d\varkappa,$$

where

$$\lambda_{\mathbf{kx}}^{ji} = \sum_{\mathbf{R}_1\mathbf{R}_2\sigma_1\sigma_2} q_i^{\sigma_1}(\varkappa)\, e^{-i\varkappa R_1}\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\tau_{\mathbf{R}_2}^{\sigma_2},$$

$$\tau_{\mathbf{R}}^{\sigma} + \sum_{\mathbf{R}_2\sigma_2}\tau_{\mathbf{R}_2}^{\sigma_2}\beta_{\mathbf{R}_2\mathbf{R}}^{\sigma_2\sigma} = q_j^{\sigma}(\mathbf{k})\, e^{i\mathbf{k}\mathbf{R}}, \qquad (14)$$

$$\beta_{\mathbf{R}_2\mathbf{R}}^{\sigma_2\sigma} = \frac{V}{(2\pi)^3}\sum_i \frac{1}{m}\int \frac{d\varkappa}{\mu_i(\varkappa) - \omega^2 - i0}$$

$$\times \sum_{R_1\sigma_1} q_i^{\sigma_1}(\varkappa)\, e^{-i\varkappa R_1}\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2} q_i^{\sigma}(\varkappa)\, e^{i\varkappa R},$$

V is the volume of the unit cell, $\mu_i(\kappa)$ is the dispersion law of the i-th oscillation mode, and $q_i(\mathbf{k})$ are the polarization vectors.

Let us consider the case of greatest interest, when the phonon wavelength is large compared with the inhomogeneity dimensions. As is well known, the elastic-coefficient matrix $\Phi_{RR'}^{\sigma\sigma'}$ has the important property

$$\sum_{\mathbf{R}'}\Phi_{\mathbf{RR}'}^{\sigma\sigma'} = 0, \qquad (15)$$

which follows from the definite behavior of the forces acting on each atom when the crystal is transported as a whole. This condition is also satisfied by each of the matrices $L_{R-R'}^{\sigma\sigma'}$ and $\Lambda_{RR'}^{\sigma\sigma'}$. Then the quantities $\beta_{R_2R}^{\sigma_2\sigma}$ are small, and their sum is equal to zero:

$$\beta_{\mathbf{R}_2\mathbf{R}}^{\sigma_2\sigma} \ll 1, \quad \sum_{\mathbf{R}_2}\beta_{\mathbf{R}_2\mathbf{R}}^{\sigma_2\sigma} = 0.$$

Consequently, we can neglect the sum in (14). As a result,

$$\lambda_{\mathbf{kx}}^{ji} = \sum_{\mathbf{R}_1\mathbf{R}_2\sigma_1\sigma_2} q_i^{\sigma_1}(\varkappa)\, e^{-i\varkappa R_1}\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2} e^{i\mathbf{k}R_2} q_j^{\sigma_2}(\mathbf{k}). \qquad (16)$$

Since in primitive lattices each atom is a symmetry or inversion center, this expression can be rewritten in the form

$$\lambda_{\mathbf{kx}}^{ji} = \sum_{\sigma\sigma_2} q_i^{\sigma_1}(\varkappa)\, q_j^{\sigma_2}(\mathbf{k}) \sum_{\mathbf{R}_1\mathbf{R}_2} [\cos\varkappa R_1 \Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\cos\mathbf{k}R_2 + \sin\varkappa R_1\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\sin\mathbf{k}R_2],$$

whence, taking (15) into account, we obtain for small k and κ

$$\lambda_{\mathbf{kx}}^{ji} = \sum_{R_1\sigma_1\sigma_2} q_i^{\sigma_1} q_j^{\sigma_2}\varkappa R_1\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\mathbf{k}R_2,\ q_j^{\sigma} \equiv q_j^{\sigma}(0), \quad kr_0 \ll 1,$$

r_0 is the dimension of the inhomogeneity. The function of the scattered long-wave phonon can then be written in the form

$$\chi_{j\mathbf{k}}^{\sigma}(\mathbf{R}) = \sum_{i\sigma_1\sigma_2} q_j^{\sigma_2} q_i^{\sigma} q_i^{\sigma_1}\frac{V}{mc_i^2}\frac{1}{(2\pi)^3}\int \frac{d\varkappa}{k_i^2 - \varkappa^2 + i0}\sum_{\mathbf{R}_1\mathbf{R}_2}\mathbf{k}R_1\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\varkappa R_2 e^{i\varkappa R_2},$$

where account is taken of the fact that $\mu_i(\kappa) = c_i^2\kappa^2$, at long wavelengths, and the notation $k_i^2 c_i^2 = \omega^2$ is introduced (c_i is the velocity of the phonon of the i-th mode; i = 1, 2, 3). Retaining only terms proportional to 1/R, we obtain the asymptotic form of this function at large distances:

$$\chi_{j\mathbf{k}}^{\sigma}(\mathbf{R}) = \frac{V}{4\pi}\sum_{i\sigma_1\sigma_2} q_i^{\sigma} q_j^{\sigma_2} q_i^{\sigma_1}\frac{1}{mc_i^2}\sum_{\mathbf{R}_1\mathbf{R}_2}\mathbf{k}R_1\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\mathbf{k}_i' R_2\frac{e^{ik_iR}}{R} \quad (\mathbf{k}_i' \equiv k_i\mathbf{R}/R).$$

We see that a phonon with polarization σ belonging to the j-th oscillation mode forms, after scattering, three diverging waves corresponding to the three vibration modes in the lattice. The cross section for the scattering of the phonon of the j-th mode, as a result of which the phonon of the i-th mode is obtained, is given by the expression

$$d\sigma_{\mathbf{jk},i\mathbf{k}'}^{\sigma\sigma} = \left(\frac{V}{4\pi mc_i^2}\right)^2 (q_i^{\sigma})^2\left\{\sum_{\sigma_1\sigma_2} q_i^{\sigma_1} q_j^{\sigma_2}\sum_{\mathbf{R}_1\mathbf{R}_2}\mathbf{k}R_1\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\mathbf{k}_i' R_2\right\}^2 d\Omega', \qquad (17)$$

where $d\Omega' = 2\pi\sin\alpha\, d\alpha$, and α is the angle between the directions of the incoming and scattered phonons. Averaging (17) over the modes and over the polarizations of the incident phonons, and summing over the modes and polarizations of the scattered phonons, we obtain a general formula for the cross section for the scattering of a phonon by a local defect in a primitive lattice of any symmetry:

$$d\sigma_{\mathbf{kk}'} = \frac{V^2}{3(4\pi mc^2)^2}\sum_{\sigma_1\sigma_2}\left\{\sum_{\mathbf{R}_1\mathbf{R}_2}\mathbf{k}R_1\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_2}\mathbf{k}'R_2\right\}^2 d\Omega'.$$

In the case of a cubic lattice this yields

$$d\sigma_{\mathbf{kk}'} = \left(\frac{a^3}{4\pi mc^2}\right)^2\sum_{\sigma_1}\left\{\sum_{\mathbf{R}_1\mathbf{R}_2}\mathbf{k}R_1\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{\sigma_1\sigma_1}\mathbf{k}'R_2\right\}^2 d\Omega',$$

and if the interaction between the displacements of the atoms in perpendicular directions can be neglected, then

$$d\sigma_{\mathbf{kk}'} = \left(\frac{a^3}{4\pi mc^2}\right)^2\left\{\sum_{\mathbf{R}_1\mathbf{R}_2}\mathbf{k}R_1\Lambda_{R_1R_2}\mathbf{k}'R_2\right\}^2 d\Omega'. \qquad (18)$$

For concreteness, let us consider the case when the defect is a vacancy, and confine ourselves to the interaction between the nearest atoms. Then

$$\mu(\mathbf{k}) = -2(L_1/m)(3 - \cos k_x a - \cos k_y a - \cos k_z a),$$

from which we see that L_1 is connected with the speed of sound by the relation

$$c^2 = -(a^2/m)L_1.$$

On the other hand, the condition (15) enables us to express all the elements of the matrix $\Lambda_{RR'}$ in terms of a single element. Recognizing also that in the case of a vacancy $\Lambda_{00} = -L_0$, we obtain

$$\Lambda_{00} = -6\frac{mc^2}{a^2}, \quad \Lambda_{0\delta} = \frac{mc^2}{a^2} = -\Lambda_{\delta\delta}.$$

Substituting in (18) and summing, we obtain the phonon-vacancy scattering cross section

$$d\sigma_{\mathbf{k}\mathbf{k}'} = \frac{a^2}{(2\pi)^2}(ka)^4(\mathbf{n}\mathbf{n}')^2 d\Omega', \quad \mathbf{n} = \frac{\mathbf{k}}{k}, \quad \mathbf{n}' = \frac{\mathbf{k}'}{k}. \tag{19}$$

If the defect is a substitutional atom, then this quantity must also be multiplied by the "intensity" of the perturbation $\Lambda^2 = (\Lambda_{00}/L_{00})^2$. In view of the complete formal similarity of the expressions for the functions of the scattered phonon and electron[3], formula (19) also gives the cross section for the scattering of long-wave electrons by a vacancion in the plane-wave approximation.

We note also that if the unit cell contains more than one atom, then condition (15) is replaced by

$$\sum_{\mathbf{R}'s'} \Phi_{\mathbf{R}\mathbf{R}'}^{ss'\sigma\sigma'} = 0 \tag{20}$$

(s is the number of the atom in the cell), and in lieu of (16) we get the matrix

$$\lambda_{\mathbf{k}\mathbf{x}}^{ij} = \sum_{\mathbf{R}_1\mathbf{R}_2 ss'\sigma\sigma'} q_i^{s\sigma}(\varkappa)\, e^{-i\varkappa\mathbf{R}_1}\Lambda_{\mathbf{R}_1\mathbf{R}_2}^{ss'\sigma\sigma'} e^{i\mathbf{k}\mathbf{R}_2} q_j^{s'\sigma'}(\mathbf{k}), \tag{21}$$

whose elements, generally speaking, do not vanish as $k \to 0$. If, however, at least one of the indices i and j pertains to the acoustic mode, then $\lambda_{00}^{ij} = 0$. This follows directly from (20) and (21), if it is recognized that the polarization vectors for the acoustic modes do not depend on the number of the atom in the cell. Thus, the optical and acoustic vibrations become separated. The expansion of the scattering cross section in powers of the wave vector begins with a constant for the optical phonons and with k^4 for the acoustic ones. At low temperatures, however, the number of optical phonons is exponentially small and they can exert no significant influence on the defecton motion.

MEAN FREE PATH

We start from the energy and momentum conservation laws. Let p and m^* be the wave vector and the mass of the defecton, and k the wave vector of the phonon. The same quantities after collision will be marked by primes. Thus, we have

$$\mathbf{p} + \mathbf{k} = \mathbf{p}' + \mathbf{k}',$$

$$\frac{\hbar^2 p^2}{2m^*} + \hbar\omega_k = \frac{\hbar^2 p'^2}{2m^*} + \hbar\omega_{k'}.$$

Recognizing that for long waves $\omega_k = ck$ and the defecton velocities are small compared with the speed of sound, and also recognizing that the phonon momentum is small, $\hbar k \ll m^* c$, we obtain

$$k' - k = \frac{k}{p_0}(\mathbf{p}\mathbf{n}' - \mathbf{p}\mathbf{n}) - \frac{k^2}{p_0}(1 - \mathbf{n}\mathbf{n}'), \quad p_0 \equiv \frac{m^* c}{\hbar}.$$

This is the change in the magnitude of the phonon wave vector as a result of one collision. Obviously, the total change of the wave vector of the phonon gas per second is given by the integral

$$q = \frac{3c}{(2\pi)^3}\int n(k)\,(k - k')\, d\sigma_{\mathbf{k}\mathbf{k}'} d\mathbf{k},$$

where $n(k) = (e^{\hbar\omega k/T} - 1)^{-1}$ is the distribution function of the bosons, and the factor 3 takes into account the three possible phonon polarizations. After integrating over the angles we obtain

$$q = \frac{4ca^6}{(2\pi)^3 p_0}\int dk \frac{k^8}{e^{\hbar ck/T} - 1}.$$

At low temperatures ($T \ll \hbar c$) the main contribution to the integral is made by small $ka \ll 1$. Consequently, the integration region can be extended to infinity. We obtain ultimately

$$q = \frac{4\hbar}{m^* a^3}\frac{\Gamma(9)\zeta(9)}{(2\pi)^3}\left(\frac{T}{\hbar c}\right)^9 \approx 0{,}4\frac{\hbar}{m^* a^3}\left(\frac{8T}{T_D}\right)^9, \tag{22}$$

where T_D is the Debye temperature.

Since the collisions with the phonons were assumed to be elastic, it follows that (22) also gives the change of the magnitude of the defecton wave vector. Let us define the free path time τ as the time during which the defecton momentum changes by an amount equal to the momentum itself. Then

$$\tau = \frac{p}{q} \approx 2{,}5\frac{m^* a^3}{\hbar} p\left(\frac{T_D}{8T}\right)^9,$$

and the transport mean free path is equivalent to the distance traversed during the time τ:

$$l = \tau\frac{\hbar p}{m^*} = a \cdot 2.5(pa)^2\left(\frac{T_D}{8T}\right)^9. \tag{23}$$

If the defectons obey the Bose-Einstein statistics, then at a temperature T the wave vector of the defecton is $p \sim (2m^*T/\hbar^2)^{1/2}$. Substituting in (23), we obtain

$$\frac{l}{a} \approx 0{,}6\frac{m^* T_D}{\hbar^2}a^2\left(\frac{T_D}{8T}\right)^8.$$

We see that the mean free path depends strongly on the temperature. At low temperatures ($T \ll T_D/8$) it is large compared with the interatomic distances, and the defecton behaves like a quasiparticle with wave vector p. If $T \gg T_D/8$, then the defecton is localized and its further motion is determined by the diffusion jumps to neighboring cells.

A similar analysis can be carried out for the scattering of electrons by a defecton. The main difference is that the electrons have a quadratic dispersion and obey Fermi-Dirac statistics. Therefore the wave-vector loss in the collision is given by

$$q = \frac{2a^6}{(2\pi)^3}\int dk\, F(k)\,(1 - F(k))\,(k - k')\, v_e\, d\sigma_{\mathbf{k}\mathbf{k}'},$$

where $F(k) = [\exp\{\hbar^2 k^2/2MT\} + 1]^{-1}$ is the fermion distribution function, $v_e = \hbar k/M$ is the velocity of an electron with momentum $\hbar k$ and mass M, and

$$k - k' = {}^1/_2\mu(\mathbf{p}\mathbf{n} - \mathbf{p}\mathbf{n}') + \mu k(1 - \mathbf{n}\mathbf{n}'), \quad \mu = M/m^* \ll 1.$$

At low temperatures $T \ll \hbar^2/2Ma^2$, the main contribution to the integral is made by small $ka \ll 1$, and

the integration region can be extended to infinity, after which the integral can be evaluated. Thus,

$$q = \frac{2\hbar}{3\pi^3 m^* a^3}(2^{5/2}-1)\Gamma\left(\frac{9}{2}\right)\zeta\left(\frac{7}{2}\right)\left(\frac{T}{T_c}\right)^{9/2} \approx 1{,}5\frac{\hbar}{m^* a^2}\left(\frac{T}{T_c}\right)^{9/2},$$

and consequently the lifetime is

$$\tau \sim \frac{2}{3}pa\frac{m^* a^2}{\hbar}\left(\frac{T}{T_c}\right)^{9/2}, \quad T_c = \frac{\hbar^2}{Ma^2},$$

and the mean free path is $l \approx \frac{2}{3}a(pa)^2(T_C/T)^{9/2}$.

In view of the large value of T_C, all the temperatures at which the crystal does not melt are "low" and the mean free path is very large. Therefore collisions with electrons exert no influence on the defecton motion.

We note also that the foregoing analysis is meaningful at not too large defect concentrations. Otherwise the scattering of defectons by defectons is most important. The small width of the defecton band leads to a large cross section of this process. This is particularly easy to see in the case of an elastically-isotropic crystal, when the defects are interstitial atoms. As is well known[4], their interaction energy at large distances is given by

$$V(R) = V_0(a/R)^6,$$

where $V_0 \sim mc^2$. Then the effective scattering cross section is given in the quasiclassical approximation by the expression

$$\sigma = 2\pi a^2 \sin\frac{3\pi}{10}\cdot\Gamma\left(\frac{3}{5}\right)\left(\frac{3\pi}{8}\right)^{1/5}\left[\frac{V_0 m^* a^2}{\hbar^2}\frac{\lambda}{a}\right]^{2/5}. \qquad (24)$$

the condition for the validity of which is the inequality

$$(\lambda/a)^4 \ll V_0 m^* a^2/\hbar^2.$$

Substituting in (24) $V_0 \sim mc^2$ and $m^* a^2/6\hbar^2 = 1/\epsilon$, we obtain

$$\sigma \sim 2\pi a^2\left(6\frac{mc^2}{\varepsilon}\frac{\lambda}{a}\right)^{2/5}.$$

In view of the small width of the defecton band $\epsilon \ll mc^2$, the scattering cross section may turn out to be quite large.

In the other limiting case, when

$$(ka)^2 \ll V_0 m^* a^2/\hbar^2,$$

we have

$$\sigma \sim 2\pi a^2\left(\frac{V_0 m^* a^2}{\hbar^2}\right)^{1/2} \sim 2\pi a^2\left(\frac{6mc^2}{\varepsilon}\right)^{1/2}.$$

The author thanks I. M. Lifshitz for valuable hints and for repeated discussions of the work.

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Translated by J. G. Adashko
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