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Contribution to the theory of defectons in quantum crystals

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Deformation produced in a quantum crystal by the presence of a point defect is considered. It is shown that a bound defecton state with deformation of the lattice can be produced in the one-dimensional case. It is shown that the deformation moves together with the defect with constant velocity without changing shape. In the three-dimensional case, the bound state is produced at deformation dimensions for which the continual approximation can be used.

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As shown by Andreev and I. Lifshitz, [1] at low temperatures point defects in quantum crystals are transformed into quasiparticles – defectons. A quantum theory of defectons, based on a microscopic model, was constructed by one of us. [2] Defectons connected with motion of complexes of defects were considered by Andreev and Meĭerovich. [3,4] They have also shown that even in a three-dimensional crystal there can exist defectons with one or two degrees of freedom. In these papers the lattice deformation around the defect was assumed specified, and its influence on the defecton spectrum was taken into account. A one-dimensional model of a quantum crystal with a defect was considered in, [5] where it was shown that a self-consistent state can be produced, such that the defect moves together with the deformation it produces. The appearance of this state is mathematically connected with the soliton solutions of the nonlinear Schrödinger equation. In the approximation used in, [5] no account was taken of the change of the probability of a transit of a defect to a neighboring node as a result of the lattice deformation.

In this paper we consider both a one-dimensional and a three-dimensional crystal with a defect. In the harmonic approximation, the system Hamiltonian can be written in the form

$$\hat{H}=\sum_{\mathbf{R},\alpha}\frac{m}{2}(\dot{\xi}_{\mathbf{R}}^{\alpha})^2(1+\mu B_{\mathbf{R}}^{+}B_{\mathbf{R}})+\frac{1}{2}\sum_{\mathbf{R}\mathbf{R}'\alpha\beta}L_{\mathbf{R}-\mathbf{R}',\xi_{\mathbf{R}}^{\alpha}\xi_{\mathbf{R}'}^{\beta}}^{\alpha\beta}+\frac{1}{2}\sum_{\mathbf{R}}\Lambda_{\mathbf{R}}B_{\mathbf{R}}^{+}B_{\mathbf{R}}-\frac{1}{2}\sum_{\mathbf{R}\mathbf{R}'}A_{\mathbf{R}-\mathbf{R}'}B_{\mathbf{R}}^{+}B_{\mathbf{R}}, \tag{1}$$

where $\xi_{\mathbf{R}}^{\alpha}$ is the α component of the displacement vector of the atom situated at the site R compared with its equilibrium position in a perfect crystal; $\mu=(M-m)/m$, where M and m are respectively the masses of the impurity and of the host lattice atom;

$$\Lambda_{\mathbf{R}}=\sum_{\mathbf{R}'}\Lambda_{\mathbf{R}\mathbf{R}'}(\xi_{\mathbf{R}}-\xi_{\mathbf{R}'}) \tag{2}$$

is the difference between the interaction energy of the defect with the remaining atoms, and the interaction energy of the host atom with them. The second sum in (1) describes the potential energy of an ideal crystal in the harmonic approximation; $B_{\mathbf{R}}^{+}$ and $B_{\mathbf{R}}$ are the Bose operators of defect creation and annihilation at the site R; $A_{\mathbf{R}-\mathbf{R}'}$ is the amplitude of the probability of the transfer of a defect from site R to site R′.

The solution of the Schrödinger equation

$$i\hbar\partial\Psi/\partial t=\hat{H}\Psi \tag{3}$$

will be sought in the form of an expansion

$$\Psi=\sum_{\mathbf{R}}a_{\mathbf{R}}(t)\Psi_{\mathbf{R}}, \tag{4}$$

where $\Psi_{\mathbf{R}}=B_{\mathbf{R}}^{+}|0\rangle$ is the wave function of the system with a defect localized at the site R; $|0\rangle$ is the wave function of the ideal crystal. Naturally, the coefficients $a_{\mathbf{R}}$ should satisfy the normalization condition

$$\sum_{\mathbf{R}}|a_{\mathbf{R}}|^2=1. \tag{5}$$

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The quantities $\Lambda_{\mathbf{R}}$ and $A_{\mathbf{R}-\mathbf{R}'}$ depend on the displacements $\xi_{\mathbf{R}}{}^{\alpha}$ of the atoms. In the approximation linear in the displacements we have

$$\Lambda_{\mathbf{R}} = \Lambda + \sum_{\rho\alpha} \Lambda_{\rho}{}^{\alpha} \xi_{\mathbf{R}+\rho}^{\alpha}, \quad \Lambda_{\rho}{}^{\alpha} \equiv (\partial \Lambda_{\mathbf{R},\,\mathbf{R}+\rho} / \partial \xi_{\mathbf{R}}{}^{\alpha})_{\xi_{\mathbf{R}}{}^{\alpha} = \xi_{\mathbf{R}+\rho}^{\alpha}} = -\Lambda_{-\rho}^{\alpha}, \tag{6}$$

$$A_{\mathbf{R}-\mathbf{R}'} = A_{\mathbf{R}-\mathbf{R}'}^{0} + \sum_{\alpha} A_{\mathbf{R}-\mathbf{R}'}^{\alpha} (\xi_{\mathbf{R}}^{\alpha} - \xi_{\mathbf{R}'}^{\alpha}), \quad A_{\mathbf{R}-\mathbf{R}'}^{\alpha} \equiv (\partial A_{\mathbf{R}-\mathbf{R}'} / \partial \xi_{\mathbf{R}}{}^{\alpha})_{\xi_{\mathbf{R}}{}^{\alpha} = \xi_{\mathbf{R}'}^{\alpha}}$$
$$= -A_{\mathbf{R}'-\mathbf{R}}^{\alpha} \tag{7}$$

For simplicity we shall take into account only the transitions of the defect to the nearest lattice sites. The Hamiltonian of the system then becomes

$$\hat{H} = \frac{1}{2}\Lambda + \frac{m}{2}\sum_{\mathbf{R}\alpha} (\dot{\xi}_{\mathbf{R}}{}^{\alpha})^2 (1 + \mu B_{\mathbf{R}}{}^{+} B_{\mathbf{R}}) + \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'\alpha\beta} L_{\mathbf{R}-\mathbf{R}'}^{\alpha\beta} \xi_{\mathbf{R}}{}^{\alpha} \xi_{\mathbf{R}'}^{\beta}$$
$$+ \frac{1}{2}\sum_{\mathbf{R}\rho\alpha} \Lambda_{\rho}{}^{\alpha} \xi_{\mathbf{R}+\rho}^{\alpha} B_{\mathbf{R}}{}^{+} B_{\mathbf{R}} - \frac{1}{2}\sum_{\mathbf{R}\delta} A_{\delta}{}^{0} B_{\mathbf{R}}{}^{+} B_{\mathbf{R}+\delta}$$
$$+ \frac{1}{2}\sum_{\mathbf{R}\delta\alpha} A_{\delta}{}^{\alpha} (\xi_{\mathbf{R}}{}^{\alpha} - \xi_{\mathbf{R}+\delta}^{\alpha}) B_{\mathbf{R}}{}^{+} B_{\mathbf{R}+\delta}, \tag{8}$$

where δ runs over only the nearest neighbors of the defect.

Substituting the expansion (4) in the Schrödinger equation (3) with the Hamiltonian (8), we obtain the following system of equations for the amplitudes:

$$i\hbar \frac{\partial a_{\mathbf{R}}}{\partial t} = \Big(\varepsilon_0 + T_0 + U_0 + \frac{\mu m}{2} \dot{\xi}_{\mathbf{R}}{}^{2} + \frac{1}{2}\sum_{\rho\alpha} \Lambda_{\rho}{}^{\alpha} \xi_{\mathbf{R}+\rho}^{\alpha}\Big) a_{\mathbf{R}}$$
$$+ \frac{1}{2}\sum_{\delta} A_{\delta}{}^{0} (a_{\mathbf{R}+\delta} - a_{\mathbf{R}}) + \frac{1}{2}\sum_{\delta\alpha} A_{\delta}{}^{\alpha} (\xi_{\mathbf{R}}{}^{\alpha} - \xi_{\mathbf{R}+\delta}^{\alpha}) a_{\mathbf{R}+\delta}, \tag{9}$$

where $\epsilon_0 = \frac{1}{2}(\Lambda + \gamma A^0)$ (γ is the number of nearest neighbors),

$$T_0 = \frac{m}{2}\sum_{\mathbf{R}\alpha} (\dot{\xi}_{\mathbf{R}}{}^{\alpha})^2, \quad U_0 = \frac{1}{2}\sum_{\mathbf{R}\mathbf{R}'\alpha\beta} L_{\mathbf{R}-\mathbf{R}'}^{\alpha\beta} \xi_{\mathbf{R}}{}^{\alpha} \xi_{\mathbf{R}'}{}^{\beta}.$$

It is important in what follows that the defecton velocity is much less than the speed of sound in the crystal and the lattice atoms have time to become adjusted to its motion. This means that the variables $\xi_{\mathbf{R}}{}^{\alpha}$ and $\dot{\xi}_{\mathbf{R}}{}^{\alpha}$ can be determined from the condition that the functional

$$H = \langle \Psi | \hat{H} | \Psi \rangle = \varepsilon_0 + T_0 + U_0 + \frac{\mu m}{2} \sum_{\mathbf{R}} \dot{\xi}_{\mathbf{R}}{}^{2} a_{\mathbf{R}}{}^{*} a_{\mathbf{R}}$$
$$+ \frac{1}{2}\sum_{\mathbf{R}\rho\alpha} \Lambda_{\rho}{}^{\alpha} \xi_{\mathbf{R}+\rho}^{\alpha} |a_{\mathbf{R}}|^2 + \frac{1}{2} A \sum_{\mathbf{R}\delta} (a_{\mathbf{R}+\delta} - a_{\mathbf{R}}) a_{\mathbf{R}}{}^{*}$$
$$+ \frac{1}{2}\sum_{\mathbf{R}\delta\alpha} A_{\delta}{}^{\alpha} (\xi_{\mathbf{R}}{}^{\alpha} - \xi_{\mathbf{R}+\delta}^{\alpha}) a_{\mathbf{R}}{}^{*} a_{\mathbf{R}+\delta}, \tag{10}$$

which plays the role of the Hamilton function, be a minimum with respect to the coordinates $\xi_{\mathbf{R}}{}^{\alpha}$ and the momenta $p_{\mathbf{R}}{}^{\alpha} = m(1 + \mu |a_{\mathbf{R}}|^2) \dot{\xi}_{\mathbf{R}}{}^{\alpha}$. To this end, we write down the Hamiltonian equation and, eliminating the variables $p_{\mathbf{R}}{}^{\alpha}$, we obtain the following system of equations for the displacements:

$$m \frac{\partial}{\partial t}\Big[(1 + \mu |a_{\mathbf{R}}|^2) \frac{\partial \xi_{\mathbf{R}}{}^{\alpha}}{\partial t}\Big] = \sum_{\mathbf{R}'\beta} L_{\mathbf{R}-\mathbf{R}'}^{\alpha\beta} \xi_{\mathbf{R}'}^{\beta}$$
$$+ \frac{1}{2}\sum_{\rho} \Lambda_{\rho}{}^{\alpha} |a_{\mathbf{R}+\rho}|^2 + \frac{1}{2}\sum_{\delta} A_{\delta}{}^{\alpha} (a_{\mathbf{R}}{}^{*} a_{\mathbf{R}+\delta} + a_{\mathbf{R}} a_{\mathbf{R}+\delta}^{*}). \tag{11}$$

Thus, it is necessary to solve simultaneously the systems of equations (9) and (11). Since we shall be interested hereafter in deformations whose characteristic dimension is much larger than the lattice constant, it is convenient to go over to the continual limit and regard the amplitudes $a_{\mathbf{R}}$ and atom displacements $\xi_{\mathbf{R}}{}^{\alpha}$ as functions of one continuous variable $\mathbf{r}$. Then Eqs. (9) and (11) take the form

$$i\hbar \frac{\partial a}{\partial t} = \Big(\varepsilon_0 + T_0 + U_0 + \frac{\mu m}{2} \dot{\xi}^2 + \sum_{\alpha} \Lambda^{\alpha} \frac{\partial \xi^{\alpha}}{\partial r_{\alpha}}\Big) a$$
$$+ \frac{1}{2}\sum_{\alpha} A_{\alpha}{}^{\alpha} \frac{\partial^2 a}{\partial r_{\alpha}{}^2} + \sum_{\alpha} A^{\alpha} \frac{\partial \xi^{\alpha}}{\partial r_{\alpha}} a, \tag{12}$$

$$m \frac{\partial}{\partial t}\Big[(1 + \mu |a|^2) \frac{\partial \xi^{\alpha}}{\partial t}\Big] = \sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \frac{\partial^2 \xi^{\beta}}{\partial r_{\gamma} \partial r_{\delta}} + (\Lambda^{\alpha} + A^{\alpha}) \frac{\partial |a|^2}{\partial r_{\alpha}}, \tag{13}$$

where

$$T_0 = \frac{m}{2}\int \dot{\xi}^2 d\mathbf{r}, \quad U_0 = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \int C_{\alpha\beta\gamma\delta} u_{\alpha\beta} u_{\gamma\delta} d\mathbf{r},$$
$$u_{\alpha\beta} = \frac{1}{2}\Big(\frac{\partial \xi^{\alpha}}{\partial r_{\beta}} + \frac{\partial \xi^{\beta}}{\partial r_{\alpha}}\Big)$$

ONE-DIMENSIONAL CASE

We consider first a one-dimensional chain with a defect atom. (We note once more that one-dimensional defecton motion can result either from strong anisotropy of the crystal or from specific singularities of the motion of complexes made up of defects.[3]) In this case the fundamental equations (12) and (13) reduce to the following:

$$i\hbar \frac{\partial a}{\partial t} = \Big(\varepsilon_0 + T_0 + U_0 + \frac{\mu m}{2} \dot{\xi}^2 + \lambda \frac{\partial \xi}{\partial x}\Big) a + \frac{1}{2} A \frac{\partial^2 a}{\partial x^2}, \tag{14}$$

$$m \frac{\partial}{\partial t}\Big[(1 + \mu |a|^2) \frac{\partial \xi}{\partial t}\Big] = m s^2 \frac{\partial^2 \xi}{\partial x^2} + \lambda \frac{\partial |a|^2}{\partial x}, \tag{15}$$

where

$$T_0 = \frac{m}{2}\int \dot{\xi}^2 dx, \quad U_0 = \frac{m s^2}{2}\int \Big(\frac{\partial \xi}{\partial x}\Big)^2 dx,$$

$\lambda = A^1 + \Lambda^1$ and s is the speed of sound.

We are interested in solutions corresponding to the motion of the defecton and the deformation with constant velocity v. We therefore seek a solution in the form $\xi = \xi(x - vt)$, $|a|^2 = f(x - vt)$. A natural condition is also that the deformation vanish far from the defect. Integration of (15) then yields for the vector of the deformation $u = \partial \xi / \partial x$

$$u(x,t) = -\frac{\lambda}{m s^2 (1 - \beta^2)} \frac{|a(x,t)|^2}{1 - \mu\beta^2 |a|^2 / (1 - \beta^2)}, \quad \beta = \frac{v}{s}. \tag{16}$$

Substituting (16) in (14) we obtain for the amplitude $a(x,t)$ the following nonlinear integro-differential equation

$$i\hbar \frac{\partial a}{\partial t} = (\varepsilon_0 + T_0 + U_0) a - \frac{\lambda^2}{m s^2 (1 - \beta^2)} \frac{|a|^2}{1 - \mu\beta^2 |a|^2 / (1 - \beta^2)} a$$
$$+ \frac{1}{2} A \frac{\partial^2 a}{\partial x^2} + \frac{\mu \beta^2 \lambda^2}{2 m s^2 (1 - \beta^2)^2} \frac{|a|^4}{1 - \mu\beta^2 |a|^2 / (1 - \beta^2)} a. \tag{17}$$

If we denote by $\mathcal{L}$ the characteristic dimension of the deformation, then $|a|^2 \sim \mathcal{L}^{-1}$. Since this dimension is large compared with the lattice constant, we need retain in (17) only the first few powers in the expansion in $\mathcal{L}^{-1}$. Discarding terms of order $\mathcal{L}^{-3}$ and higher, we

obtain the Schrödinger nonlinear equation

$$i\hbar\frac{\partial a}{\partial t}=(\varepsilon_0+T_0+U_0)a-\frac{\lambda^2}{ms^2(1-\beta^2)}|a|^2a+\frac{1}{2}A\frac{\partial^2 a}{\partial x^2}. \qquad (18)$$

In this approximation, the deformation vector $u(x, t)$ is given by

$$u(x,t)=-\frac{\lambda}{ms^2(1-\beta^2)}|a(x,t)|^2.$$

This expression has a simple physical meaning – the deformation is proportional to the probabilistic distribution of the defecton over the lattice, and the proportionality coefficient is equal to the total change of the chain length. (This can be easily verified by integrating (16) with account taken of the fact that the amplitude $a(x, t)$ is normalized to unity.)

The solution of (18), normalized to unity and assuming a zero value at infinity, is of the form

$$a(x\ t)=\frac{1}{\sqrt{2\mathscr{L}}}\exp[i(kx-\varphi-\omega t)]\Big/\operatorname{ch}\left(\frac{x-x_0-vt}{\mathscr{L}}\right), \qquad (19)$$

where $k=\hbar v/A=m^*v/\hbar$ coincides with the wave vector of the free defecton, x_0 is the defecton coordinate, v is the defecton velocity, and the constant φ depends on the initial phase. The energy of the defecton connected with the deformation is

$$\hbar\omega=\varepsilon_0+\frac{\hbar^2v^2}{2A}-\frac{2}{3}\frac{A}{(2\mathscr{L}_0)^2}\frac{1-5\beta^2}{(1-\beta^2)^3},$$

and the dimension of the deformation is $2\mathscr{L}$, where $\mathscr{L}=\mathscr{L}_0(1-\beta^2)$, $\mathscr{L}_0=ms^2\epsilon/\lambda^2$, and ϵ is the width of the defecton band. The kinetic and potential energies are

$$T_0=\beta^2U_0,\quad U_0=\frac{\lambda^4}{6m^2s^4\varepsilon(1-\beta^2)^3}=\frac{A}{3\mathscr{L}^2(1-\beta^2)}.$$

The deformation around the defect is described by the formula

$$u(x,t)=\frac{\lambda^3}{4Am^2s^4(1-\beta^2)}\operatorname{sech}^2\left(\frac{x-x_0-vt}{\mathscr{L}}\right).$$

It moves together with the defecton with constant velocity and about a change of shape. It is interesting to note that the dimension and shape of the deformation depend on the velocity. Relations of similar kind were obtained earlier for crowdions in crystals.[6]

If the excitation energy is represented in the form of the sum of the rest E_0 and the kinetic energy K, then

$$E_0=\varepsilon_0-\frac{\varepsilon}{3(2\mathscr{L}_0)^2},\quad K=\frac{\hbar^2v^2}{2A}+\frac{A}{6\mathscr{L}_0^2}\frac{\beta^2(2+3\beta^2-\beta^4)}{(1-\beta^2)^3}.$$

We see thus that a bound state of the defecton is energywise more favored. If the excitation rate is small compared with the speed of sound, then the exitation moves along the chain like a particle with an effective mass

$$M^*=m^*+A/(3s^2\mathscr{L}_0^2),$$

that is close to the effective mass of the free defecton.[5]

The condition for the applicability of the continual approximation is the inequality

$$\lambda^2/\varepsilon ms^2\ll 1-\beta^2. \qquad (20)$$

We note that the free defecton cannot pass through regions where the potential varies over the lattice constant by more than the width of the energy gap. The condition (20) indicates that the defecton can move together with its own potential well whose variation over the lattice constant is much larger than the band width ($\Lambda^1\gg\epsilon$).

If $A<0$, which corresponds to a negative effective mass of the free defecton, the solution obtained above is unstable. In this case, however, there exist stable solutions in the short-wave part of the spectrum (which corresponds to the low-lying states). This can be easily seen if we seek the solution of the Schrödinger equation in the form

$$\Psi=\sum_n e^{i\varkappa n}a_nB_n^+|0\rangle$$

in place of (4).

If we retain in (17) also the terms of next order of smallness ($\propto\mathscr{L}^{-7/2}$) we obtain another linear equation

$$i\hbar\frac{\partial a}{\partial t}=(\varepsilon_0+T_0+U_0)a-\frac{\lambda^2}{ms^2(1-\beta^2)}|a|^2a+\frac{1}{2}A\frac{\partial^2 a}{\partial x^2}+\mu\frac{\lambda^2\beta^2}{2ms^2(1-\beta^2)^2}|a|^4a. \qquad (21)$$

As shown in [7], Eq. (21) also has soliton solutions. If $\mu>0$, corresponding to a heavy defect, the normalized solution of (21) can be written in the form

$$a(x,t)=\left(\frac{1}{2\mathscr{L}}\frac{\operatorname{tg}\eta}{\eta}\right)^{1/2}\exp[i(kx-\omega t-\varphi)]\left[1+\frac{1}{\cos\eta}\operatorname{ch}\left(\frac{x-x_0-vt}{L}\right)\right]^{-1},$$

$$k=\frac{\hbar v}{A},\quad \eta=\frac{\lambda\beta}{s(1-\beta^2)}\left(\frac{\mu}{3Am}\right)^{1/2},\quad L=\frac{Ams^2}{\lambda^2}(1-\beta^2)\frac{\eta}{\operatorname{tg}\eta}=\frac{1}{2}\mathscr{L}\frac{\eta}{\operatorname{tg}\eta},$$

$$\hbar\omega=\varepsilon_0+T_0+U_0+\frac{\hbar^2v^2}{2A}-\frac{\lambda^4}{8Am^2s^4(1-\beta^2)^2}\left(\frac{\operatorname{tg}\eta}{\eta}\right)^2\qquad T_0=\beta^2U_0,$$

$$U_0=\frac{\lambda^2}{4Lms^2(1-\beta^2)\eta^2}\left\{2\sin^2\frac{\eta}{2}-(\eta-\sin\eta)\operatorname{ctg}\eta\right.$$

$$\left.+\frac{\mu}{2L\eta}\frac{\beta^2}{1-\beta^2}[(\eta-\sin\eta)(1+3\operatorname{ctg}^2\eta)+\operatorname{tg}^2\frac{\eta}{2}((\eta+1)\sin^2\eta-1)]\right\}. \qquad (22)$$

If $\mu<0$, then η becomes imaginary and the solution of (21) is given by formulas (22), in which the trigonometric functions must be replaced by the corresponding hyperbolic ones.

We note that both the term $\sim a^5$ and all the remaining ones, which can appear when (16) is expanded further, contain an additional small parameter β^2. If η is small, meaning low velocities or small μ, the solution (22) goes over into (19).

THREE-DIMENSIONAL CASE

Consider an isotropic three-dimensional crystal with a defect. The initial equations (12) and (13) then take the form

$$i\hbar\frac{\partial a}{\partial t}=\left(\varepsilon_0+T_0+U_0+\frac{\mu m}{2}\dot{\xi}^2\right)a+\frac{1}{2}A\Delta a+\sum_\alpha(\Lambda^\alpha+A)\frac{\partial\xi_\alpha}{\partial r_\alpha}a, \qquad (23)$$

$$\frac{\partial}{\partial t}\left[(1+\mu|a|^2)\frac{\partial\xi^\alpha}{\partial t}\right]=s^2\Delta\xi^\alpha+\frac{\Lambda^\alpha+A}{m}\frac{\partial}{\partial r_\alpha}|a|^2, \qquad (24)$$

where

$$T_0=\frac{m}{2}\int\dot{\xi}^2\,dr,$$

$$U_0=\frac{c_1}{2}\sum_{\alpha\beta}\int\frac{\partial\xi^\alpha}{\partial r_\alpha}\frac{\partial\xi^\beta}{\partial r_\beta}dr+\frac{c_2}{2}\sum_{\alpha\beta}\int\frac{\partial\xi^\alpha}{\partial r_\beta}\frac{\partial\xi^\alpha}{\partial r_\beta}dr;$$

c_1 and c_2 are constants expressed in terms of the elastic moduli of the medium.

A direct solution of this system is difficult, and we shall use a different approach. We point out that in the one-dimensional case the kinetic energy is of the order of β^2 compared with the potential energy. Thus, to find the shape of the deformation it suffices to find the minimum of the functional (10) without taking the kinetic energy into account. We shall also disregard the change that the lattice deformation introduces into the probability amplitude of the defect transfer. It can be shown that in this case, too, the deformation is proportional to the probability of finding the defect in a given site. The functional (10) thus takes the form

$$U=\Lambda+\sum_{\mathbf{R}\delta}A_\delta a_{\mathbf{R}}^*a_{\mathbf{R}+\delta}-G\sum_{\mathbf{R}}(a_{\mathbf{R}}^*a_{\mathbf{R}})^2, \tag{25}$$

where G is a measure of the elastic energy. In analogy with the one-dimensional case, we seek the solution in the continual approximation in the form

$$a_{\mathbf{R}}=\varphi(\mathbf{R})e^{i\mathbf{k}\mathbf{R}}.$$

Substituting in (25), we get

$$U=\Lambda+\varepsilon(\mathbf{k})+\frac{A}{V_0}\int_{V_0}(\nabla\varphi)^2\,d\mathbf{R}-\frac{G}{V_0}\int_{V_0}\varphi^4\,d\mathbf{R},$$

where $\epsilon(\mathbf{k})$ is the dispersion law of the free defecton, V_0 is the crystal volume, and φ and $\nabla\varphi$ are assumed equal to zero on the boundary of the volume. For simplicity we assume that $V_0=V_\infty$. Then the normalization condition takes the form

$$\frac{1}{V_0}\int_{V_\infty}\varphi^2\,d\mathbf{R}=1. \tag{26}$$

We choose the trial function in the form of the spherically symmetrical function

$$\varphi(\mathbf{R})=\left(\frac{3}{\pi^3\mathcal{L}^3}\right)^{1/4}\operatorname{sech}\left(\frac{|\mathbf{R}-\mathbf{R}_0|}{\mathcal{L}}\right),$$

where $\mathcal{L}$ is the dimension of the deformation region and $\mathbf{R}_0$ is the radius vector of the defect. We define the function χ as follows:

$$\chi=\frac{U-\Lambda-\varepsilon(k)}{|A|}=\frac{1}{V_0}\int[(\nabla\varphi)^2-\varphi^4]\,d\mathbf{R}. \tag{27}$$

For a one-dimensional chain it takes the form

$$\chi_1=\frac{1}{3}\left[\operatorname{sign}A\,\mathcal{L}^{-2}-\frac{G}{|A|}\mathcal{L}^{-1}\right]. \tag{28}$$

Figure 1 shows a plot of the function χ_1 at $G/|A|=0.2$. If $A>0$, the minimum is reached at $\mathcal{L}_m=2A/G$. As already noted, for $A<0$ the solution is unstable and χ_1 has no minimum.

$$\chi_3=\operatorname{sign}A\,\frac{\pi^2+12}{3\pi^2}\frac{1}{\mathcal{L}^2}-\frac{2(\pi^2-6)}{\pi^3}\frac{G}{|A|}\frac{1}{\mathcal{L}^3}. \tag{29}$$

Figure 2 shows a plot of χ_3 for $G/|A|=130$. In contrast to the one-dimensional case, there is no minimum in the continual approximation at either $A>0$ or $A<0$. The function χ_3 becomes negative for the dimensions

$$1<\mathcal{L}<\frac{G}{\alpha|A|}\qquad\alpha=\frac{\pi^3}{6}\frac{\pi^2+12}{\pi^2-6}\sim 30$$

The continual approximation is valid then if $G/|A|\gg\alpha$. We shall show that the absence of a minimum is due to the use of the continual approximation. To this end we set up in lieu of (27) the function χ in the site representation:

$$\chi=\sum_{\mathbf{R}\delta}(a_{\mathbf{R}}^*a_{\mathbf{R}+\delta}-a_{\mathbf{R}}{}^0a_{\mathbf{R}}{}^0{}_{+\delta})-\frac{G}{|A|}\sum_{\mathbf{R}}|a_{\mathbf{R}}|^4, \tag{30}$$

where $a_{\mathbf{R}}{}^0=N^{-1/2}e^{i\mathbf{k}\mathbf{R}}$. With decreasing dimension $\mathcal{L}$ of the deformation, as $\mathcal{L}\to 1$, it is obvious that $U>\Lambda+\epsilon(\mathbf{k})$. We see thus that the function (30) should have a minimum outside the region of applicability of the continual approximation.

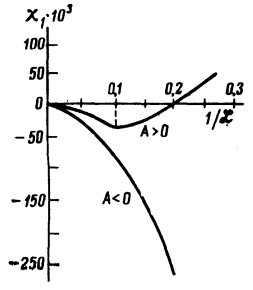

FIG. 1.

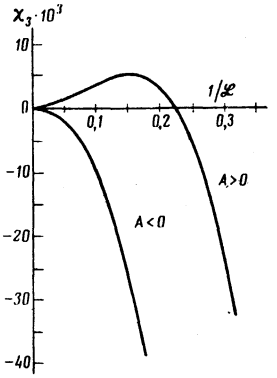

FIG. 2.

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Anisotropy of the scattering of conduction electrons by dislocations in aluminum

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The de Haas–van Alphen effect was used to measure the broadening Γ, due to electron scattering by dislocations, of the Landau levels of the electrons of the β and γ sections of the Fermi surface of aluminum. The dislocations were produced by uniaxial dilatation of the samples directly in the course of the measurements at 1.3 K, at a load $\sigma \parallel [111]$, and in a magnetic field $\mathbf{B} \parallel [1\bar{1}0]$. It was observed that Γ depends strongly on the position of the electron orbit on the Fermi surface and on the dislocation density. A ratio $\Gamma_\gamma/\Gamma_\beta = 3.5$ is obtained for dislocation densities $D \sim 10^8$, and decreases to 2 with increasing D. An increase in the areas S of the extremal sections of the Fermi surface is observed at the same time when the degree of uniaxial deformation $\Delta V/V$ is increased. The values of $\mu = -(3/2)(\Delta S/S)/(\Delta V/V)$ were measured and found to be 90 and 60 for the β and γ sections, respectively. These values of μ were used to calculate the anisotropy of the broadening of the Landau levels in accord with Watts' theory [Phys. Cond. Matt. 19, 125 (1975)]. The values obtained are in satisfactory agreement with the results of the direct measurements.

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1. INTRODUCTION

We have investigated the scattering of conduction electrons by dislocations in aluminum with the aid of a procedure based on the measurements of the amplitude of the de Haas–van Alphen effect, followed by calculation of the Dingle temperature[1] that characterizes the collision broadening Γ of the Landau levels. Particular attention was paid to the study of the relation between the Dingle temperature for electrons on different sections of the Fermi surface, a relation governed by the anisotropy of the scattering in momentum space.

In the case of electron scattering by point defects, the Dingle temperature χ_i and the (non-transport) electron collision frequency τ_i^{-1} in a zero magnetic field, averaged over the i-th electron orbit, are in essence equivalent characteristics of the scattering[1]:

$$X_i = \Gamma_i/\pi k = \hbar/2\pi k\tau_i. \tag{1}$$

The connection between the Dingle temperature and the characteristics of electron scattering by dislocations in a zero magnetic field has not yet been rigorously established. We shall therefore regard the measured Dingle temperature as an autonomous characteristic of the scattering, and use relation (1) to calculate the effective frequency of the collisions with the dislocations in a magnetic field when we compare the obtained data with the results of the investigation of scattering by other methods.

The dependence of the Dingle temperature on the electronic characteristics and on the parameters of the dislocation system was investigated theoretically in a number of papers.[4-10] This dependence is clearly seen from the Watts formula[7] calculated on the basis of the mechanism of "dephasing of the quantum oscillations":

$$X_i = \frac{\hbar e F_i^2}{kcm_c^i B} \begin{cases} \langle\mu\rangle_i^2 \overline{\epsilon^2}, & \xi_i = R_i^2 D \ll 1, \\ \langle\mu^2\rangle_i \overline{\epsilon^2} l/L_i, & \xi_i \gg 1, \end{cases} \tag{2}$$

where B is the magnetic field, D is the dislocation density, R is the Larmor radius, F is the oscillation frequency, $\epsilon = \Delta V/V$ is the change of the volume in the uniaxial deformation, l is the correlation length (see[7]), L is the length of the classical electron trajectory, and $\Delta F/F = -(2/3)\mu\epsilon$.

If we assume that $\overline{\epsilon^2} \sim D$ and $l \sim D^{-1/2}$ then, as seen from (2), $X \sim D^{1/2}$ in the case of large dislocation densities ($\xi \gg 1$) and $X \sim D/B$ in the case of small dislocation densities ($\xi \ll 1$). This agrees with the results of Vinokur,[8] who calculated the probability of the scattering of conduction electrons by dislocations in the Born approximation.

It should be noted that the quantities $\overline{\epsilon^2}$ and l in formulas (2) are not uniquely determined by the dislocation density D. Thus, for example, the formation of dislocation dipoles decreases $\overline{\epsilon^2}$, although the dislocation density may not change in this case. For this reason, and also because the existing experimental methods of determining the dislocation density are not accurate enough, the comparison of the experimental and theoretical dependences of the Dingle temperature on the dis-

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