commensurate ones.

We note that all our results were obtained in the self-consistent field approximation and we did not take phase fluctuations into account. In a purely one-dimensional system, such fluctuations are important; allowance for them jointly with consideration of commensurability effect is reported by Brazovskiĭ *et al.*[20] In quasi-one-dimensional compounds with sufficiently strong interaction of the CDW on different chains or in layered compounds, the phase fluctuations are not so important, especially far from the temperature at which the three-dimensional CDW structure appears.

We note in conclusion that our results can apparently be used not only for compounds with CDW, but also to other systems in which structural transitions to a non-commensurate phase are observed.[21]

In conclusion, we are deeply grateful to L. V. Keldysh, as well as to V. L. Ginzburg and to the participants of his seminar, for useful discussions.

[1)] Macmillan's analysis is in fact fully equivalent to Dzyaloshinskiĭ's earlier investigation of helicoidal magnetic structures.[12]

[2)] We note that a relation similar to that in Fig. 1 was observed numerous times in different systems; e.g.,[6].

[3)] Similar results are arrived at also by a consistent quantization procedure.[17]

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Continual theory of tunnel self-trapping

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A theory is developed for tunnel self-trapping of electrons (or of Frenkel excitons) as they interact with acoustic and nonpolar optical phonons. It is assumed that the electron-phonon interaction is strong enough, so that the size of the self-trapping barrier exceeds greatly the lattice constant and the continual theory can be used. It is shown that in these two cases the tunneling picture is entirely different. In the interaction with the optical phonons, the decisive contribution is made by quasiclassical trajectories with a spatial scale on the order of the barrier size. In interaction with acoustic phonons, on the contrary, the optimal trajectories have a scale much smaller than the barrier size. Explicit expressions for the transparency of the self-trapping barrier are obtained for both cases.

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A sufficiently strong electron-photon interaction produces in a crystal self-trapping of electrons (excitons) into states with scale dimensions equal to the lattice constant. They are called small-radius polarons, condensons, and polarizing or deforming excitons. The character of the resultant final states (for example, single-site or quasimolecular formation) are determined mainly by quantum-chemical considerations and is practically independent of the type of the phonons with which the dominant interaction takes place. On the contrary, the process of formation of a self-trapped state from a band state is decisively affected by the type of the electron-phonon interaction. Thus, for example, in a polarization interaction with optical phonons the self-trapping, i.e., the transition to the polaron state, always takes place without a barrier.[1] On the contrary, if

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short-range interactions predominate, then the self-trapping usually entails the surmounting of the potential barrier that separates the self-consistent band and self-trapped states.[2] At low temperatures, the self-trapping barrier is overcome by tunneling. We have here an analogy with quantum formation of the embryos of low-temperature phase transitions,[3,4] the only important difference being that in the self-trapping process the tunneling of the nuclei is accompanied by complete restructuring of the electron ψ function—from a band function to a localized function.

We calculate below the exponents for tunnel self-trapping of electrons and of Frenkel excitons when they interact with acoustic and with nonpolar optical phonons. We confine ourselves to situations in which the tunneling can be described within the framework of continual models.

1. QUALITATIVE ANALYSIS

The main feature of the energy spectrum of electrons (or excitons) that interact strongly with acoustic or nonpolar optical oscillations is the possible existence of free (band) and self-trapped states. One of us has shown[2] that for all the short-range interactions both types of solutions (both band and self-trapping) are in a rigorous sense self-consistent solutions (unlike the case of long-range polarization optical interactions). There is therefore, generally speaking, no alternative between the formation of band and self-trapping states, i.e., they can exist simultaneously. Recent experiments on the coexistence of free and self-trapped excitons in noble gases,[5-7] in iodides of alkali metals,[8,9] and in some other crystals[10] agree fully with this statement.

To compare the competing quantities, we write down the quantities with dimension of energy (E_B, ω_D, C, and $\rho s^2 v$) that are involved in the theory of electron-phonon interaction, and confine ourselves for concreteness to the case of interaction with acoustic phonons.

Here E_B is the width of the conduction band, C is the deformation potential, ω_D is the phonon Debye frequency, s is the speed of sound, and v is the volume per atom. The last two energies are in fact usually encountered as the combination $E_{FC} \approx C^2/2s^2v$ corresponding to the Franck-Condon energy, i.e., to a lowering of the energy of the system (compared with the centroid of the electron spectrum) when the electron is self-trapped. It is also convenient, following[11], to introduce the dimensionless parameters

$$\Lambda \approx E_{FC} \Big/ \left(\frac{E_B}{2}\right), \quad \lambda \approx E_{FC}\omega_D \Big/ \left(\frac{E_B}{2}\right)^2.$$

The condition for the coexistence of free and self-trapped states consists mainly in the requirement that the electrons by "light": $E_B \gg \omega_D$.[2] In addition, for self-trapped states to be formed the electron-phonon coupling must be strong enough: $\Lambda \gtrsim 1$ (for details see Refs. 12, 2, 13–15). An estimate of Λ in terms of the fundamental constants yields $\Lambda \sim 1$, so that the conditions for self-trapping should on the whole be favorable. The average electron range in the free state can be large. Indeed, the level width $\Delta\epsilon$ connected with the spontaneous phonon emission is $\Delta\epsilon/\epsilon \sim \lambda \sim \Lambda\omega_D/E_B$, where ϵ is the electron energy. We see that at $\Lambda \sim 1$ the parameter λ can be small in terms of the usual adiabatic parameter $\omega_D/E_B \sim (m/M)^{1/2}$.

Perfectly analogous arguments can be advanced for the interaction with nonpolar optical vibrations; in this case $E_{FC} = \gamma^2\omega_0$, where ω_0 is the vibrational frequency and γ is the dimensionless coupling constant.

The energy diagram is shown in Fig. 1. It contains the total energy $U(Q)$ of the system when the nuclei are at rest as a function of the configuration coordinate Q that describes the lattice deformation. Curves 1 and 2 correspond to the adiabatic potentials of the nuclei under conditions when the electron is on a lower discrete level. It is seen that the discrete level can arise at a finite (curve 1) or infinitesimally small (curve 2) deformation energy. In either case, however, the potential barrier remains finite. Its minimal value $W \sim E_B/\Lambda^2$[11] corresponds to a saddle on the $U(Q)$ surface. We emphasize that the existence of the barrier W (the self-trapping barrier) is peculiar to the relaxation from band states.

Let us examine the nonradiative relaxation of a system at $T = 0$ from a band state to a self-trapping state. If $W \gg \omega_0/2$, then the bottleneck is the system tunneling, shown by the wavy line in Fig. 1; the subsequent cascade process of vibrational relaxation along the curve 1 will be relatively faster. This is precisely the situation that will be considered below. On the contrary, at $W \lesssim \omega_0/2$ the probability of the first stage is high and the limit is imposed by the second stage of the relaxation.

The rate of the vibrational relaxation was already estimated in several papers.[16,17] The probability of tunneling through the self-trapping barrier has not yet been calculated, and sometimes sight is lost of the very fact that such a barrier exists. Yet in a number of cases it is precisely the tunneling probability which should govern the self-trapping rate.

If $W \gg \omega_0/2$ (i.e., $\Lambda\lambda \ll 1$), then we can use the quasiclassical approximation for the description of the tunneling of the nuclear subsystem. On the contrary, the electron motion must be described by quantum theory, since the electron is constantly in the lower state and the very existence of the self-trapping barrier is entirely connected with the kinetic energy of the electron.

There is also the question of the errors introduced by the use of adiabatic potentials in region where the adi-

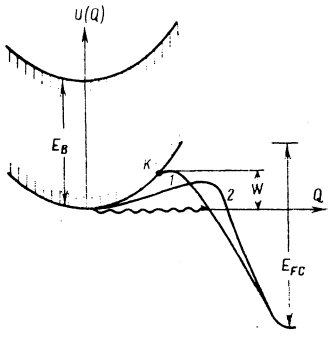

FIG. 1.

abatic approximation is not valid, namely to the left of the point K, and also near K on curve 1 of Fig. 1. It is, however, easily seen that the quasiclassical integral over the region to the left of K coincides exactly with $|\Psi|^2$ for the configuration K, i.e., with the quantum-mechanical probability of the nuclear configuration at which the local level is produced for the electron; Ψ is the nuclear wave function. The nonadiabaticity influences therefore only the pre-exponential factor, which we shall not calculate, and does not change the argument of the exponential.

The last question to be discussed here concerns the feasibility in practice of determining the adiabatic potentials, which we must have to calculate the quasiclassical integrals. The point is that self-trapped states (condensons, deforming excitons) have a spatial scale on the order of the lattice constant[1)], as established in the initial paper of Deĭgen and Pekar.[12] Yet the characteristic spatial scale of the barrier is $r_0 \sim \Lambda d$, where d is the lattice constant. In the case of strong coupling, the barrier can therefore be described in the macroscopic approximation,[19] and this uncovers definite possibilities of developing also a macroscopic theory for the rates of tunnel self-trapping.[2)] According to the results of Fugol' and Tarasova,[20] the case $\Lambda \gg 1$ is apparently realized in light inert gases.

2. FUNDAMENTAL EQUATIONS

Naturally, $U(Q) \geq 0$ along the entire tunneling path. Since we are dealing with a classically forbidden region of Q, we introduce, as usual, the imaginary time $\tau = it$ and change to imaginary action $S \to iS$. In this notation, the quasiclassical representation of the phonon wave function (with the electron in the ground quantum state) takes the form[3,4]

$$\Psi = e^{-S}, \tag{1}$$

where S is the extremal action:

$$S = \min \int L\, d\tau, \quad L = \frac{1}{2}\sum_q \dot{Q}_q \dot{Q}_{-q} + U(Q), \tag{2}$$

Q_q are the normal coordinates, $\dot{Q}_q = dQ_q/d\tau$, and L is the Lagrange function with imaginary time and corresponds to classical motion with potential energy $-U(Q)$. In the case of tunneling with a total energy $\mathcal{E} = 0$ (cf. Fig. 1), the two terms in L are equal and

$$S = \min \int \sum_q \dot{Q}_q \dot{Q}_{-q}\, d\tau. \tag{3}$$

The minimization is over all the phonon trajectories with $\mathcal{E} = 0$ joining the free state with one of the states on the surface $U(Q) = 0$ to the right of the barrier. It is subsequently necessary to minimize S over the finite states and to separate those states that make the decisive contribution to the tunneling. Eliminating now the first term of L, we obtain the Maupertuis principle:

$$S = \min \int 2U\, d\tau = \min \int (2U)^{1/2}\, ds, \quad ds^2 = \sum_q dQ_q\, dQ_{-q}. \tag{4}$$

The phonon Lagrange function that includes the electron-phonon interaction is

$$L = \frac{1}{2}\sum_q \dot{Q}_q \dot{Q}_{-q} + \frac{1}{2}\sum_q \omega_q^2 Q_q Q_{-q} + \min_\psi \int \left\{ \frac{1}{2} |\nabla\psi|^2 + \sum_q \Gamma_q Q_q e^{iqr} |\psi|^2 \right\} dr; \tag{5}$$

it is assumed that the normalization condition $\|\psi\| = 1$ is satisfied. The integral term in (5) is the energy $E(Q)$ of the electron at a fixed lattice deformation.

For acoustic phonons we have $\omega_q = sq$ and $\Gamma_q = Cq/(\rho V)^{1/2}$, where ρ is the density. Introduction of the dimensionless variables

$$r \to \frac{mC^2}{\rho s^2} r, \quad \tau \to \frac{mC^2}{\rho s^3}\tau, \quad Q_q \to \frac{Q_q}{(ms^2)^{1/2}} \tag{6}$$

transforms the Lagrange function into $L = g_A \mathcal{L}$, where $g_A = \rho^2 s^4/m^3 C^4$. The dimensionless Lagrange function $\mathcal{L}$ takes in the coordinate representation the form

$$\mathcal{L} = \frac{1}{2}\int \left(\frac{\partial Q}{\partial \tau}\right)^2 dr + \frac{1}{2}\int (\operatorname{div} Q)^2\, dr + \min_\psi \int \left\{ \frac{1}{2} |\nabla\psi|^2 + \operatorname{div} Q |\psi|^2 \right\} dr. \tag{7}$$

In the same notation,

$$S = \sigma_A \mathcal{L}, \quad \sigma_A = \rho s/m^2 C^2. \tag{8}$$

For optical phonons $\omega_q = \omega_0$ and $\Gamma_q = \gamma\omega_0 (2\omega_0 v/V)^{1/2}$. The transformations

$$r \to 2m\omega_0 v\gamma^2 r, \quad \tau \to \frac{\tau}{\omega_0}, \quad Q_q \to \frac{Q_q}{2m^{3/2} v\omega_0^2 \gamma^2} \tag{9}$$

lead to the relation $L = g_O \mathcal{L}$, where $g_O = (4m^3 v^2 \omega_0^2 \gamma^4)^{-1}$ and the dimensionless Lagrange function is

$$\mathcal{L} = \frac{1}{2}\int \left(\frac{\partial Q}{\partial \tau}\right)^2 dr + \frac{1}{2}\int Q^2(r)\, dr + \min_\psi \int \left\{ \frac{1}{2} |\nabla\psi|^2 + Q(r) |\psi|^2 \right\} dr. \tag{10}$$

The action is transformed into

$$S = \sigma_O \mathcal{L}, \quad \sigma_O = 1/4m^3 v^2 \omega_0^3 \gamma^4. \tag{11}$$

The formulas for g_A and G_O determine the scale of the barrier W. In both cases $W \sim E_B/\Lambda^2$ in accord with[11]. At the same time, σ_A and σ_O determine the scale of the action, for which we obtain different estimates in these cases:

$$\sigma_A \sim \frac{1}{\lambda} \sim \Lambda \frac{W}{\omega_0}, \quad \sigma_O \sim \frac{1}{\lambda\Lambda} \sim \frac{W}{\omega_0}. \tag{12}$$

To determine the numerical coefficients in σ_A and σ_O we must find the optimal trajectories $Q_q(\tau)$. Recognizing the difficulty of this problem and the need for using variational methods we investigate this problem by two different methods and compare the results.

3. TWO-PARAMETER APPROXIMATION

We limit the class of trajectories in Q space to spherically symmetrical wells with Gaussian profiles:

$$\operatorname{div} \mathbf{Q}(\mathbf{r}) = -Qe^{-\beta r^2}, \quad Q(\mathbf{r}) = -Qe^{-\beta r^2} \tag{13}$$

for acoustic and optical phonons, respectively. Then the trajectory in Q space is determined by the relations $Q = Q(\tau)$ and $\beta = \beta(\tau)$. The lattice deformation energy is

$$U_{\text{def}} = \frac{1}{2}\sum_{\mathbf{q}} \omega_{\mathbf{q}}^2 Q_{\mathbf{q}} Q_{-\mathbf{q}} = \frac{Q^2}{2}\left(\frac{\pi}{2\beta}\right)^3 \tag{14}$$

We calculate the electron energy in the field of the deformed lattice by means of the variational function $\psi \propto \exp(-\alpha r^2)$:

$$E(Q\beta|\alpha) = \frac{3}{2}\alpha - Q\left(\frac{2\alpha}{\beta+2\alpha}\right)^{3/2} \tag{15}$$

The condition $E'_\alpha = 0$ for the determination of α reduces to

$$Q\frac{(2\alpha)^{1/2}2\beta}{(\beta+2\alpha)^{5/2}} = 1. \tag{16}$$

Since this equation is easy to solve for Q, it is convenient to eliminate Q and operate in the subsequent examination of the region $E < 0$, in which the electron has a local level, not on the $Q\beta$ plane but on the $\alpha\beta$ plane.

The localization line, i.e., the boundary between the region of the free motion and the localization region, is determined by the condition $E = 0$, which reduces when account is taken of (16) to

$$\beta = 4\alpha. \tag{17}$$

The right-hand boundary of the tunneling region is determined by the condition $U = U_{\text{def}} + E = 0$, or, taking (16) into account

$$\frac{1}{16}\left(\frac{\pi\beta}{2}\right)^{3/2}\frac{(\beta+2\alpha)^5}{\alpha\beta^3} = \frac{\alpha}{2}\left(4\frac{\alpha}{\beta} - 1\right). \tag{18}$$

A plot of $\beta = \beta(\alpha)$ as described by this equation is shown in Fig. 2. The minimum of the curve corresponds to

$$\beta_{\min} = (3/2)^6\pi^3/2 \approx 397.$$

The left-hand branch moves slowly away from the line $\beta = 4\alpha$, and its slope $\beta/\alpha \to 4$. The right-hand branch is given by $\beta \propto \alpha^{4/3}$. It is obvious that a direct meaning is possessed only by that part of the $\alpha\beta$ plane which lies to the right of the line $\beta = 4\alpha$. In the region of the free states we must operate with the original variables $Q\beta$, and the mapping of the trajectory sections corresponding to free motion on the $\alpha\beta$ plane is purely arbitrary.

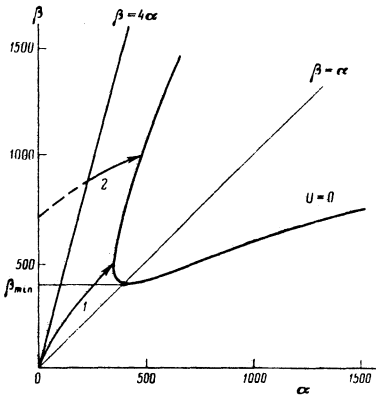

FIG. 2. Diagram, on a $\alpha\beta$ plane, corresponding to the two-parameter approximation. The line $\beta = 4\alpha$ corresponds to the instant when a local level appears for the electron (the localization line). The entire region to the right of this line is the localization region. The region to the left corresponds arbitrarily to the region of the free motion of the electron. The curve $U = 0$ is the locus of the end points for the trajectories corresponding to transitions into the self-trapping states.

To calculate the action in accord with formula (4) we must express the length element ds in terms of the variables $Q\beta$ and $\alpha\beta$. This is easily done by using (13). Without writing out the rather cumbersome resultant equations, we note that they are different for acoustic and optical phonons. Accordingly, the optimal trajectories are also different, and we therefore consider these cases separately.

1. Acoustic phonons

We consider first trajectories of type 1 (Fig. 1) that extend entirely over the region of the trapped states. For example, on the straight-line trajectories we have $ds \propto \beta^{-5/4}d\beta$ and $U^{1/2} \propto \beta^{1/4}$ (at small $\beta \ll \beta_{\min}$), and therefore the integral (4) diverges logarithmically at small β. The same holds for all trajectories of type 1; they are therefore ineffective.

We consider now trajectories of type 2 (Fig. 2), on which the localization sets in only at finite β. On these trajectories the integral consists of two contributions: over the free region and over the localization region. In the free region for the acoustic phonons with $\omega_{\mathbf{q}} = q$, all $\mathbf{Q}_{\mathbf{q}}(\tau) = \mathbf{Q}_{\mathbf{q}}e^{iq\tau}$. Considering the trajectories that start at $\tau = -\infty$ with $\mathbf{Q}_{\mathbf{q}}(-\infty) = 0$ and at $\tau = 0$, we get

$$\mathcal{S}_{\text{free}} = \min\int_{-\infty}^{0}\sum_{\mathbf{q}}\dot{\mathbf{Q}}_{\mathbf{q}}(\tau)\dot{\mathbf{Q}}_{-\mathbf{q}}(\tau)\,d\tau = \frac{1}{2}\min\sum_{\mathbf{q}} q\mathbf{Q}_{\mathbf{q}}\mathbf{Q}_{-\mathbf{q}}. \tag{19}$$

The minimum must be calculated subject to the additional condition that the deformation $\{\mathbf{Q}_{\mathbf{q}}\}$ lie on the localization line ($e = 0$). The Schrödinger equation that follows for ψ from (7) admits on the localization line of the group $\mathbf{r} \to \lambda\mathbf{r}$, $\mathbf{Q} \to \mathbf{Q}/\lambda$. Under this transformation, $\mathbf{Q}_{\mathbf{q}} \to \lambda^{1/2}\mathbf{Q}_{\mathbf{q}}$. Therefore $\mathcal{S}_{\text{free}}$ is invariant according to (19) and is determined exclusively by the functional form $\mathbf{Q}(r)$. If the Gaussian approximation (13) is used, $\mathcal{S}_{\text{free}} = 1.5^5\pi/8$. Since $\mathcal{S}_{\text{free}}$ does not depend on β, the optimal trajectory is determined by the contribution

from the localization region. Calculating in this region the integral (4) over the horizontal segments between the line $\beta = 4\alpha$ and the curve $U = 0$, we obtain $S_{loc} \approx 50\,\beta^{-1/2}$ at $\beta \gg \beta_{min}$. Thus, the contribution from the free region to the action predominates, and the transparency is maximal at $\beta \gg \beta_{min}$, with $S \lesssim 3.0$.

These calculations lead to interesting conclusions. The tunnel self-trapping is effected predominantly not over the scales Λd corresponding to the spatial dimension of the self-trapping barrier with minimal height (near the saddle point), but over scales $r \ll \Lambda d$. Since we have used from the very outset the continual approximation, we must confine ourselves to consideration of the region $d \ll r \ll \Lambda d$. In this entire region the action is approximately the same, and it corresponds therefore in principle to a large phase space and to a large preexponential factor. Unfortunately, the dimension of the region is substantially contracted by the large numerical factor $\beta_{min}^{1/2} \approx 20$, and we therefore write out here specially the criterion for the existence of such a region: $mC^2 \gg 20\rho s^2 d$.

Since the lower edge of the tunneling region corresponds to microscopic dimensions, the sign of the corrections to the continual theory assumes a significant role. If the corrections decrease the barrier transparency, then the results remain in force. But if they increase the transparency, then tunneling over microscopic scales $r \sim d$ becomes predominant and the results provide only an upper limit for S.

2. Optical phonons

In this case $ds \propto \beta^{-3/4} d\beta$ on the trajectories of type 1 (Fig. 2) and the integral diverges. For the class of straight-line trajectories, the minimum of S is reached at $\beta = 2\alpha$, and then $S \approx 438$. The competing trajectories are of type 2. On the free segment $S_{free} = \frac{1}{4} 1.5^5 (\pi/2)^{3/2} \beta^{1/2} \approx 3.74 \beta^{1/2}$, and in the localization region S decreases with increasing β, and integration over the horizontal segments leads to $S_{loc} \to 50$ as $\beta \to \infty$. The optimum $S \approx 187$ is reached at $\beta_{opt}^{1/2} \approx 26$, and the integrals over the free-motion and localization regions make approximately equal contributions. Since this number is markedly lower than that obtained for the ray trajectories, we give preference to trajectories of type 2.

Thus, optical phonons tunnel via configurations that have symbolically a spatial scale $r_{tun} \sim \Lambda d$. Numerically, however, the scale is smaller since β_{opt} is large. Thus, for example $r_{tun} \approx r_0/5$, where r_0 is the radius of the electron wave function for configurations near the saddle point.[19,21]

4. ELIMINATION OF PHONON COORDINATES

The approach described in the preceding section explains clearly the difference between the tunneling in interaction with acoustic and optical phonons, and describes the character of the optimal trajectories. A more consistent and general formalism, however, is obtained by a different approach, based on the fact that the phonon variables enter the Lagrangian (5) only quadratically and linearly. Therefore the problem can be solved exactly in terms of the phonon variables and these variables can be eliminated. The problem then reduces to variation of the action, which depends exclusively on $\psi(\mathbf{r}\tau)$. This way corresponds fully to the general formalism of polaron theory, where the determination of the stationary states reduces to variation of the known functional $J[\psi]$.[1]

We shall consider the cases of acoustic and optical phonons separately.

1. Acoustic phonons

According to (27) and (7)

$$\mathcal{S} = \min_{\psi Q} \int \left\{ \frac{1}{2} \left(\frac{\partial \mathbf{Q}}{\partial \tau} \right)^2 + \frac{1}{2} (\operatorname{div} \mathbf{Q})^2 + \frac{1}{2} |\nabla \psi|^2 + |\psi|^2 \operatorname{div} \mathbf{Q} \right\} d\mathbf{r} d\tau. \tag{20}$$

We are interested in those trajectories with energy $\mathcal{E} = 0$ which begin at the point $\mathbf{Q} = 0$ at $\tau = -\infty$ (nonlocalized states) and end at $\tau = 0$ on the surface

$$U(Q) = \frac{1}{2} \int (\operatorname{div} \mathbf{Q})^2 d\mathbf{r} + \min_{\psi} \int \left\{ \frac{1}{2} |\nabla \psi|^2 + |\psi|^2 \operatorname{div} \mathbf{Q} \right\} d\mathbf{r} = 0. \tag{21}$$

From the energy conservation law

$$\mathcal{E} = \frac{1}{2} \int \left(\frac{\partial \mathbf{Q}}{\partial \tau} \right)^2 d\mathbf{r} + U(Q) = 0 \tag{22}$$

it follows that at the end point of the trajectory, corresponding to tunnel self-trapping we have $\partial \mathbf{Q}/\partial \tau = 0$.

Minimization of $\mathcal{S}$ with respect to $\mathbf{Q}$ yields Euler's equation:

$$\partial^2 \mathbf{Q}/\partial \tau^2 + \Delta \mathbf{Q} + \nabla |\psi|^2 = 0, \tag{23}$$

which must be solved under the conditions

$$\mathbf{Q}|_{\tau = -\infty} = 0, \quad \left. \frac{\partial \mathbf{Q}}{\partial \tau} \right|_{\tau = 0} = 0. \tag{24}$$

A solution satisfying the conditions (24) is

$$\mathbf{Q} = \nabla \int_{-\infty}^{\infty} G(\tau - \tau', \mathbf{r} - \mathbf{r}') |\psi(\mathbf{r}'\tau')|^2 d\mathbf{r}' d\tau', \tag{25}$$

where

$$G(\mathbf{r}\tau) = \int e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}') - i\omega(\tau - \tau')} \frac{1}{k^2 + \omega^2} \frac{d\mathbf{k}}{(2\pi)^3} \frac{d\omega}{2\pi} \tag{26}$$

is the Green's function of the four-dimensional Laplace

operator, and $|\psi|^2$ is continued in even fashion into the region $\tau > 0$.

Substituting (25) in (20), using (23), and extending the integration with respect to τ to $+\infty$, we obtain the functional

$$\mathcal{S} = \frac{1}{2}\min_{\psi}\int\left\{\frac{1}{2}|\nabla_r\psi(R)|^2 + \frac{1}{2}|\psi(R)|^2\Delta_r\int G(R-R')|\psi(R')|^2 d^4R'\right\}, \tag{27}$$

which depends exclusively on $\psi(R)$; here $R = \mathbf{r}\tau$. From (27) follows Euler's equation

$$-\frac{1}{2}\Delta_r\psi + \psi\Delta_r\int G(R-R')|\psi(R')|^2 d^4R' = E(\tau)\psi(R). \tag{28}$$

Since the second term on the left is equal to $\psi\,\mathrm{div}\,\mathbf{Q}[\psi]$, according to (25) it follows that $E(\tau)$ is the electron level for the deformation $\mathbf{Q}(\mathbf{r}\tau)$.

According to (26), the Green's function $G(R)$ is a homogeneous function of R of degree -2. This yields a sort of "virtual theorem" for the action. Introducing the trial function $\chi = \varkappa^{3/2}\psi(\varkappa\mathbf{r}, \varkappa\tau)$, where $\psi(\mathbf{r}\tau)$ is the extremal of $\mathcal{S}$, and differentiating $\mathcal{S}$ with respect to $\varkappa$, we get

$$\frac{d\mathcal{S}[\chi]}{d\varkappa}\Big|_{\varkappa=1} = \frac{1}{2}\int\psi^*(R)\left\{-\frac{1}{2}\Delta_r\psi(R) + \psi(R)\Delta_r\int G(R-R')|\psi(R')|^2 d^4R'\right\} d^4R = \frac{1}{2}\int_{-\infty}^{\infty} E(\tau)\,d\tau = 0. \tag{29}$$

Since $E(\tau)$ is the ground-state energy, it follows that $E(\tau) \leqslant 0$; in the free state $E = 0$, and in the localized one $E < 0$. This leads to a rigorous proof of the conclusion arrived at above (see Sec. 3) that the extremal trajectories have an almost free character: the time of passage through the localized states τ_0 tends asymptotically to zero on going to the exact extremal. But since the lattice velocity is finite, this means that localization sets in at infinitesimally small radii. Therefore the behavior of the system is singular as $\tau_0 \to 0$. An analysis of the limiting expression for the action at small τ_0 leads to the formula

$$\mathcal{S} = \min_{\psi}\left\{\frac{1}{2}\left(\int\frac{1}{2}|\nabla\psi(\mathbf{r})|^2 d\mathbf{r}\right)^2 \times\left[\int|\psi(\mathbf{r})|^2\Delta_r G(\mathbf{r}-\mathbf{r}', 0)|\psi(\mathbf{r}')|^2 d\mathbf{r}d\mathbf{r}'\right]^{-1}\right\}; \tag{30}$$

Here $\psi(\mathbf{r}) = \psi(\mathbf{r}, \tau = 0)$. Its derivation is given in the Appendix.

It is remarkable that expression (30) depends only on the functional form of ψ at $\tau = 0$ (i.e., in the localized state) and does not change when it undergoes a scale transformation. This agrees with the results of Sec. 3 and with the fact that we calculate the limit as the spatial and temporal localization scales tend to zero. The physical meaning that can be ascribed to this limit has already been discussed in Sec. 3.

Substituting in (30) of the trial function $\psi \propto \exp(-\alpha r^2)$ leads to $\mathcal{S} = 9\pi^2/32 \approx 2.78$, which refines somewhat the result of Sec. 3.

2. Optical phonons

The initial formulas differ from the case of acoustic phonons only in that div $\mathbf{Q}(\mathbf{r})$ is replaced by $Q(\mathbf{r})$ in (20) and (21). The Euler equation for the displacements

$$\partial^2 Q/\partial\tau^2 - Q - |\psi|^2 = 0 \tag{31}$$

should be solved with boundary conditions analogous to (24). Its solution is

$$Q(\mathbf{r}\tau) = \int_{-\infty}^{\infty} G(\tau-\tau')|\psi(\mathbf{r}\tau')|^2 d\tau', \quad G(\tau-\tau') = -\int_{-\infty}^{\infty}\frac{e^{-i\omega(\tau-\tau')}}{1+\omega^2}\frac{d\omega}{2\pi}; \tag{32}$$

it is assumed that $|\psi|^2$ is continued in even fashion into the region $\tau > 0$.

After eliminating Q, the action is represented in the form of the functional

$$\mathcal{S} = \frac{1}{2}\min_{\psi}\int d\mathbf{r}\int_{-\infty}^{\infty}\left\{\frac{1}{2}|\nabla_r\psi(\mathbf{r}\tau)|^2 + \frac{1}{2}|\psi(\mathbf{r}\tau)|^2\int_{-\infty}^{\infty} G(\tau-\tau')|\psi(\mathbf{r}\tau')|^2 d\tau'\right\} d\tau, \tag{33}$$

whose variation yields the Euler equation for ψ:

$$-\frac{1}{2}\Delta\psi(\mathbf{r}\tau) + \psi(\mathbf{r}\tau)\int_{-\infty}^{\infty} G(\tau-\tau')|\psi(\mathbf{r}\tau')|^2 d\tau' = E(\tau)\psi(\mathbf{r}\tau). \tag{34}$$

The individual terms in (33) are homogeneous with respect to pure spatial transformations. This enables us to obtain a virial theorem by introducing the trial function $\chi = \varkappa^{3/2}\psi(\varkappa\mathbf{r}, \tau)$ and varying $\mathcal{S}$ with respect to $\varkappa$:

$$\frac{d\mathcal{S}[\chi]}{d\varkappa}\Big|_{\varkappa=1} = \int d\mathbf{r}\int_{-\infty}^{\infty}\left\{\frac{1}{2}|\nabla_r\psi|^2 + \frac{3}{4}|\psi(\mathbf{r}\tau)|^2\int_{-\infty}^{\infty} G(\tau-\tau')|\psi(\mathbf{r}\tau')|^2 d\tau'\right\} d\tau = 0. \tag{35}$$

Subtracting (35) from (33) and using (34), we get

$$\mathcal{S} = -\int_{-\infty}^{0} E(\tau)\,d\tau. \tag{36}$$

It is seen from (36) that tunneling through the region $E < 0$ occupies a finite time interval, in accord with the

conclusions of Sec. 3.

Before we proceed to the approximate determination of $\mathcal{S}$, we make the following remark. If the problem is rigorously formulated, the condition (21) does not change the extremal trajectories, and merely selects the ones that bring the system to definite final states; we have therefore determined the extremal trajectories above by simply varying $\mathcal{S}$. In the approximate solution of the problem, however, it is necessary to make especially sure that the trajectories land on the surface $U(Q)=0$. This is easiest to do by introducing a Lagrange multiplier, i.e., by defining the functional

$$\mathcal{S}_\lambda=\min_{\psi Q}\left\{\int dr\int_{-\infty}^{0}d\tau\left(\frac{1}{2}\left(\frac{\partial Q}{\partial\tau}\right)^2+\frac{1}{2}Q^2+\frac{1}{2}|\nabla\psi|^2+|\psi|^2Q\right)+\lambda\int dr\left(\frac{1}{2}Q^2+\frac{1}{2}|\nabla\psi|^2+|\psi|^2Q\right)_{\tau=0}\right\}, \tag{37}$$

and obtaining its minimum under the conditions

$$Q(\tau=-\infty)=0,\quad U(Q)|_{\tau=0}=0.$$

Variation with respect to Q at $\tau\neq 0$ leads to the Euler equation (31), and at $\tau=0$ to the boundary condition

$$\left[\frac{\partial Q}{\partial\tau}+\lambda(Q+|\psi|^2)\right]_{\tau=0}=0. \tag{38}$$

On going to the exact solution, $\lambda\to 0$ and (38) goes over into

$$(\partial Q/\partial\tau)|_{\tau=0}=0.$$

We define the trial function in the form

$$\psi(r\tau)=\begin{cases}\psi_0(r) & \text{if}\quad -\tau_0<\tau<0\\ V^{-1/2}\to 0 & \text{if}\quad \tau<-\tau_0.\end{cases} \tag{39}$$

The solution of (31) with the boundary condition (38) is then

$$Q(r\tau)=T(\tau)|\psi_0(r)|^2,$$
$$T(\tau)=-1+\frac{1}{2}\exp(-\tau-\tau_0)-\frac{\lambda-1}{2(\lambda+1)}\exp(\tau-\tau_0),\quad \tau>-\tau_0. \tag{40}$$

We determine the function ψ_0 from the condition that it satisfy (34) at $\tau=0$:

$$-{}^1/_2\Delta\psi_0+T(0)|\psi_0|^2\psi_0=E\psi_0. \tag{41}$$

At $T(0)<0$ Eq. (41) easily reduces to the standard equation investigated numerically by Zakharov, Sobolev, and Synakh.[21] The lowest eigenvalue is

$$E=-\frac{4}{T^2(0)}E_0,\quad E_0\approx 1.5^2\frac{\pi^2}{2}. \tag{42}$$

Using the virial theorem for Eq. (41)[3)]

$$\frac{1}{2}\int|\nabla\psi_0|^2dr=-\frac{3}{4}T(0)\int|\psi_0|^4dr \tag{43}$$

jointly with (40), we can express all the integrals in $\mathcal{S}$ and U in terms of T and E_0. As a result we arrive at the expressions

$$\mathcal{S}=E_0\min_{\tau_0}\left\{\frac{12}{T^2(0)}(\tau_0+\lambda)-\frac{8}{T^3(0)}\left(-\tau_0-\lambda+\frac{1}{2}+\frac{\lambda-1}{2(\lambda+1)}e^{-2\tau_0}\right)\right\} \tag{44}$$

$$U(\tau)=E_0\left\{\frac{12}{T^2(0)}-\frac{8}{T^3(0)}\left(\frac{1}{2}T^2(\tau)+T(\tau)\right)\right\}. \tag{45}$$

The equation $U(\tau=0)=0$, which defines λ, enables us to get $T(0)=-\frac{1}{2}$ and eliminate λ from (44) with the aid of (40). The result is

$$\mathcal{S}=16E_0\min_{\tau_0}\{3-\tau_0-4e^{-\tau_0}+2e^{-2\tau_0}\}. \tag{46}$$

This expression is meaningful only at τ_0 such that $U(\tau)\geq 0$, and the equality is reached only at $\tau=0$. It can be verified that this condition is satisfied only at $\tau_0\leq\ln 2$. Thus, in the class of trial functions, the minimum of the action is reached at $\tau_0=\ln 2$ and is equal to $\mathcal{S}=8(3-2\ln 2)E_0\approx 12.9E_0\approx 143$, which likewise improves the result of Sec. 3. The tunneling time in dimensional units is $\tau_0=\ln 2/\omega_0$, i.e., it is of the order of the reciprocal frequency of the optical phonon.

5. CONCLUSION

Thus, analysis of tunnel self trapping by two different methods leads to a single picture of the phenomena and to close values of the numerical parameters. The main conclusion reduce to the following. Although the very fact of coexistence of free and self-trapped states and the presence of the self-trapping barrier are common to electron (exciton) interactions with acoustic and nonpolar optical phonons, the pictures of the tunnel self-trapping are entirely different. For the optical phonons, the optimal quasiclassical trajectories pass over a spatial scale $\sim\Lambda d$ corresponding to the spatial extent of the minimum-height barrier. Therefore if the coupling force is strong enough ($\Lambda\gg 1$) the trajectories lie entirely in the region of applicability of the continual theory.

On the contrary, for acoustic phonons the action reaches a minimum on trajectories corresponding to tunneling in the region of asymptotically narrow barriers. It remains almost unchanged, however, in the scale region $r\ll\Lambda d$. Therefore the continual theory, which determines the contribution made to the transition probability from the region $d\ll r\ll\Lambda d$, yields either the total probability or its lower bound (see Sec. 3).

The barrier transparency can be characterized by the

quantity $D = e^{-2S}$. The final result takes a particularly simple form for optical phonons. Assuming the dimensionless barrier height $W = 4E_0$ that follows from the virial theorem[19] and using the formulas for σ_0 and g_0 (Sec. 2), we have ultimately

$$D_0 \approx \exp\left(-6.5\frac{W}{\omega_0}\right), \quad W \approx \frac{11.2}{m^3 v^2 \omega_0^2 \gamma^4}, \tag{47}$$

i.e., the transparency is expressed directly in terms of the barrier height and the phonon frequency. For acoustic phonons

$$D_A \approx \exp(-5.6\rho s/m^3 C^2). \tag{48}$$

In either case, refinement of the calculation of S should decrease the numerical factor in the exponent and hence increase the transparency.

The determination of D for noble gases is made difficult both by the simplification of the model (the excitons are in fact noticeably different there from Frenkel excitons[16a] and have a degenerate band) and by the fact that m and C are known for them only quite roughly. If we use nevertheless the parameter values $\rho \sim 1.5$ g/cm^3, $s \approx 10^5$ cm/sec, $m \approx 3\times 10^{-27}$ g, and $C \approx 2$ eV, which are close to the real ones, then we obtain the quite reasonable $\log D \approx -4$.

Analysis of the experimental data has led recently to the conclusion that in a number of crystal the trapping of carriers by some local levels is accompanied by a strong deformation of the lattice.[22,23] The method developed above can be applied also to this situation, provided only that the barrier lies in the macroscopic region.

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APPENDIX

DERIVATION OF FORMULA (30)

We define a class of trial functions in analogy with (39), with $\psi_0 = \psi_0(r/r_0)$, where ψ_0 is a normalized function with localization radius r_0 and is to be determined. Using the homogeneity of G, we obtain from (27) an expression for the action in the limit as $\tau \to 0$:

$$S = \frac{\tau_0}{r_0^2}\frac{1}{2}\int |\nabla_\xi \psi_0|^2 d\xi + \frac{1}{2}\left(\frac{\tau_0}{r_0^2}\right)^2 \int |\psi_0(\xi)|^2 \Delta_\xi G(\xi - \xi', 0)|\psi_0(\xi')|^2 d\xi d\xi'. \tag{A.1}$$

where $\xi = r/r_0$. Minimizing S with respect to $\lambda = \tau_0/r_0^2$ we get

$$\lambda = -\frac{1}{2}\int |\nabla_\xi \psi_0|^2 d\xi \left[\int |\psi_0(\xi)|^2 \Delta_\xi G(\xi - \xi', 0)|\psi_0(\xi')|^2 d\xi d\xi'\right]^{-1}. \tag{A.2}$$

Substitution of (A.2) into (A.1) leads directly to (30).

It remains to verify the satisfaction of the condition (21) when the trial function is so chosen. The Euler equation for the extremals of the functional (30) is

$$-\frac{1}{2}\Delta_\xi \psi + \lambda\psi \int \Delta_\xi G(\xi - \xi', 0)|\psi(\xi')|^2 d\xi' = 0, \tag{A.3}$$

with λ defined by (A.2). Comparison of (27) with (A.3) leads to $E(\tau = 0) = 0$. Substitution of (25) and (39) in (21) shows that in the limit as $\tau_0 \to 0$ and at constant $\lambda = \tau_0/r_0^2$ the first term is vanishingly small compared with the remaining two and can be omitted. The vanishing of the sum of the two remaining terms is ensured by the equality $E(\tau = 0) = 0$.

[1)] Provided only that nonlinearity and anharmonicity do not alter the results excessively.[18]

[2)] In this respect the picture recalls somewhat the quantum production of embryos near the lability point.

[3)] Analogous to the "1:2:3:4 theorem" in polaron theory.

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Temperature dependence of the electron specific heat and effective mass

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The temperature dependence of the electron specific heat is investigated. The Éliashberg method is used to obtain a general formula including the function $g(\omega)=\alpha^2(\omega)F(\omega)$ and the universal function $Z(T/\omega)$; an expression is found for $Z(x)$; this formula can be used to describe the nonmonotonic $C_e(T)$ dependence at all temperatures for an arbitrary electron-phonon interaction. Calculations are made for specific metals and the available experimental results are analyzed. The question of the temperature and carrier-density dependences of the mass is considered. An approximate method is suggested for obtaining information on the function $g(\omega)$.

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We shall consider the temperature dependence of the electron specific heat and effective mass. The electron–phonon interaction is known to affect considerably the characteristics of an electron system. The question of the renormalization of the electron mass associated with this interaction was investigated (for $T=0$) by Migdal.[1] The state of the phonon system varies with rising temperature. Excitation of thermal phonons results in temperature dependences of the electron characteristics. The temperature dependence of the effective mass has been observed in cyclotron resonance studies.[2-5] These studies have been carried out in the temperature range $T \lesssim 6°$ K, i.e., for $T \ll \omega_D$.

The electron–phonon interaction causes the temperature dependence of the electron specific heat to deviate from the simple linear law. This has been observed experimentally on several occasions.[6-9] Éliashberg[10] developed a method based on the exact expression for the thermodynamic potential. He obtained a general expression for the entropy and showed that allowance for the electron–phonon interaction results, in the $T\to 0$ limit, in an additional contribution $\Delta C_e(T) \propto T^3 \ln(\omega_D/T)$. The question of the temperature dependence of the electron specific heat $C_e(T)$ and effective mass $m^*(T)$ has also been investigated by others[11,12] (see also Grimvall's review [13]). Fradin[14] calculated analytically the dependence $C_e(T)/T$ throughout the temperature range in the Einstein model of the phonon spectrum. The asymptotic behavior of $C_e(T)$ in the limits $T\to 0$ and $T\to\infty$ was investigated by Masharov.[15] We shall use the Éliashberg method to obtain relationships which describe the dependence $C_e(T)$ throughout the investigated temperature range for an arbitrary electron–phonon interaction and we shall apply these relationships to some specific substances.

The influence of the phonon system on the electron characteristics is known to be described by the function $g(\omega)=\alpha^2(\omega)F(\omega)$ [$F(\omega)$ is the density of the phonon states and $\alpha^2(\omega)$ describes the electron–phonon interaction]. The function $g(\omega)$ can be determined with high accuracy by investigating superconductors using the tunnel spectroscopy methods and it is known for many metals (see Figs. 2 and 3 below).[16-18]

The deviation of the dependence $C_e(T)$ from linearity can be expressed directly in terms of the function $g(\omega)$ (see below). We shall use the available tunnel data to plot curves describing the behavior of the specific heat and mass in several metals. We shall compare the predicted behavior with the available experimental data.

We shall present the results in three sections. In the first section we shall consider the temperature dependence of the electron specific heat. We shall discuss the available experimental data, the question of the separation of the phonon contribution, etc. In the second section we shall deal with the problem of the temperature and carrier-density dependences of the effective mass. In the third section we shall consider the possibility of obtaining information on the function $\alpha^2(\omega)$ describing the electron–phonon interaction.

1. ELECTRON SPECIFIC HEAT

The electron–phonon interaction results in deviation of the temperature dependence of the electron specific heat from the simple linear law. As mentioned above, the $C_e(T)$ dependence has been considered in several papers.[11-13] We shall solve this problem in its general form for an arbitrary electron–phonon interaction constant for all temperatures.

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