Self-trapped electron and hole states

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The basic ideas and results of the theory of self-trapped electron and hole states are reviewed. The basic features of self-trapping as an important and quite general phenomenon as well as the basic types of self-trapped states (polarons, fluctuons, and electron pairs with a negative correlation energy) are studied. The characteristic features of self-trapping on defects in a crystal lattice, in disordered systems, and in amorphous structures are compared with self-trapping in regular crystals. Some pressing problems in the modern theory of self-trapped electron and hole states in solids are noted or briefly discussed.

CONTENTS

1. INTRODUCTION

The interaction of a charge carrier (electron or hole) with a medium is often strong and substantially changes its "bare," for example, Bloch, state in the undeformed medium. Thus the local deformation of the medium induced by the field of an electron can create a potential well, in which the electron is trapped; at the same time the electron follows adiabatically the slow changes in the deformation and, therefore, "feels" the instantaneous potential well, maintaining the stationary nature of the well and of the corresponding deformation of the medium with its field. Such a self-consistent, in the sense indicated, state of the electron is said to be self-trapped (ST)[1)]; it can be substantially more favorable energetically than the "bare" state. In an external electric field the self-trapped electron is subject to a force, which is transmitted to the medium and causes the translational motion of the electron, accompanied by a matched motion of the deformation of the medium. Such self-trapped electrons can be current carriers, determining the conductivity and other kinetic effects. The study of self-trapping phenomena, self-trapped quasiparticle states, and concomitant effects in condensed media (crystals, amorphous materials, some liquids, and even dense gases) now comprises a quite important part of the theory of solids and other condensed systems. The purpose of this paper is to review the basic ideas and results of this theory. In fact, self-trapped states of current carriers can be important in nonmetallic systems, primarily in semiconductors, and we shall be concerned with them below.

The phenomenon of self-trapping was predicted by Landau over 50 years ago (1933).[1] In his pioneering work he showed that an electron, strongly deforming the crystal lattice surrounding it, acquires in the instantaneous, local, potential well that is formed a discrete energy level below the bottom of the Bloch conduction band, and this level corresponds to the self-trapped state. Actually, the case of a short-range "local" potential of the deformed (three-dimensional) lattice was discussed, and it was shown qualitatively that the electron makes a transition into the self-trapped state by overcoming an energy barrier with a corresponding activation energy. Landau's concept was qualitatively extended to the case of a long-range local potential of the deformed lattice of an ionic crystal by Mott (1937) and others.[2,3] Pekar (1946) first developed a systematic theory of self-trapped states—polarons with a large radius, arising as a result of the

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strong long-range interaction of the electron with the polarization phonons in an ionic crystal.[4,5] In this case the transition into the self-trapped state occurs without overcoming a barrier, and the polarons must be the main current carriers.[5]

On the other hand, Frenkel' (1936)[6] predicted the possibility of a different type of self-trapping, which occurs without the overcoming of an energy barrier and in which the local deformation of the vibrating lattice follows the position of the quasiparticle, identified as an exciton with a small radius in the crystal (see also Ref. 7). It was first noted in Ref. 6 that in a regular crystal a self-trapped quasiparticle undergoes translational motion "as if it pulled a heavy load of atomic displacements," i.e., because of the inertia of the accompanying deformation of the lattice its effective mass is much larger than that of a free quasiparticle.

The general theoretical approach developed in Ref. 8 allowed the interpretation of both possible types of self-trapped states, predicted by Landau[1] and Frenkel',[2] as limiting cases of self-trapping for "light" wide-band ($D \gg \hbar\omega_{ph}$) and "heavy" narrow-band ($D \lesssim \hbar\omega_{ph}$) quasiparticles in the crystal; D is the width of the bare Bloch band in a perfect crystal and $\hbar\omega_{ph}$ is the characteristic energy of the phonons interacting with the electron (quasiparticle).

The formulation of the theory of the polaron as the problem of determining the spectrum of a nonrelativistic particle interacting with a boson (phonon) field led to the development of a number of general methods in the theory of self-trapped states (see Refs. 9–13). In this connection the term "polaron" became a synonym for the self-trapped state of an electron in a harmonic crystal lattice with a linear response of the medium (see Sec. 2 and, in part, Sec. 3). The characteristic features of self-trapped states on defects in a crystal lattice are discussed in Sec. 3 (see, for example, Ref. 14). Self-trapped states with large radius—fluctuons, arising in a disordered medium accompanying the nonlinear response of the medium, are studied in Sec. 4.[15,16] Another type of self-trapped, predominantly two-electron, state in amorphous systems is discussed in Sec. 5.[17,18] In all these sections and, as a rule, in the theory of self-trapped states in general, multielectronic correlations are assumed to be unimportant and are not explicitly taken into account; this apparently gives an adequate description of the real situation in the nonmetallic systems studied. Finally, some results, unsolved problems, and further possibilities for the theory of self-trapped states are discussed in the concluding section.

The theory of polarons in crystals is reviewed in Refs. 5, 13, and 19–22 and the theory of fluctuons is reviewed in Ref. 23 and 24–28. In this paper we review the present status of the theory of the basic models and types of self-trapped electron and hole states in solids—their common features and differences. The main attention is devoted to the general aspects of the theory of self-trapped current carriers, their conductivity, and related effects.[2)] In this connection, in comparing theory with experiment for the main types of self-trapped states only those experimental data which indicate more or less reliably the realizability of such states in solids are briefly noted in the corresponding sections. The list of references is unavoidably not exhaustive and is only representative.

2. SELF-TRAPPED STATES IN A REGULAR CRYSTAL

Self-trapped polaron states in a crystal, which are primarily discussed in this section, are actually determined by the linear response of the medium (linear coupling between the deformation and the field of the electron) in a harmonic lattice. On the other hand, self-trapped states in an antiferromagnetic crystal can be determined by the nonlinear response of the medium (see Sec. 2g).

a) Hamiltonian of the electron-phonon system

The simplest model is usually used to analyze the general properties of self-trapped polaron states in crystals: 1) the bare Bloch band of the current carrier is not degenerate and is isotropic with the dispersion law $\varepsilon(\mathbf{k}) \approx k^2/2m$ in the effective-mass (m) approximation, or

$$\varepsilon(\mathbf{k}) \approx -\tfrac{1}{2} D + J \sum_{g} \cos(\widehat{\mathbf{kg}})$$

with $D \approx 2zJ$ in the nearest-neighbor approximation (z) with a tunneling amplitude $J(g) \equiv J$, $|g| \approx a$ (the bottom of the band $(\varepsilon(\mathbf{k}))_{min} = 0$ is the zero reference point of the energy and a is the interatomic distance); 2) the interaction (electronic transitions) between the Bloch states of the conduction electrons and holes are not important for a sufficiently large energy gap E_g between the true, or effective, band edges; 3) the electron-phonon coupling is linear with respect to atomic displacements (q). (The effects of degeneracy and anisotropy of the bands are discussed in Sec. 2d and the interband interaction is discussed in Sec. 5a.) For the model under study the Hamiltonian of the electron-phonon system includes the kinetic energy operator of the electrons $\hat{K}_e$ the interelectronic interaction operator $\hat{U}_e$, the phonon-energy operator $\hat{\mathscr{H}}_{ph}$, and the electron-phonon interaction operator $\hat{\mathscr{H}}_{int}$ (see, for example, Refs. 5, 13, 21, and 24)[3)]:

$$\hat{\mathscr{H}} = \hat{K}_e + \hat{U}_e + \hat{\mathscr{H}}_{ph} + \hat{\mathscr{H}}_{int}, \tag{2.1}$$

where $\hat{\mathscr{H}}_{ph} = \Sigma_\lambda \omega_\lambda \hat{N}_\lambda$, $\hat{N}_\lambda \equiv b_\lambda^+ b_\lambda (\lambda \equiv \mathbf{f}, j)$, $\mathbf{f}$ is the quasimomentum, and $j = 1, 2, 3, \ldots$ is the number of the phonon branch. For typical semiconductors (Ge, A_3B_5, etc.) and ionic crystals (NaCl, etc.) with sufficiently large D (> 1 eV) the single-electron approximation, in which[5,9,13,19,21]

$$\hat{K}_e = \varepsilon(\mathbf{k}),\ \varepsilon(\mathbf{k}) \approx \frac{k^2}{2m} \quad \text{for} \quad |\mathbf{k}|a \ll \pi,\ \ \varepsilon(\mathbf{k}) \ll D, \tag{2.2}$$

$$\hat{\mathscr{H}}_{int} = N^{-1/2} \sum_{\lambda} w_\lambda q_\lambda \exp(i\mathbf{fR}) \quad \text{for} \quad \mathbf{R} \equiv \{\mathbf{r} \text{ or } \mathbf{l}\},$$

$$q_\lambda = b_\lambda + b_{-\lambda}^+; \tag{2.3}$$

is usually applicable, in the isotropic-continuum approximation (for $|\mathbf{k}|a \ll \pi$, $|\mathbf{f}|a \ll \pi$)

$$\hat{\mathscr{H}}_{int} = \int d\mathbf{r}'\, Z(\mathbf{r}, \mathbf{r}')\, \Delta_0(\mathbf{r}'), \tag{2.4}$$

$$\hat{\mathscr{H}}_{ph} = K_{ph} + \tfrac{1}{2} S_0 \int d\mathbf{r}\, \Delta_0^2(\mathbf{r}); \tag{2.5}$$

where N is the number of cells in the normalizing volume $V_0 \equiv N v_0$, $v_0 \equiv |g|^3 \approx a^3$ (or $v_0 \approx a^d$, $d = 3, 2, 1$). $\hat{K}_{ph}$ is the kinetic energy operator for the vibrations, $\Delta_0(\mathbf{r})$ is the defor-

mation field, S_0 is the deformation constant, and $Z(\mathbf{r}, \mathbf{r}')$ describes the coupling between the electrons ($\mathbf{r}$) and the continuum ($\mathbf{r}'$). In (2.3), as usual, we assume that the electron-phonon coupling constants w_λ are independent of the quasimomentum of the electron ($\mathbf{k}$), i.e., in the site ($\mathbf{l}$, $\mathbf{R} \equiv \mathbf{l} - \mathbf{l}' \approx g$) or coordinate ($\mathbf{r}$, $\mathbf{R} \equiv \mathbf{r} - \mathbf{r}'$) representations $w_\lambda(\mathbf{r}) \approx w_\lambda \delta(\mathbf{r})$ or $w_\lambda(\mathbf{l}) \approx w_\lambda \delta_{\mathbf{l},0}$. This approximation is adequate for evaluating the integrals appearing in the theory, containing, aside from $w_\lambda(\mathbf{r} - \mathbf{r}')$, the smooth functions $f(\mathbf{r}, \mathbf{r}')$, because $w_\lambda(\mathbf{r} - \mathbf{r}')$, just as $J(\mathbf{r} - \mathbf{r}')$, decays exponentially with increasing $|\mathbf{r} - \mathbf{r}'|$ (see Refs. 21 and 22).

The single-band Hamiltonian $\hat{\mathscr{H}}$ is invariant under combined translation $\hat{Q}$ of electrons and centers of vibration, so that the spectrum has a band structure $\{\mathscr{E}_v(\mathbf{K})\}$, determined by the quantum numbers $v(..., N_\lambda, ...)$ and the total quasimomentum $\mathbf{K}$ (N_λ is the number of phonons, $N_\lambda = 0, 1, 2, ...$). The group velocity in such a band is given by $\mathbf{V}_v(\mathbf{K}) = \partial \mathscr{E}_v(\mathbf{K})/\partial \mathbf{K} = 0$ with suitable $\mathbf{K} = \mathbf{K}_0 \equiv \mathbf{K}_0^{(v)}$ ($\mathbf{K}_0 = 0$ for an isotropic band $\mathscr{E}_v(\mathbf{K})$).

The type of interaction $\hat{\mathscr{H}}_{\text{int}}$ is determined by the specific dependences of ω_λ and w_λ on $\mathbf{f}$ (see, for example, Refs. 5, 21, 22, and 24). Thus for the case of polarization ($\mathbf{p}$) phonons (at least in three-dimensional systems) and $|\mathbf{f}|a \ll \pi$

$$\omega_{\mathbf{f}}^{(\mathrm{p})} \approx \omega_{\mathrm{p}} = \text{const}, \quad w_{\mathbf{f}}^{(\mathrm{p})} \approx \sqrt{4\pi\alpha\lambda_{\mathrm{p}}}\,\omega_{\mathrm{p}}(|\mathbf{f}|v_0)^{-1},$$
$$Z^{(\mathrm{p})}(\mathbf{r}, \mathbf{r}') \approx E_{\mathrm{L}}^{(\mathrm{p})} |\mathbf{r} - \mathbf{r}'|^{-2}, \quad E_{\mathrm{L}}^{(\mathrm{p})} = \text{const}, \tag{2.6}$$

where the dimensionless coupling constant $\alpha \equiv e^2/2\varkappa\lambda_p\omega_p$, $\lambda_p \equiv (2m\omega_p)^{-1/2}$, $\varkappa^{-1} \equiv \varkappa_\infty^{-1} - \varkappa_0^{-1}$; $\varkappa_0$ and $\varkappa_\infty$ are the static and high-frequency dielectric permittivities. For the case of nonpolarization optical (o) phonons, acoustical longitudinal (ac) or piezoacoustical (pac) phonons with $|\mathbf{f}|a \ll \pi$ respectively,

$$\omega_{\mathbf{f}}^{(0)} \approx \omega_0 \equiv \text{const}, \quad w_{\mathbf{f}}^{(0)} \approx w_0 = \text{const},$$
$$Z^{(0)}(\mathbf{r}, \mathbf{r}') \approx E_{\mathrm{S}}^{(0)} \delta(\mathbf{r} - \mathbf{r}'), \tag{2.7}$$
$$\omega_{\mathbf{f}}^{(\mathrm{ac})} = s|\mathbf{f}| \ll \omega_{\mathrm{D}},$$
$$w_{\mathbf{f}}^{(\mathrm{ac})} = C|\mathbf{f}|(2M_a\omega_{\mathbf{f}}^{(\mathrm{ac})})^{-1/2},$$
$$Z^{(\mathrm{ac})}(\mathbf{r}, \mathbf{r}') \approx E_{\mathrm{S}}^{(\mathrm{ac})} \delta(\mathbf{r} - \mathbf{r}'), \tag{2.8}$$
$$\omega_{\mathbf{f}}^{(\mathrm{pac})} = s|\mathbf{f}| \ll \omega_{\mathrm{D}}, \quad w_{\mathbf{f}}^{(\mathrm{pac})} \sim |\mathbf{f}|^{-1/2},$$
$$Z^{(\mathrm{pac})}(\mathbf{r}, \mathbf{r}') \approx E_{\mathrm{L}}^{(\mathrm{pac})} |\mathbf{r} - \mathbf{r}'|^{-2}, \tag{2.9}$$

where $E_S = \text{const}$, $E_L^{(\mathrm{pac})} = \text{const}$, $M_a \equiv \rho_0 v_0$, ρ_0 is the density, s is the velocity of sound, and C is the constant in the deformation potential; usually $C \lesssim D$.

Thus the interactions (2.6) and (2.9) are long range (L) while (2.7) and (2.8) are short range (S) with respect to the length scale a.

Everywhere below, unless otherwise stated (see Secs. 2f, 3c, and 5), we have in mind single-electron self-trapped states, including polarization self-trapped states of the single-electron system (2.4).

b) Limiting cases. Self-consistent states

There are two limiting cases of polaron self-trapped states, corresponding to a wide or very narrow Bloch electronic band:

$$\omega_{\mathrm{ph}}\tau_{\mathrm{t}} \equiv 2\omega_{\mathrm{ph}}D^{-1} \ll 1 \quad \text{or} \quad \omega_{\mathrm{ph}}\tau_{\mathrm{t}} \gg 1, \tag{2.10}$$

where τ_{t} is the electron tunneling time; $\omega_{\mathrm{ph}} \equiv \{\omega_{\mathrm{p}}, \omega_0 \text{ or } \omega_{\mathrm{D}}\}$. In the limiting case of very narrow bands the ground self-trapped state is similar to a strongly localized Wannier state, both with weak and, primarily, with strong electron-phonon coupling (see Sec. 2e).

In the most important, for electrons (holes) in semiconductors, case with $\omega_{\mathrm{ph}}\tau_{\mathrm{t}} \ll 1$, primarily discussed below and studied in most works on the theory of polarons,[1-5, 9-13] the "immobile" self-trapped state with velocity $\mathbf{V}(\mathbf{K}) = 0$ and finite radius ρ_{p} is the ground state of the system, as soon as the corresponding energies of the system (2.4) E_1 and of the self-localized electron ε_1 satisfy

$$E_1 < (\varepsilon(\mathbf{k}))_{\min} \equiv 0, \quad \varepsilon_1 < 0, \quad |\varepsilon_1| \gg \omega_{\mathrm{ph}}. \tag{2.11}$$

The latter inequality, corresponding to a strong electron-phonon coupling, means that the motion of the electron in the local potential well, created in the lattice deformed by the electron, adiabatically follows the changes in the deformation in the state with the discrete level ε_1 (< 0), maintaining the existence of this deformation with its field in accordance with Landau's concept. The magnitude of the energy $|\varepsilon_1|$, characterizing such a self-consistent self-trapped ground state, and the energy $\delta_0^{(0)}$ of the deformation of the lattice by the self-trapped electron are of the same order of magnitude, $|\varepsilon_1| \sim \delta_0^{(0)}$ [see (2.16)]. The structure of polaron self-consistent self-trapped states with

$$\omega_{\mathrm{ph}}\tau_{\mathrm{t}} \ll 1, \quad |\varepsilon_1| \sim |E_1| \sim \delta_0^{(0)} \gg \omega_{\mathrm{ph}} \tag{2.12}$$

can be studied using the approach developed by Pekar[4,5] and others (see Ref. 22). This approach is based on the adiabatic approximation with $|\varepsilon_1| \gg \omega_{\mathrm{ph}}$ and the quasiclassical description of the vibrations with $\delta_0^{(0)} \gg \omega_{\mathrm{ph}}$ (b_λ, b_λ^+, and $q_\lambda \equiv b_\lambda + b_\lambda^+$ are c numbers). The problem reduces to finding the minimum energy of the system with a given quasimomentum $\mathbf{K}$, i.e., minimizing the functional $J[\psi, q_\lambda] \equiv \langle\psi|\hat{\mathscr{H}}|\psi\rangle_0$:

$$\min_{\{\psi, q_\lambda\}} J[\psi, q_\lambda] = J_0^{(\mathbf{K})} \quad \text{or} \quad \min_{(\psi)} J[\psi] = J_0^{(\mathbf{K})}, \tag{2.13}$$

with $\psi = \psi_0^{(\mathbf{K})}$ and $q_\lambda \equiv q_\lambda[\psi] = q_\lambda[\psi_0^{(\mathbf{K})}] \equiv q_\lambda^{(\mathbf{K})}$; here $J[\psi] = \min_{(q_\lambda)} J[\psi, q_\lambda]$; $\langle ... \rangle_0$ is the zeroth order approximation with respect to the small perturbation $\hat{K}_{\mathrm{ph}}$ (in the adiabatic approximation), and ψ and q_λ are the varied electronic wave function and the normal coordinates of the lattice vibrations; $J_0^{(\mathbf{K})}$ is the lowest energy of the system in the state $(\psi_0^{(\mathbf{K})}, q_\lambda^{(\mathbf{K})})$ with fixed $\mathbf{K}$. In particular, $E_1 = J[\psi_0^{(0)}] \equiv J_0^{(0)}$ is the energy of the ground state $(\psi_0^{(0)}, q_\lambda^{(0)})$ with $\mathbf{V}(\mathbf{K}) = 0$.

Consistent variations of $J[\psi, q_\lambda]$ with respect to ψ and q_λ also correspond to Pekar's condition for a self-consistent self-localized state $\psi_0^{(0)}$. Schrödinger's equation for the latter is nonlinear. This follows from the relations describing the energy of the system $J[\psi]$ and of the electron $E_e[\psi]$ as well as the change in the energy of the system $\delta[\psi]$ and the displacement of the centers of vibration $q_\lambda[\psi] = b_\lambda[\psi] + b_\lambda^+[\psi]$ in the deformed lattice with a linear response of the medium

$(q_\lambda[\psi] \propto Q_f[\psi] \equiv \langle\psi|\omega_\lambda \exp(i\mathbf{fr})|\psi\rangle)$ for a given electron state ψ:

$$J[\psi] = K_e[\psi] - \delta[\psi] = E_e[\psi] + \delta[\psi], \tag{2.14}$$

$$K_e[\psi] \equiv \langle\psi|\hat{K}_e|\psi\rangle,$$

$$\delta[\psi] = -\frac{1}{2}\langle\psi|\hat{\mathscr{H}}_{int}|\psi\rangle \equiv -\frac{1}{2}W[\psi] > 0. \tag{2.15}$$

A systematic, actually equivalent, approach in the theory of polaron self-trapped states was proposed by Bogolyubov,[9] Tyablikov,[10] and others (see Ref. 13) within the framework of the adiabatic perturbation theory which they developed, in which the kinetic energy of the lattice vibrations plays the role of a *small* perturbation. This method, as also Pekar's approach, is adequate for the analysis of polaron self-trapped states, at least for low velocities $|\mathbf{V}(\mathbf{K})| \ll s$.

It is convenient to analyze the self-trapped states with large ($\rho_p \gg a$) or small ($\rho_p < a$) radius in (2.13)–(2.15) in the **r** or **l** representations, respectively. In the general case, the following relations characteristically hold for a polaron ground self-trapped state:

$$\varepsilon_{opt} - \varepsilon_{th} \equiv \varepsilon_R \approx \delta_0^{(0)} \equiv \delta[\psi_0^{(0)}] = -\frac{1}{2}W_0^{(0)} > 0,$$

$$\varepsilon_{opt} = |\varepsilon_1| \equiv |E_e[\psi_0^{(0)}]|,$$

$$\varepsilon_{th} = |J_0^{(0)}| \equiv |E_1|, \quad W_0^{(0)} \equiv W[\psi_0^{(0)}], \tag{2.16}$$

i.e., the energy of the optical Franck-Condon transition ε_{opt} of the electron from the self-trapped state into the Bloch state (photodissociation of the polaron) exceeds the energy of the thermal transition ε_{th}; ε_R is the corresponding relaxation energy of the lattice. The structure of the polaron self-trapped states is determined by the nature of the interaction (2.3)—long-range (2.6), (2.9) or short-range (2.7), (2.8), and in the latter case also by the dimensionality d of the electronic subsystem ($d = 3, 2$, and 1), usually with a three-dimensional phonon spectrum (in this sense, below, d is usually called the dimensionality of the system). As a rule, under the conditions (2.12) we have in mind self-trapped states corresponding to low electron energies $\varepsilon(\mathbf{k}) \ll D$.

We note that the electron-phonon system under study can be approximated by a single-band [in the sense of (2.1)–(2.4)] model, at least if

$$\delta_0^{(0)} \ll E_g, \tag{2.17}$$

which usually holds in crystals in which the self-trapped states of the charge carriers are the determining ones (see Sec. 2d).

The energy of the system (2.1)–(2.3) with low velocities of the self-trapped state

$$J_0^{(K)} = J_0^{(0)} + \frac{1}{2}M_{\alpha\beta}^{-1}(\mathbf{K}-\mathbf{K}_0)_\alpha(\mathbf{K}-\mathbf{K}_0)_\beta, \quad \alpha, \beta \equiv x, y, z, \tag{2.18}$$

is determined by the effective mass tensor $M_{\alpha\beta}$ of the translational motion of the polaron (electron and accompanying deformation), i.e., by a scalar M in the case of an isotropic band, which for simplicity we shall primarily have in mind in what follows.

c) Long-range interactions. The polaron

In the simplest model (2.2)–(2.5) in the **r** representation, which is useful for the analysis of self-trapped states with a large radius $\rho \gg a$, in three-dimensional (3D) as well as 2D and 1D systems, in accordance with (2.14)–(2.15),[4,5]

$$\left.\begin{aligned} &J[\psi] \equiv J_L[\psi] = K_e[\psi] - \delta_L[\psi], \\ &K_e[\psi] \approx \int d\mathbf{r}\,|\nabla\psi(\mathbf{r})|^2 (2m)^{-1}, \\ &\delta[\psi] \equiv \delta_L[\psi] = -\frac{e}{2}\int d\mathbf{r}\,\varphi_L(\mathbf{r})\,|\psi(\mathbf{r})|^2, \\ &\varphi_L(\mathbf{r}) = -\frac{e}{\varkappa}\int d\mathbf{r}'\,|\psi(\mathbf{r}')|^2\,|\mathbf{r}-\mathbf{r}'|^{-1} \backsim r^{-1} \\ &\qquad\qquad \text{for} \quad |\mathbf{r}| \equiv r \gtrsim \rho. \end{aligned}\right\} \tag{2.19}$$

In the ground self-trapped state ($\psi = \psi_0^{(0)}, \rho = \rho_p$) the energy of the system[4,5] and the effective mass of the polaron (with $K^2 \ll 2M\omega_p$)[29] are described by the relations

$$J_0^{(0)} \equiv J_{0L}^{(0)} = -0.109\alpha^2\omega_p, \quad M = 0.02\alpha^4 m \quad (\gg m). \tag{2.20}$$

A change in the state ($\psi_0^{(0)} \to \psi$) unavoidably increases the energy $J[\psi]$ of the system. As a result, under the scale transformation $\mathbf{r} \to \gamma\mathbf{r}$ and $\psi_0^{(0)}(\mathbf{r}) \equiv \gamma^{-d/2}\psi_0^{(0)}(\gamma\mathbf{r}) \to \psi(\mathbf{r}) \equiv \psi_0^{(0)}(\gamma\mathbf{r})$ ($d = 3, 2$ or 1) the functional $J[\psi] \equiv \tilde{J}_L(\gamma)$ in general must have an absolute minimum at $\gamma = 1$, if the continuum model is adequate. Thus with (2.19)[5,25]

$$J_L[\psi] \equiv \tilde{J}_L(\gamma) = \gamma^2 K_e^{(0)} - \gamma\delta_{0L}^{(0)}, \tag{2.21}$$

where $\gamma = 2K_e^{(0)}/\delta_{0L}^{(0)} = 1$, has a unique and finite minimum. The corresponding state $\psi_0^{(0)}$, which has a finite radius in the continuum model (in which the distance a is identified with a point), actually corresponds to a smooth wave function ($\sim\exp(-r/\rho)$) with the radius $\rho \equiv a\beta^{-1}$, in addition, the radius of the ground polaron state $\psi_0^{(0)}$ (of the polaron) ρ_p is large, $\rho_p \gg a$ (see Refs. 5 and 25):

$$\left.\begin{aligned} &J_L[\psi_0^{(0)}] \equiv \bar{J}_L(\beta) = \beta^2 D - \beta\delta_{0L}^*, \\ &\rho_p \equiv a\beta_0^{-1} \approx a\alpha^{-1}(ma^2\omega_p)^{-1/2} \sim \frac{a\varkappa m_0}{m} \gg a, \\ &J_{0L}^{(0)} \equiv \bar{J}_L(\beta_0), \end{aligned}\right\} \tag{2.22}$$

where $D \equiv 1/ma^2$, $\beta = \beta_0 \approx 2\delta_{0L}^* D^{-1} (\ll 1)$ and $\delta_{0L}^* \equiv p_0 e^2/2\varkappa a \gg \delta_{0L}^*$, $p_0 \sim 1$.

It is evident that already with arbitrarily small β (i.e., also small deformations) $\bar{E}_{eL}(\beta) < \bar{J}_L(\beta) < 0$, and therefore, the Bloch state ($\beta \to 0$) is unstable with respect to a transition into the polaron state, and the transition does not involve overcoming an energy barrier. The reason evidently lies in the fact that the polaron (spherically symmetrical) potential well $\psi_L(r)$ for the electron is, for $r \gtrsim \rho (\gtrsim \rho_p)$, Coulombic; for the same reason such a self-trapped electron—a polaron with a large radius—is characterized, aside from the ground state ($\psi_0^{(0)}, n = 0$), also by a series of excited, hydrogen-like self-trapped states $\psi_n^{(0)}$ with a large radius $\rho_p^{(n)} > \rho_p \equiv \rho_p^{(0)} \gg a$ ($n = 1, 2, \ldots$).[4,5,13,21] Based on (2.21) and (2.22), the self-trapped state $\psi_0^{(0)}$, which is energetically more favorable than the Bloch states, is characterized by the relations[4,5]

$$\varepsilon_{opt} = -\varepsilon_1 = 2\delta_{0L}^{(0)} - K_e^{(0)} = \frac{3}{2}\delta_{0L}^{(0)} > 0,$$
$$\varepsilon_{th} = -E_1 = -(\varepsilon_1 + \delta_{0L}^{(0)}) = \frac{1}{2}\delta_{0L}^{(0)}, \quad (2.23)$$

$\varepsilon_{th} : K_e^{(0)}\delta_{0L}^{(0)} : \varepsilon_{opt} : |W_0^{(0)}| = 1:1:2:3:4$. It follows from the formulas (2.20), (2.22), and (2.23), in accordance with (2.12) and (2.16), that for a polaron with a large radius adiabatic strong coupling is characteristic, in the sense that

$$D > \delta_{0L}^{*} \gg \delta_{0L}^{(0)} = 2|E_1| \gg \omega_p \text{ and } D\omega_p^{-1} \gg \alpha^2 \gg \alpha_0^2 \approx 10. \quad (2.24)$$

Therefore, such polarons (Pekar polarons) can exist only in a limited range of values of α,[5,21,22] i.e., their abundance in real materials is limited; apparently, the presence of large polarons in ionic crystals (see (2.6)) has in reality not been established unequivocally.[19,21,22] The effective mass M of the polaron is large, $M \gg m$, and it is actually a measure of the inertia of the lattice polarization accompanying the motion of the self-trapped electron.[12,29] The characteristic values of ρ_p, $\delta_{0L}^{(0)}$ and M with the typical values $\alpha^2 \approx 30$, $\varkappa \approx 10$, $m_0/m \sim 1$ and $\omega_p \lesssim 0.1$ eV are $\rho_p \sim 10a$, $\delta_{0L}^{(0)} \lesssim 0.3$ eV, $M \sim 10^2 m$ (see Ref. 5). For large polarons created by the piezoacoustical interaction (2.9), the functional $J[\psi]$ coincides with (2.19).[30]

On the other hand, as soon as

$$\rho_p < a, \quad \text{i.e.} \quad \Lambda_L^{*} \equiv 2\delta_{0L}^{*} D^{-1} > 1, \quad (2.25)$$

there exists a polaron with a small radius (small polaron),[31,32,19,21] for which the quantity

$$\Phi_0^{*} \equiv \delta_{0L}^{*}\omega_p^{-1} \approx \alpha\sqrt{\frac{D}{\omega_p}} \gg 1,$$
$$\Phi_0^{*} \gg \alpha_1^{*} \gg 1, \quad \text{with} \quad \delta_{0L}^{*} \sim \tfrac{1}{3}\delta_{0L}^{(0)}; \quad (2.26)$$

plays the role of the electron-phonon coupling constant; typically $\delta\rho_{0L}^{*} \lesssim 0.3$ eV and $\Phi_0^{*} \lesssim 10$, in agreement with the condition (2.17) of single-bandedness of the model (with $E_g \gtrsim 1$ eV).

The simplest and most characteristic case here is the case of a nonadiabatic small polaron,[19,21,31,32] for which, by definition, the electron tunneling time τ_t is appreciably longer than the time τ_{ad} of mutual adjustment of the electron state and the lattice deformation: $\tau_{ad} \sim (\delta_{0L}^{*}\theta)^{-1/2}$, with characteristic energy $\theta \equiv \max\{T;\ T_0 \equiv \frac{1}{2}\omega_{ph}\}$ (see Ref. 21). (In Ref. 31 $\theta \sim T_0\sqrt{T/\delta_{0L}^{*}} < T$ for $T_0 \lesssim T \ll \delta_{0L}^{(0)}$.) Actually, for large $\Phi_0 \gg 1$ $\tau_{ad}^{-1} \gg \omega_{ph}$ [$= \omega_p$ for the model (2.19)], in accordance with (2.12); T is the temperature. In this case, when $\omega_{ph} \ll D/2 \ll \tau_{ad}^{-1}$, obviously $\rho_p a^{-1} \ll 1$ and, therefore, $\psi_0^{(0)}$ is approximated well by a Wannier electron state, $\psi_0^{(0)}(\mathbf{l}) = \delta_{\mathbf{l}\mathbf{l}_0}$. Here the electron kinetic energy operator $\hat{K}_e$ is a small perturbation in the Hamiltonian of the system. The basic second-quantized Hamiltonian $\hat{\mathscr{H}}_0 = \hat{\mathscr{H}}_{ph} + \hat{\mathscr{H}}_{int} + \hat{U}_c$ in the $\mathbf{l}$ representation is transformed, by means of the well-known canonical transformation $\exp(-\hat{S}) \equiv \exp(\hat{S}^{+})$ with $\hat{S} = \Sigma_{\mathbf{l}\sigma}\hat{S}_{\mathbf{l}}\hat{n}_{\mathbf{l}\sigma}$ and

$$\hat{S}_{\mathbf{l}} = N^{-1/2}\sum_{\lambda} X_\lambda (b_\lambda - b_{-\lambda}^{+}) \exp(i\mathbf{f}\mathbf{l}), \quad (2.27)$$

into the Hamiltonian $\tilde{\mathscr{H}} = \tilde{\mathscr{H}}_{ph} + \tilde{\mathscr{H}}_p + \tilde{U}_p$ ($\hat{n}_{\mathbf{l}\sigma}$ are the electron occupation number operators). The operator $\tilde{\mathscr{H}}_{ph} = \Sigma_\lambda \omega_\lambda \hat{N}_\lambda$ describes phonons with displaced centers ($X_\lambda = -\langle 1 = 0|\exp(i\mathbf{f}\mathbf{r})\omega_\lambda|\mathbf{l} = 0\rangle\omega_\lambda^{-1}$) and $\tilde{\mathscr{H}}_p = \Sigma_{\mathbf{l}\sigma} E_1 \hat{n}_{\mathbf{l}\sigma}$, corresponds to small polarons with site energy E_1 (measured from the electron level) and self-trapping energy W_1 characterizing the gain in energy accompanying self-trapping, $E_1 = W_1 < 0$ [in the model (2.6), $|W_1| \sim \delta_{0L}^{(0)}$]. The interpolaron interaction $\tilde{U}_p = \hat{U}_c + \hat{U}_a$ includes, aside from the Hubbard repulsion $\hat{U}_c$, an attraction $\hat{U}_a$ due to phonon exchange (see Refs. 19 and 21).

The polaron kinetic energy operator $\tilde{K}_p = \exp(\hat{S})\hat{K}_e\exp(-\hat{S})$ and the polaron tunneling amplitude operator (in the phonon number space $\hat{N}_\lambda$) between nearest neighbors $\mathbf{g}$, $\Delta_g = J\exp(\hat{S}_0 - \hat{S}_g)$, describe two substantially different types of tunneling of a small polaron: coherent and noncoherent (see Refs. 19, 21, 31, and 32). The coherent tunneling (without a change in the phonon numbers) is described by the macroscopically finite (as $N \to \infty$) amplitude

$$\Delta = J\exp(-\Phi),$$
$$\Phi = N^{-1}\sum_{\lambda} |X_\lambda|^2 \sin^2\frac{\mathbf{fg}}{2} \cdot \operatorname{cth}\frac{\omega_\lambda}{2T} \geqslant \Phi_0 \equiv \Phi \quad (T = 0), \quad (2.28)$$

determining the small-polaron band with width $D_p \approx 2z\Delta \ll D \approx 2zJ$ with the large values of the coupling parameter $\Phi_0 \gg 1$ ($\Phi_0 \sim \Phi_0^{*} \gg 1$) occurring here; Φ increases and Δ decreases as T increases, and in addition $\Phi \sim \Phi_0 T/T_0$ and Δ decay exponentially for $T \gtrsim T_0$. Actually, $D_p \ll \omega_{ph}$ and $D_p < T$ for not very low T, and the effective mass of such a small polaron $M \approx 1/D_p a^2$ is exponentially large (compared with m) due to the high inertia of the strong circumelectron deformation of the lattice accompanying translation.

Noncoherent tunneling (hopping) occurs together with the emission and/or absorption of a phonon and is described by the average probability (per 1 s) W_h, which increases with T ($W_h \to 0$ as $T \to 0$). In this sense, hopping is thermally activated; in particular, at sufficiently high temperatures $T > T_1$ hopping corresponds to a multiphonon process; $T_1 < T_0$ when $\Phi_0 \gg 1$, in particular, $T_1 \approx T_0/\ln(4\Phi_0)$ in the case (2.6). Thus when $T \gtrsim T_0$

$$W_h \simeq \frac{J^2\sqrt{\pi}\exp(-\mathscr{E}/T)}{2\sqrt{2\mathscr{E}T}}, \quad (2.29)$$
$$\mathscr{E} = N^{-1}\sum_{\lambda} 2|X_\lambda|^2 \sin^2\frac{\mathbf{fg}}{2} \cdot \omega_\lambda \equiv \gamma_1\Phi_0 T_0 \gg T_0,$$
$$\gamma_1 \sim 1; \quad \gamma_1 = 1 \quad \text{with} \quad \omega_{ph} = \omega_p. \quad (2.30)$$

As is evident from (2.28)–(2.29), the motion of a nonadiabatic small polaron is determined by hopping for $T > T_\Gamma$ or by coherent tunneling for $T < T_\Gamma$, so that the dynamic and kinetic characteristics vary nonmonotonically as a function of T, having a minimum (or maximum) at $T \approx T_\Gamma$; the general order of magnitude of the temperatures T_Γ characteristic for specific phenomena is $T_\Gamma \sim T_1$ (see Ref. 21).

The situation for an adiabatic small polaron was investigated in a number of studies (see, for example, Refs. 33 and 34). Such a polaron is described by the self-consistent state

$\psi_0^{(0)}$, whose structure and properties are determined by the specific structure of the electron-phonon coupling in a discrete lattice. From a qualitative viewpoint, the properties of such polarons fall between those of the nonadiabatic small polaron and a large polaron.

The characteristic effects produced by large polarons are determined by the fact that the effective mass of such polarons is large ($M \gg m$), the discrete spectrum includes the excited states $\psi_n^{(0)} \geqslant 1$ with energies $J_n^{(0)} > J_0^{(0)}$, and the polaron potential $\varphi_L(r) \sim r^{-1}$ for $r \gtrsim \rho_p \gg a$. Thus in a strong static uniform electric field F the polaron autoionizes with probability $p_{AI} \sim \exp(-F_I/F)$ (and is thermally ionized with probability $p_{TI} \sim \exp(-\varepsilon_I/T)$, $d\varepsilon_I/dF < 0$) for $F_1 \lesssim F \ll F_2 \sim \delta_{0L}^{(0)}/|e|\rho_p$, $F_1 \sim F_2(\delta_{0L}^{(0)} m \rho_p^2)^{-1/2} \ll F_2$, and obviously transforms into a Bloch electron with a much higher mobility for $F \gtrsim F_2$ (see Refs. 35 and 21). At the same time the conductivity can increase markedly with F when $F \approx F_{cr}$, $F_1 < F_{cr} \lesssim F_2$; typically $F_1 \sim 0.1F_2$ and $F_2 \gtrsim 10^6$ V/cm for typical values, $\delta_{0L}^{(0)} \lesssim 0.1$ eV. These and other features of the kinetics of large polarons,[12,19–22] in particular, a resonant infrared absorption band accompanying the transitions $\psi_0^{(0)} \to \psi_n$ ($n = 1, 2, \ldots$), $\omega \geqslant \omega_{21} \approx 0.14\alpha^2\omega_p$, have apparently not yet been observed.

For small polarons the main features of the conductivity $\sigma'(\omega, T) = \mathrm{Re}\,\sigma(\omega, T)$ and other kinetic coefficients are determined by the exponential smallness of the tunneling amplitude and the competition between the coherent tunneling (σ_c) and hopping (σ_h), $\sigma'(\omega) \approx \sigma_c(\omega) + \sigma_h(\omega)$. Here (see Refs. 17 and 21)

$$\sigma_c(\omega) \sim \sigma_c(1+\omega^2\tau^2)^{-1} \quad \text{for} \quad \omega < T,$$
$$\sigma_c \equiv \sigma_c(\omega = 0) \sim N_p \frac{e^2\tau}{M} \min\left\{\frac{\Delta}{T};\ 1\right\}, \tag{2.31}$$

$$\sigma_h \sim N_p |e| \mu_0 \frac{zW_h}{T} \text{ and, for } \omega > T,$$
$$\sigma_h(\omega) \propto \omega^{-1} \exp\left[-\frac{(\omega-\omega_m)^2}{2\Gamma^2}\right]; \tag{2.32}$$

where $\mu_0 \equiv |e|a^2/\hbar (\sim 1\ \mathrm{cm}^2/v \cdot \mathrm{s})$; $\omega_m \equiv 4\mathscr{E}$, $\Gamma \approx \sqrt{4\mathscr{E}\theta}$; $N_p a^3$ is the equilibrium polaron density; τ is the transport relaxation time, which does not increase with T (the formula $\sigma_c \sim N_p e^2 \tau \Delta/MT$ is valid for $\Delta < \vartheta \equiv \min\{T; T_0\}$, $\tau\vartheta \gg 1$, i.e., not just for weak scattering, $\tau\Delta \gg 1$, since for $\Delta < T$ the scattering is determined by conservation of the energy of the phonons). It follows from (2.31) and analogous formulas that the dependences $\sigma'(\omega, T)$ are nonmonotonic and have minima at $T = T_{min}$ and $\omega = \omega_{min}$ and maxima at $T = T_{max}$, $\omega = \omega_{max}$, in addition $T_{min} \sim T_\Gamma < T_0$, $\omega_{min} < \omega_{ph}$, and also $T_{max} \sim \mathscr{E} \gg \omega_{ph}$, $\omega_{max} = \omega_m \gg \omega_{ph}$ (thus $\sigma'(\omega) \approx \sigma_c(\omega)$ when $T < T_{min}$, $\omega < \omega_{min}$, but $\sigma'(\omega) \approx \sigma_h(\omega)$ when $T > T_{min}$ or $\omega > \omega_{min}$). Such nonmonotonic dependences, in particular, the wide Gaussian absorption peak at $\omega \approx \omega_m$ in the presence of a Franck-Condon transition into the Bloch state, and the analogous dependences $\tilde{\sigma}(F; T) \approx \sigma'(\omega_F, T)$ with $\omega_F \equiv |e|Fa > T$ in a strong field F, characteristic for small polarons and partially observed experimentally, are discussed in greater detail, for example, in Refs. 17 and 21.

On the whole, the many unusual properties of self-trapped polaron states are determined by multiphonon transitions, due to the significant difference between the local deformations of the lattice in the initial and final states of the system for $\Phi_0 \gg 1$ (see Refs. 5, 13, 19, 22).

The theory of self-trapped polaron states in crystals is studied in many works, including a number of reviews (see, for example, Refs. 5, 13, 19–22). Thus the method of adiabatic perturbation theory[9,10] for a large polaron is substantially developed in Refs. 38 and 39, while the theory of a small polaron is further developed in Ref. 40.

d) Short-range and "mixed" interactions in 3D systems. Small polarons

The functionals $J_S[\psi]$ and $E_{eS}[\psi]$ in the simplest model (2.5) of an isotropic continuum, taking into account (2.7) or (2.8) and (2.14), (2.15), have the same form as (2.14), but[41,8,25,42,22]

$$\delta_S[\psi] = \frac{1}{2}\int d\mathbf{r}\,|\psi(\mathbf{r})|^2 \varphi_S(\mathbf{r}),$$
$$\varphi_S(\mathbf{r}) = \int d\mathbf{r}' Z_S(\mathbf{r}, \mathbf{r}')|\psi(\mathbf{r}')|^2 \approx E_S|\psi(\mathbf{r})|^2. \tag{2.33}$$

The scale transformation $\mathbf{r} \to \gamma\mathbf{r}$ leads for the 3D systems studied here to the relation

$$J_S[\psi] = \tilde{J}_S(\gamma) = \gamma^2 K_e'^{(0)} - \gamma^3 \delta_{0S}^{(0)}, \tag{2.34}$$

instead of (2.21), so that $\tilde{J}_\sigma(\gamma)$ does not have a lower bound. This function has two minima, $\tilde{J}_S(\gamma) = 0$ at $\gamma = 0$, i.e., $\rho = \infty$, and $\tilde{J}_S(\gamma) \to -\infty$ as $\gamma \to \infty$, i.e., $\rho \to 0$, which in the continuum model corresponds to Bloch states at the bottom of the conduction band and a self-trapped state with a small radius ($\rho_p < a$).[41] The latter essentially has the same properties and is characterized by the same relations, in particular, (2.25)–(2.32), as a small polaron, which was discussed in Sec. 2c. In this connection, in general, the self-trapped state with a small radius in the electron-phonon system (2.1)–(2.5) is called a polaron with a small radius or a small polaron, in particular, a nonadiabatic small polaron ($\rho_p < a$). Such a self-trapped state is realized when

$$\Lambda > \Lambda_c, \quad \Lambda = 2|W_1|D^{-1} \approx \delta_{0S}^{(0)} D^{-1}, \tag{2.35}$$

where the critical value Λ_c lies, roughly speaking, between 1 and 10 (see Ref. 25). Nevertheless, unlike the case (2.21), in the case (2.34), generally speaking, the self-trapped state with a finite radius, i.e., actually a self-trapped polaron state with a large radius ($\rho_p \gg a$), is not realized in the continuum model.

The long-range interaction (2.6) [or (2.9)], existing in ionic crystals together with the short-range interaction, can appreciably change the nature and conditions of formation of the self-trapped state of the electron.[25] Thus when both types of interactions are associated with the same phonon branch (for example (2.8) and (2.9) for acoustical phonons), aside from the contribution $\delta_L[\psi] + \delta_S[\psi]$ to $\delta[\psi]$, there also arises a mixed term[25,22]:

$$\delta_{mix}[\psi] = 2E_S E_L S_0^{-1} \int\int d\mathbf{r}\, d\mathbf{r}' |\psi(\mathbf{r})|^2 |\psi(\mathbf{r}')|^2 |\mathbf{r} - \mathbf{r}'|^{-2}, \tag{2.36}$$

which under a scale transformation contributes an additional term $-\gamma^2 \delta_{mix}[\psi_0^{(0)}]$ in (2.34). For $\Lambda_S < 1$, when a

small polaron with short-range coupling would not exist, the contributions $\delta_L[\psi]$ and $\delta_{mix}[\psi]$ to $\delta[\psi]$ can lead to the formation of a self-trapped polaron state with a large radius in the region of quite large $\alpha^2 > \alpha_1^2$, including also smaller values of α^2 than in the case (2.21) (with $E_S = 0$), since $\alpha_1^2 < \alpha_0^2 \approx 10$ (see Ref. 25).

In the situation under study, corresponding to wide electron bands ($D \gg \omega_{ph}$) and described, in particular, by the relations (2.27), the inequality $|W_1|\omega_{ph}^{-1} \gg 1$ must obviously be satisfied for $\Lambda > \Lambda_c$, so that a small polaron corresponds to very strong electron-phonon coupling, $\Phi_0 \gg 1$. An expression analogous to (2.33) in the **l** representation permits evaluating $\delta_{0S}^{(0)} = c_1 E_S a^{-3}$, $c_1 \sim 1$ with $\Sigma_1 |\psi(\mathbf{l})|^4 \sim a^{-3}$, so that $\Lambda_S^{(ac)} = c_2 C^2/M_a s^2 D$, $c_2 \sim 1$ and $\Lambda_S^{(opt)} \sim w_0^2/D\omega_0$ with $D = 1/ma^2$; if $C = c_3 D$, $D = c_4 E_{at}$ $s/a = c_5\sqrt{m_0/M_a}\,E_{at}$ with $E_{at} = m_0 e^4/\hbar^2$, assuming that $c_3 \sim c_4 \sim c_5 \sim 1$, then $\Lambda_S^{(ac)} \sim 1$ (see Ref. 22). It may be assumed here that in (nonmetallic) crystals it is precisely the short-range coupling with acoustic phonons which determines the appearance of self-trapped states differing qualitatively from the Bloch states in the band and that the ground state of the electron is mainly a small polaron with its characteristic properties. Some of these effects have indeed been observed for holes in wide-gap crystals—alkali-halide crystals (AHC)[43]—and in cryogenic crystals[44] as well as in some transition-metal compounds (see, for example, Refs. 19–21, 45). The effects of the self-trapped states of the current carriers, however, have not been observed in diamond-like semiconductors (Ge, A_3B_5, etc.), in which the value of $\Lambda_S^{(ac)}$ lies between roughly 0.1 and 1. This fact, in accordance with Refs. 46 and 22, can be linked to the smallness of the energy gap E_g in such materials, $E_g \ll D$ (actually, $E_g \lesssim 1$ eV), since for $\Lambda_S > \Lambda_c$, i.e., $|W_1| > E_g$, the crystal would become unstable with respect to spontaneous creation of electron-hole pairs and a phase transition into the wide-gap dielectric phase.

In the case (2.34) an analysis of the critical points (minima, saddle points, etc.) of the adiabatic local potential $\Psi_0(q)$ in the configuration space (q) in the ground self-trapped state,

$$\Psi_0(q) = \varphi_0(\Delta) = \frac{1}{2} S_0 \int d\mathbf{r} \Delta_0^2(\mathbf{r}) + \int\int d\mathbf{r}\, d\mathbf{r}' |\psi_0^{(0)}(\mathbf{r}')|^2 Z_S(\mathbf{r}, \mathbf{r}') \Delta_0(\mathbf{r}'), \quad (2.37)$$

yields more accurate properties of the electron states noted above than in the case (2.21) (see Refs. 22 and 25). Namely, small polarons correspond to a local ($\Lambda_S < 1$) or absolute ($\Lambda_S > 1$) minimum of $\Psi_0(q)$ with a finite deformation ($q = q_0 \neq$), i.e., to a metastable or stable (ground) state of the system, and is characterized by $\Phi_0 \sim |W_1|\omega_{ph}^{-1} \gg \Lambda_S$, i.e., by a very strong coupling, $\Phi_0 \gg 1$ for $\Lambda_S > 1$. On the other hand, the Bloch states near the bottom of the band are also self-consistent, corresponding to the local (for $\Lambda_S > 1$) or absolute (for $\Lambda_S < 1$) minimum of $\Psi_0(q)$ at $q = 0$, and are characterized by the coupling constant $\alpha_{ac} \sim \Lambda_S^{(ac)}\sqrt{m/M_a}$ and by the lifetime $\tau(\varepsilon)$ of an electron with energy ε, $(\varepsilon\tau(\varepsilon))^{-1} \sim \alpha_{ac}$, in addition, $\alpha_{ac} \ll \Lambda_S^{(ac)}$ and α_{ac} is small ($\alpha_{ac} < 1$) for actual, not very large $\Lambda_S^{(ac)}$ ($\lesssim 10$). The transition from the stable self-trapped state to the stable Bloch state accompanying a decrease in Λ_S is discontinuous at the critical value $\Lambda_S = \Lambda_c$, as expected from physical considerations (see Refs. 22, 25, 42 and also Ref. 47).

On the whole, the situation described above corresponds to the existence of an energy barrier in q space between the minima $\Psi_0(0)$ and $\Psi_0(q_0)$ of the adiabatic potential $\Psi_0(q)$—the self-trapping barrier, in accordance with Landau's initial idea (see Ref. 22). This barrier is significant when its height is $H_b \gg \omega_b/2$, where ω_b is the characteristic frequency of the phonons determining the barrier, for example, $\omega_b^{(opt)} \sim \omega_0$ or $\omega_b^{(ac)} \sim s/r_b$, where r_b is the spatial size of the barrier. The estimates of H_b and r_b from dimensional considerations have the following form in the continuum model[8,48,22]:

$$H_b = c_1' \left(\frac{E_S}{2}\right)^{-2} m^{-3} \sim E_S r_b^{-3} \sim D\Lambda_S^{-3},$$

$$r_b \sim mE_S \sim a\Lambda_S, \quad c_1' \sim 1 \quad (2.38)$$

(more precisely $c_1' = 1.11$[49,22]). These estimates are valid, at least, for $r_b \gg a$, i.e., $\Lambda_S \gg 1$, and the last condition, according to Refs. 50 and 48, holds in light cryogenic crystals, for example, Ne. When this condition does not hold, the estimates of H_b depend on the specific structure of the lattice and are therefore difficult to obtain. In the general case, however, it may be assumed that H_b increases with m and decreases as Λ_S increases, so that the self-trapping barrier is determined not solely by purely lattice properties, but also by the nature of the formation (decay) of the site wave packet—the self-trapped state at a site. We note that the long-range $\delta_L[\Psi]$ and the "mixed" $\delta_{mix}[\Psi]$ interactions lower the self-trapping barrier as E_L increases right to the point at which the barrier vanishes.[22,25,42]

The presence of a self-trapping barrier can lead, for $\Lambda_S^{(ac)} > 1$, to the coexistence of the ground self-trapped and metastable Bloch states, since the latter can still decay slowly, $(\tau(\varepsilon)\varepsilon)^{-1} \sim \alpha_{ac} \ll 1$ for $\alpha_{ac} \ll \Lambda_S^{(ac)}$ (see, for example, Refs. 8, 22, 45, 50). This phenomenon, as also the presence of the self-trapping barrier in general, can lead to significant features in the kinetic phenomena (for example, conductivity, since the mobility of the Bloch electron is much greater than the mobility of a small polaron) and optical effects (see, above, Refs. 22, 48, 51). The self-trapping time τ_{ST} in the presence of a self-trapping barrier has been investigated theoretically in a number of studies,[22,48,51–54] in particular, a systematic theory at low temperatures was developed in Ref. 53. (The theoretical analysis has something in common with the analysis of the quantum diffusion time τ_D; see, for example, Refs. 17 and 55.) The theory of the coexistence of Bloch and self-trapped states in crystals has also been discussed in other studies (see, for example, Ref. 56). On the other hand, the existence of small polarons and their characteristic effects, in particular, the coexistence effects, in crystals with a significant relative fraction of short-range electron-phonon interactions has been experimentally observed in a number of compounds of transition and rare-earth metals ($LaCoO_3$, V_2O_5, $SrTiO_3$, etc.), in which $D/2 \lesssim 0.1$ eV and $\{|W_1|,$

$\mathscr{E}\} \lesssim 0.3$ eV (see Ref. 45 and 20) and, most reliably, for holes in AHC[43] and cryogenic Ar crystals.[44]

e) 1D and 2D systems. Band-structure effects in 3D systems. Extremely narrow bands

The properties and conditions of existence of self-trapped electron states in 1D systems with a dominant short-range electron-phonon coupling can differ substantially from those in 3D systems. For such systems the scale transformation $\mathbf{r} \to \gamma\mathbf{r}$ in the isotropic continuum model leads to the formula

$$J_S[\psi] \equiv \tilde{J}_S(\gamma) = \gamma^2 K_e^{(0)} - \gamma^d \delta_{0S}^{(0)}, \quad d = 1, 2, \tag{2.40}$$

instead of (2.34). Thus when $d = 2$ (in layered, strongly anisotropic 3D crystals or on their surfaces, etc.) the ratio of both terms $\delta_{0S}^{(0)}/K_e^{(0)}$ is independent of γ and, according to (2.33) is determined by the value of the parameter $mE_S/2$, whose critical value is $(mE_S/2)_{cr} = 2.88$.[49,48,22] When $mE_S/2 < 2.88$ the self-trapped state does not exist, while for $mE_S/2 > 2.88$ a small self-trapped state does exist ($\rho_p \lesssim a$) and the self-trapping barrier is absent (the anisotropy of the phonon spectrum was studied in Ref. 57). The absence of a self-trapping barrier in 2D and 1D systems follows from (2.38) with the substitution $m^3 \to m_1 m_2 m_3$, $m_3 \to \infty$ (2D) or $m_2 \to \infty$, $m_3 \to \infty$ (1D) ($m_{1,2,3}$ are the effective masses of the anisotropic band).[48] In a 1D system the ground self-trapped state is a small ($\rho_p \lesssim a$) or even a large ($\rho_p \gg a$) polaron, since $J_S[\psi]$ is similar to $J_L[\psi]$ in a 3D system [see (2.21)]. The theory of self-trapped states in 1D systems (at dislocations or polymer chains, etc.) is developed in detail in a number of studies.[8,31,58–60]

Specific electron self-trapped states with radius $\rho_p \gtrsim a$, similar to the strong-coupling polaron with a coupling constant $\alpha_*^2 \sim \sqrt{M_a/m_0} \sim 10$ and effective mass $M \sim \alpha_*^4 m$, can exist in 1D Peierls-Fröhlich dielectrics: the main self-trapped excitation is a soliton, which can have a charge $e^* = e$ with zero spin or can be neutral ($e^* = 0$) with spin 1/2, and self-trapping occurs without a barrier within a time of $\sim 10^{-13}$s.[61,62] Such remarkable self-trapped states have been observed in polyacetylene chains.[61,62] The interaction between the chains can distort or destroy such states.[61]

The degeneracy of the electron band, which is usually taken into account by replacing the operators K_e from (2.2) and $\hat{\mathscr{H}}_{int}$ from (2.3) by matrix expressions whose rank is equal to the degeneracy factor (see, for example, Ref. 63), can qualitatively change some characteristics of polaron self-trapped states and lead to the appearance of new types of such states. As shown in Ref. 64, band degeneracy leads to spontaneous symmetry breaking of the self-trapping barrier, which acquires an elongated or flattened shape and, therefore, plays a substantial role in the kinetics of self-trapping. In this connection band degeneracy can lead to low-symmetry (accompanying symmetry breaking of the lattice) small polaron states, in particular, a two-center (quasimolecular) state, for example a V_K center in AHC[43] or a R_2^+ center in the cryogenic crystal Ar.[44] Such low-symmetry self-trapped states can play an important role in the formation and transformation of defects (see Refs. 42–44, 22, 51). Band degeneracy also lowers the symmetry of the large Pekar polaron (2.19)–(2.24), for which rotational degrees of freedom appear also.[64] The spherical symmetry of the large polaron is also lost in the case of a multi-ellipsoidal anisotropic (nondegenerate) band.[65]

A small ($\rho_p > a$) self-trapped state can be the ground state of a wide-band electron ($D \gg \omega_{ph}$) even in cases of electron-phonon coupling stronger than required by the criteria (2.24) and (2.34). This can occur, in particular, for a high-energy Bloch electron in certain regions of $\mathbf{k}$ space, for example, in the region where the effective mass is negative (or large and positive); such self-trapped states and their coexistence with Bloch states can be manifested in nonequilibrium electron phenomena.[28]

In the case of extremely narrow electron bands ($D/2\omega_{ph} < 1$) the ground state of the electron is similar to a small polaron ($\psi_0^{(0)}(\mathbf{l}) = \delta_{\mathbf{l},\mathbf{l}_0}$) with arbitrary coupling with phonons, while the self-trapping barrier is actually absent (see Refs. 21 and 22). The dependence of the tunneling probability $\Delta(T)$, $W_h(T)$ on T, however, can differ significantly from that for small polarons. This difference arises when the electron tunneling amplitude $J(q)$ depends strongly on the atomic displacements q. In this case, the tunneling actually occurs in the presence of atomic configurations close to the extremal configuration [$q = q^*(T)$], arising due to the competition between the strong increase in $J(q)$ and the decrease in the probability $P(q)$ of atomic displacements as the displacements increase.[66] This "fluctuation formation" of lowered barriers leads to a growth of $\Delta(T)$ with T in contrast to the drop for small polarons.

$$\Delta \approx J(q^*) \exp[-\Phi(T) - \varphi(T)], \quad \varphi(0) \gg \{\Phi(0), 1\}, \tag{2.42}$$

since $\varphi(T)$ decreases with T. On the other hand, W_h/Δ^2 grows with T, and the region of T in which hopping predominates can become much larger than the characteristic region for a small polaron. For an electron, the extremal configuration can correspond to an adjacent pair of atoms[67,17] (compare the motion of R_2^+ centers in Ar).[44]

f) Two-electron self-trapped state. Bipolarons

The polaron two-electron self-trapped state with energy E_2 can become energetically more favorable than the single-electron state with energy E_1 when the effective correlation energy of the pair is negative[68]:

$$\begin{aligned} U &= E_2 - 2E_1 \\ &= U_c + W_2 - 2W_1 < 0, \ W_n < 0 \ (n = 1, 2) \end{aligned} \tag{2.43}$$

(W_2 is the self-trapping energy of the pair). In this case, an effective attraction exists in this pair, since the attraction due to the exchange of phonons predominates over the interelectron repulsion with characteristic energy $U_c > 0$. The properties and physical conditions for the existence of such self-trapped pairs, whose singlet $\sigma = \sigma_1 + \sigma_2 = 0$ ground state is usually considered and is often called a bipolaron state, are

studied in a number of works (see, for example, Refs. 13 and 68–72).

The properties and criteria for the realization of a bipolaron with a large radius $\rho_{2p}(\sim\rho_p \gg a)$, and an effective mass $M_2 \sim M$ in a 3D system—an ionic crystal—due to the long-range interaction (2.6) was studied in Ref. 69, and it was assumed that aside from (2.24) the very strong restriction $\varkappa_\infty \varkappa_\infty^{-1} < 0.05$ (i.e., $\varkappa_0 \gtrsim 10^2$ for $\varkappa_\infty \gtrsim 5$) must be satisfied. In this case both $U_c(\sim e^2/\varkappa_0 \rho_p)$ and $|U|$ (if $U<0$), $|U| \lesssim 0.1|E_1|$ ($\lesssim 0.01$ eV with $|E_1| \lesssim 0.1$ eV) would have been small. However, it can by no means be assumed that the existence of a self-consistent ground state of a singlet bipolaron with a large radius in a 3D system has been unequivocally established. There is also apparently no experimental evidence for the existence of large bipolarons in 3D systems (see, for example, Ref. 13). As was actually pointed out (see Ref. 42b), the long-range interaction (2.6) [or (2.9)], which screens the interelectron repulsion, can lead in 3D systems to the formation of "weak-coupling" bipolarons (bipolarons with a large radius, etc.), $|U| \ll |W_1|$, only because of the quantum properties of the interacting particles; short-range interactions of the type (2.7) or (2.8), which lead to the existence of stable bipolarons with a small radius (small bipolarons), are more likely to be significant here.

For small bipolarons and polarons in the system (2.27), it is evident that $W_2 = 4W_1$, so that $U<0$ with $U_c < 2|W_1|$ (see Refs. 67–72). Typical estimates $|W_1| \sim 0.1C^2/M_a s^2 \lesssim 0.1-0.3$ eV[19–21] and $U_c \lesssim 0.3$ eV[73] suggest that both $U<0$ and $U>0$ with $U_c \lesssim 0.1$–0.3 eV can occur. In this connection, it may be expected that small bipolarons will exist in transition metal compounds with large $\varkappa_0 (\gg \varkappa_\infty)$ and/or $\omega_D \omega_{ph}^{-1} \gg 1$. Accordingly, it was found experimentally in Ref. 74 that the current carriers in WO_3 are single-center bipolarons, and in Refs. 70–71 it is conjectured that two-center polarons (Ti^{3+}–Ti^{3+}) determine the ground state of the Ti_4O_7 crystal. The mobility of such a bipolaron must be significantly lower than the mobility of a small polaron (see Refs. 70–72); small bipolarons and polarons can coexist in the system.[4)]

It is not difficult to see from the foregoing that for small enough $U_c(<2|W_1|)$ small bipolarons can exist, even when the electron-phonon coupling is not strong enough for a small polaron to form [see (2.35)]. Moreover, two-electron states with $U<0$, reminiscent of a Cooper pair,[75] can also form in the presence of weak electron-phonon coupling: 1) in regions of $\mathbf{k}$ space where the effective mass of the band electron $m(\mathbf{k})(>0)$ is large or $m(\mathbf{k})<0$ (see, for example, Refs. 28, 60, 76 and 2) in 1D and partly in 2D systems with electron-phonon interaction (2.3).[77] Spinless charged pairs of coupled solitons can exist in Peierls-Fröhlich dielectrics.[61,62]

g) Self-trapped electrons in an antiferromagnet

In an antiferromagnetic wide-gap semiconductor the ground state of the conduction electron can be a self-trapped state with a large radius ($\rho_M \gg a$); this state is often called a spin polaron.[26,27] The spin polaron appears as a result of the s–d (s–f) exchange coupling of the electron with the spins S_a of the surrounding magnetic atoms, when $D \gg |A_0|S_a \gg T_N$; A_0 is the coupling parameter and T_N is the Néel point. In the process of self-trapping, in a definite region with large radius $\rho_M \gg a$ around the electron the spins of the atoms (S_a) are oriented along the spin ($A_0>0$) or opposite to the spin ($A_0<0$) of the electron (σ); far from the boundary inside this region the angle θ_0 between the spins (S_a,σ) is virtually independent of the electron field. In this sense there exists a nonlinear response of the medium, in contrast to the linear response for polaron self-trapped states. As also in (2.13), the energy E_{1M} and radius ρ_M of the spin polaron is determined by minimizing the energy of the system $J_M^{(0)}[\psi]$ (in the continuum model):

$$J_M^{(0)}[\psi] \equiv J_M[\psi]_{\nabla(K)=0} \approx -\frac{1}{2}|A_0|S_a + K_e(\rho) + U_M(\rho), \tag{2.44}$$

where $K_e(\rho) \approx 1/2m\rho^2$; $U_M(\rho) \approx \beta_d T_N (\rho/a)^d$, $\beta_d \sim 1 (d = 3,2,1)$. Here, for $d=3$

$$\rho_M \approx a\left(\frac{D}{T_N}\right)^{1/5} \text{ and } J_M[\psi_0^{(0)}]$$

$$= E_{1M} \approx -\frac{1}{2}|A_0|S_a + c_1 D^{3/5} T_N^{2/5} < 0, \tag{2.45}$$

with $T_N \leqslant c_2 |A_0 S_a|^{5/2} D^{-3/2}$; $c_1 \sim 1$, $c_2 \sim 0.1$. The spin polaron is a self-consistent self-trapped state with a large radius for an electron in the region of the other almost ferromagnetic phase which the electron creates; as T increases, this self-trapped state is destroyed.[26,27,78,79,5)] Such self-trapped states can also arise in the antiferromagnetic phase of a Hubbard semiconductor (see Refs. 80, 78). The interaction of the electron with the phonons increases the stability of the spin polaron (see, for example, Ref. 79). But for very strong electron-phonon coupling the current carrier is most likely a small polaron in the antiferromagnetic crystal, whose motion has singularities. Thus, according to Ref. 83, the hopping of a small polaron at temperatures $T<T_N$ between different magnetic sublattices is accompanied by a change in the surrounding spin configuration, and the activation energy of hopping conductivity $\mu_h \sim \mu_0 z W_h/T$ [see (2.32)] increases by an amount $\sim T_N$; this effect has apparently been observed in NiO.[6)]

3. SELF-TRAPPED STATES ON DEFECTS IN A CRYSTAL LATTICE

A defect in a crystal lattice, including an impurity center, which attracts an electron can facilitate the formation of the ground self-trapped state of the electron when such a state does not exist in the regular crystal. This phenomenon is called extrinsic self-trapping. It is desirable to distinguish the situation in which the defect is a trapping center, in the sense that in the absence of self-trapping it corresponds to at least one bound state and a discrete level of the electron in the interband gap, from the alternative situation in which the defect does not have such a discrete level in the gap.

a) One-electron self-trapped state on a trapping center

The simplest situation is a trapping center with a long-range attractive field $\varphi_d(r) = -\varepsilon_d a_B r^{-1}$ with $\varepsilon_d = Z_0 e^2/\varkappa_0 a_B$. The radius of the ground electronic state of such a center, in the absence of self-trapping, is $a_B = \varkappa_0/me^2$ and here is a discrete level $\varepsilon_B = -me^4 Z_0^2/2\varkappa^2$ in the gap; in semiconductors $a_B \gg a$ and $|\varepsilon_B| \ll E_g$ (shallow level) for typical values of $\varkappa_0^2 \gg 1$ and $m < m_0$. For a system with long-range electron-phonon coupling (2.6) or (2.9), within the framework of Pekar's approach, the ground self-trapped state of the trapping center corresponds to a unique, finite minimum of the functional of the system (analog of the functional (2.21) in the continuum model)

$$J_L^{(d)}[\psi] \equiv \tilde{J}_L^{(d)}(\gamma) = \gamma^2 K_e^{(0)} - \gamma\delta_{0L}^{(0)}, \tag{3.1}$$

where $\gamma = 2K_e^{(0)}/\delta_{0L}^{(d)} = 1$, $\delta_{0L}^{(d)} = \delta_{0L}^{(0)} + \bar{\varphi}_d^{(L)}$. The polaron binding energy at a trapping center for a bound polaron with a large radius ($\rho_p^{(d)} \gg a$)[84,25] is given by

$$E_{1p}^{(d)} = E_1 + |\varepsilon_B| = -\frac{1}{2}\delta_{0L}^{(d)}$$

$$= -\frac{1}{2}\delta_{0L}^{(0)}\left[1 + \frac{4Z_0\varkappa}{\varkappa_0}\left(1 + \frac{3}{4}\frac{Z_0\varkappa}{\varkappa_0}\right)\right], \tag{3.2}$$

with $\bar{\varphi}_d \equiv -\int d\mathbf{r}\varphi_d(\mathbf{r})|\psi_0^{(0)}(\mathbf{r})|^2 > 0$, $E_1 \equiv J^{(d)}[\psi_0^{(0)}]$.

The criterion for extrinsic self-trapping, $0.109\alpha^2 \times (1 + \bar{\varphi}_d/0.109\alpha^2\omega_p) \gg 1$, can be satisfied for smaller values of α^2 than in (2.24), so that a bound polaron can exist when a polaron state is not realized in the regular lattice (for example, when $\alpha^2 < 10$ and $\bar{\varphi}_d \gg \omega_p$). The polaron self-trapping can appreciably increase (by $\sim\bar{\varphi}_d$) the width of the impurity gap and convert a center with a shallow electronic level in the gap ($|\varepsilon_B| \ll E_g$) into a deep center. As also for polaron self-trapped states in a crystal [see (2.23) and (2.31)] $\varepsilon_{opt} - \varepsilon_{th} \approx \delta_{0L}^{(0)} \gg \omega_{ph}$, and the absorption spectrum contains wide bands and at least one no-phonon line corresponding to a resonant transition between the $\psi_0^{(0)}$ state and the first excited self-consistent state (see Refs. 5 and 85).

The situation is qualitatively different in a 3D system with short-range electron-phonon coupling (2.7) or (2.8). The corresponding functional

$$J_S^{(d)}[\psi] \equiv \tilde{J}_S^{(d)}(\gamma) = \gamma^2 K_e^{(0)} - \gamma^3\delta_{0S}^{(0)} - \gamma\bar{\varphi}_d^{(S)}, \tag{3.3}$$

aside from minima corresponding to the starting shallow electron level ε_B and (in the limit $\gamma \to \infty$) a bound small polaron, may or may not have a minimum (for finite γ) for a bound polaron with a larg radius, when $(K_e^{(0)})^2 \gtrsim 3\delta_{0S}^{(0)}\bar{\varphi}_d^{(S)}$. In this case, in contrast to the case (3.2), states with shallow and deep (polaron) levels coexist (they are separated by barriers in q space), and the transition from one type of stable state to another with increasing Λ (with $\Lambda = \Lambda_c^{(d)} \sim 1$) is discontinuous, as in the case $\bar{\varphi}_d = 0$ (see Sec. 2d). For 1D systems in the limit $\gamma^3\delta_{0S}^{(0)} \to \gamma\delta_{0S}^{(0)}$ in (3.3) the situation is similar to the situation described in the case of (3.2).

The structure of a self-trapped polaron state on a short-range trapping center depends on the specific configurations of the defect and the type of electron-phonon coupling. In the cases (2.7) and (2.8) the quantity $|W_1^{(d)}| = |W_1| + \bar{\varphi}_d$ plays the role of the binding energy of the self-trapped state, instead of $|W_1|$, and the ground state on the defect is self-trapped when $|W_1^{(d)}| > D/2$, even when the criterion (2.35) does not hold, as soon as $\bar{\varphi}_d$ is large enough. This apparently happens for some donors in InSb crystals, in whose regular lattice self-trapping does not occur (see Ref. 86). The situation is analogous in the cases (2.6) and (2.9) with the substitution $\delta_{0L}^{(0)} \to \delta_{0L}^{(d)}$ in (2.24) or $W_1 \to W_1^{(d)}$ in (2.25) (see Refs. 25, 51, 87).

A self-trapped state can form on a changing center (short-range defect with a changing configuration) even in the absence of electron-phonon coupling. The role of such a defect is played by a Jahn-Teller defect[88–90,93] or an off-center (a noncentral ion, see Refs. 17, 91). Thus the interaction of an electron with the local mode of the displacements q of atoms in a Jahn-Teller defect, which partially or completely removes the degeneracy of the populated term,[89] can lead to a self-trapped state with a small radius with energy $E_1 < 0$, when the interaction energy $V_{e-JT} = \varepsilon_1(q) - \varepsilon_1(0)$ is high enough; $\varepsilon_1(q)$ is the electron term of the defect. In the simplest model,[89] in which the significant displacements are harmonic, $E_0(q) \approx (1/2)kq^2$ and $V_{e-JT}(q) \approx -\lambda_{JT}q$, the one-electron state with small radius corresponds to the term

$$E_1 = E_1(q_1) \equiv \min E_1(q) \simeq \min\left[\varepsilon_1(q) + \frac{1}{2}kq^2\right]$$

$$= \varepsilon_1(0) + W_1^{(JT)} < \varepsilon_1(0), \tag{3.4}$$

where $q = q_1 \simeq \lambda_{JT}k^{-1} \ll a$ and, for the trapping center, $\varepsilon_1(0) \equiv \varepsilon_1^0 < 0$. The binding energy $|W_1^{JT}|$ and the equilibrium displacement q_1 can be significant, $\omega_D \ll |W^{(JT)}| \lesssim 0.3$ eV, $q_0 \ll q_1 \lesssim 0.1$ Å ($\ll a$) for typical values of the quasielastic constant $k \approx k^{(0)} \approx 10 - 30$ eV/Å^2 and of the, in this sense, strong coupling parameter $a\lambda_{JT}$ (~ 3 eV) (q_0 is a typical value of the amplitude of zero-point vibrations, $q_0 \ll 0.1$ Å). Such a self-trapped state is stable (ground state), being populated under equilibrium conditions when $E_1 < \zeta$, as soon as the correlation energy for the two-electron state of the defect $U > 0$ (ζ is the electron chemical potential).

An example of such Jahn-Teller defects, on which self-trapped states form, is the V vacancy in the p-Si crystal,[90] for which according to Ref. 89 the starting state is V^{2+}, and also $\varepsilon_1^0 - E_v \simeq 0.32$ eV, $\lambda_{JT}a \simeq 2.25$ eV, $q_1 \simeq 0.15$ Å, $k \simeq 15$ eV/(Å)^2, and at the same time $|W_1^{(JT)}| \approx 0.17 - 0.19$ eV $\ll E_g \simeq 1.2$ eV (and $\rho_p \approx a$). However, the one-electron self-trapped state on a V^+ vacancy is only metastable; the stable state is either the V^{2+} state or the two-electron self-trapped V^0 state, for which $U < 0$ (see Sec. 3c).[89,90]

For an off-center with z_0 ($\geqslant 2$) close ($\Delta r \ll a$) equilibrium positions of the atom (ion) in the crystal, small $k \ll k^{(0)}$, i.e., significant anharmonicity of the vibrations (Li^+ ion instead of K^+ in KCl, etc.; see Ref. 91) is characteristic. For such a changing defect (see Refs. 92, 17, 93) the one-electron self-trapped state corresponds to the term

$$E_1 \equiv E_1(q_1) \equiv \min E_1(q) \simeq \min\left[\varepsilon_1(q) + \frac{1}{2}kq^2 + C_0q^4\right]$$

$$\equiv \varepsilon_1^0 + W_1^{(off)} < \varepsilon_1^0, \tag{3.5}$$

with $\varepsilon_1(q)-\varepsilon_1^0 \equiv V_{e-off}(q) \simeq -\lambda_1 q+\lambda_2 q^2+\lambda_4 q^4$, $\lambda_1>0$, $C_0>0$, $\lambda_2<0$ and $\lambda_4>0$, where $Ca_0^2 \lesssim k^{(0)}$, $Ca_0^4 \gtrsim \lambda_4 a_0^4 \sim \lambda_1 a_0 \sim |\lambda_2| a_0^2$ with characteristic atomic (ionic) radius $a_0 \sim 1$ Å. The one-electron self-trapped state, arising in the presence of quite strong coupling between the electron and the displacement q of the ion in the off-center, the state is qualitatively similar to the state on a Jahn-Teller defect, but the quantitative characteristics can, of course, differ substantially. Thus q_1 and the binding energy $|W_1^{(off)}|$ can be much larger, for example, 0,1 eV $\lesssim |W_1^{(off)}| \lesssim 1$ eV ($|W_1^{(off)}| < E_g/2$) and $a_0 \gtrsim q_1 \gtrsim 0.1$ Å with $\lambda_1 a \sim 3$ eV, $0.01\, k^{(0)} \lesssim k \lesssim 0.1\, k^{(0)}$ (see Sec. 5b and also Refs. 17 and 18 for a more detailed discussion). An example of such a defect is an impurity In^{3+} ion replacing the Cd^{2+} ion in the CdF_2 crystal—a one-electron stable self-trapped state with a small radius in the model (3.5) could correspond to the substitution In^{2+} ion in CdF_2 with $U>0$ which has been studied in detail (see, for example, Ref. 87).

As also for a conduction electron, for an electron at a trapping center in a 3D system a self-trapping barrier, generally speaking, exists so that a self-trapped state with a small radius and a weakly bound state with a large radius can coexist. In models of a trapping center, similar to the models (2.33)–(2.38), in which q_1 is not very large, $q_0 \ll q_1 \ll a_0$, as a rule, the curves of the adiabatic potentials $\Psi_0(q)$ for the ground self-trapped state and $\Psi_1(q)$ for the metastable weakly bound state have the form of the curves shown schematically in Fig. 1a with the characteristic optical and nonradiative transitions, including luminescence (radiative, "vertical" transition $I \to 0$). On the other hand, in the model (3.5) and similar models, in which q_1 is large, $q_1 \lesssim a_0$, and the schematic form of $\Psi_0(q)$ and $\Psi_1(q)$ is more likely similar to the curves in Fig. 1b. In this case, the luminescence is actually suppressed, and the lifetime of the populated metastable "weakly bound" (τ_{SL}^{*T}) and band (τ_{SL}^{**T}) states can be large, $\tau_{EL} \gg \omega_D^{-1}$, i.e., they can give rise to delayed photocurrents and other similar effects at low temperatures T (see Refs. 14, 87, 93–95).

b) One-electron self-trapped states on changing defects

One-electron self-trapped states in imperfect crystals can also form in systems which do not have filled local levels in the undeformed lattice as a result of the restructuring of the electron spectrum accompanying a corresponding deformation of the local atomic configuration. In this case, as shown in the theory developed in Ref. 14, self-trapped states can arise not only in the form of discrete levels in the gap in the spectrum, but also in the form of resonance levels with virtually zero width in the allowed bands. The potential of the defect in Ref. 14 is approximated, for simplicity, by a rectangular well (V_d) with a level $\varepsilon_1(q)$, lying above the Fermi level in the absence of deformation, $\varepsilon_1(0)>\zeta$. This level moves deeper into the gap as the deformation, actually the amplitude q (>0) of the "breathing" mode of the displacements accompanying the symmetrical expansion of the coordination sphere around the defect, increases. In this case, as soon as the level $\varepsilon_1(q)$ is, for all practical purposes, not repelled from the edge of the valence band, it can move into the band as q increases further (compare Sec. 5c).

A real localized state appears when the energy $\varepsilon_1(q)<\zeta$, i.e., the level is occupied by an electron. This effect was called in Ref. 14 impurity self-trapping. The corresponding self-trapped state arises with a finite deformation of the lattice ($q=q_1>q_c$), for which the minimum energy of the system is given by

$$E_1(q) \simeq \varepsilon_1(q)+\frac{1}{2}kq^2 \tag{3.6}$$

with $\varepsilon_1(q) \simeq \tilde{\varepsilon}-\lambda_0 V_d \delta^2(q)+\lambda_0^2 V_d \delta^3(q)$, $\tilde{\varepsilon}=\text{const}>\zeta \equiv \varepsilon_1(q_c)>\varepsilon_1(q_1)$, $\delta(q) \equiv (d(q)-d_a)d_a^{-1}$, $d_a=\text{const}$, $d(q)=d_0+\gamma_0 q$, $\gamma_0=\text{const}$, $\lambda_0=\pi^2/4$. The energy of the stable self-trapped state of the electron $E_1=E_1(q_1) \equiv \min E_1(q)$ and the height of the self-trapping barrier H_b^*, corresponding to the minimum ($q=q_1$) and maximum ($q=q_2$) of the energy change $\Delta E(q)$ accompanying the deformation of the lattice, were obtained in the form

$$\begin{aligned} E_1=E_1(q_1) &\simeq \tilde{\varepsilon}-\frac{16}{27\pi^2}V_d(1-\xi)^3 \\ &\quad +\frac{4}{3}V_d\xi(1-\xi)\delta_0(>\varepsilon_1(q_1)), \\ H_b^*=\Delta E(q_2) &=\frac{1}{4}\pi^2\xi\left(\delta_0+\frac{2\sqrt{\tilde{\varepsilon}-\zeta}}{\pi\sqrt{V_d}}\right), \end{aligned} \tag{3.7}$$

where $\xi \equiv k/4\gamma_0^2 m/V_d^2$, $k \equiv M_a\omega_0^2$ and $\delta_0 \equiv |\delta(0)|$. In this case both $E_1>0$ and $E_1<0$ relative to the other minimum

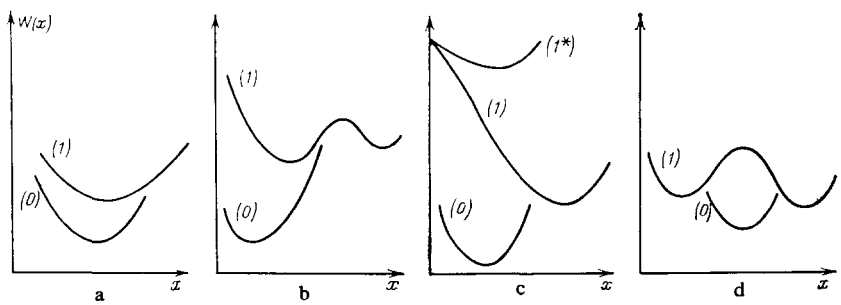

FIG. 1. Typical examples of possible dependences of the adiabatic potential of the ground (0) and excited (1), (1*) states on the configuration of the variable (q or x).

$\Delta E(q)$, the bottom of the conduction band, $\Delta E(q) = 0$ at $q = 0$ can occur. The conditions for the existence of the self-trapped state, $\xi \sim (M_a/m\gamma_0^2)(\omega_0/V_d) \ll 1$ and $\delta_0 \ll 1$, can be satisfied in the presence of a soft mode with frequency $\Delta E(q) = 0$ in the phonon spectrum of the crystal.

When $E_1 > 0$ the level of the metastable quasilocal self-trapped state of the electron stabilizes ζ, $\zeta = E_1$ if the number of electrons N_e is less than the number of defects N_d under study (and the number of other defects is small). Violation of the condition of equilibrium $\zeta = E_{11}$ with $N_e = \text{const}$ leads to transitions of electrons from metastable self-trapped states into Bloch states when $\zeta < E_1$ (or, conversely, when $\zeta > E_1$) with overcoming of a barrier (the self-trapping barrier for $\zeta > E_1$). On the other hand, when $E_1 < 0$ the localized ground self-trapped state has a thermal activation energy $|E_1|$ and is separated from the metastable Bloch states by the self-trapping barrier with a height $H_b'^* = H_b^* + |E_1|$. The situation for such a changing defect most likely corresponds to the schematic diagram in Fig. 1b (in the absence of a "weakly bound" electron state). The times of tunneling transitions for low $T \ll \omega_0$, $\tau_0 \equiv \tau(T = 0)$ and thermally activated transitions $\tau \propto \exp(-H_b/T)$, $H_b = \{H_b^*$ or $H_b'^*\}$ are exponentially large $\tau \gg \omega_0^{-1} (\gg \omega_D^{-1})$. The threshold energy of optical transitions from the self-trapped state into the Bloch state is $\varepsilon_{opt} = \zeta - \varepsilon_1(q_1)$ when $E_1 > 0$ or $\varepsilon_{opt} = |\varepsilon_1(q_1)|$ when $E_1 < 0$. In this case, long-time nonequilibrium effects (photocurrents, etc.), which can vanish rapidly as T increases, are expected. It is assumed in Ref. 14 that this model (3.6)–(3.7) adequately describes the unusual picture of nonequilibrium processes at low temperatures $T(\lesssim 20$ K) and the stabilization of ζ observed in the narrow-gap ($E_g \simeq 0.32$ eV) semiconductor $Pb_{1-\bar{c}}Sn_{\bar{c}}Te$ (In) ($\bar{c} \lesssim 0.2$). Here the In^{3+} ion, which replaces the main Pb^{4+} ion,[94,95] apparently corresponds to the changing defect which self-traps the electron.

The theory of self-trapped states of an electron on a changing defect, presented in Ref. 93, is developed in application to the model proposed there, associated most likely with the Jahn-Teller effect or some other in a certain sense similar effect. In this model the rearrangement of the local atomic configuration of the defect is accompanied by the appearance of a discrete level of the electron $\varepsilon_1(q)$ and its displacement into the gap; in addition, the energy of the defect with the trapped electron $\Lambda_i = \text{const}$, $\Lambda_1 \geqslant 0$, $\Lambda_2 \gtrless 0$, $\Lambda_4 > 0$, $C_1 = \text{const} > 0$) is given by

$$E_1(q) = \varepsilon_1(q) + \frac{1}{2}kq^2 + C_1q^4, \quad [q > 0, \quad k \ll k^{(0)},$$
$$\varepsilon_1(q) \simeq \tilde{\varepsilon}_0 - \Lambda_1 q + \Lambda_2 q^2 + \Lambda_4 q^4, \quad \tilde{\varepsilon}_0 > \zeta; \tag{3.8}$$

where the linear term $-\Lambda_1 q$ can characterize (for $\Lambda_2 > 0$) the coupling with the Jahn-Teller displacement, while the term $\Lambda_2 q^2$ (for $\Lambda_2 < 0$) can correspond to coupling with the soft phonon mode. For typical $\Lambda_1 a_0 \sim 1$ eV and small $\omega_0 \ll \omega_D$ for the case of a single populated term $\varepsilon_1(q) < \zeta$, the energy of the system $E_1(q)$ here also has two minima, corresponding to the Bloch (at the bottom of the band) and self-trapped states of an electron with finite $q = q_1$. These states are separated by a maximum (barrier), while the energy of the system $E_0(q) = (1/2)kq^2 + C_1q^4$ with an unpopulated term has a single minimum corresponding to the Bloch state at the bottom of the band (with $q = 0$). Such a model can describe a defect with a self-trapping barrier and a metastable state of the electron, a Bloch (with a self-trapped ground state) or a self-trapped state (Fig. 1c). In the model (3.8), which can be used, in particular, to interpret the electron properties of $Pb_{1-\bar{c}}Sn_cTe(In)$ ($\bar{c} \lesssim 0.2$) at low temperatures T, the changing defect in this crystal can be, in accordance with Refs. 94 and 95, a vacancy or a substitution In^{3+} ion.

A common feature of the models (3.6), (3.8), and (3.5), which can describe the appearance of a stable bound self-trapped state on a changing defect, is the presence of nonlinear electron-atom interactions and/or anharmonicities of the local atomic configuration. This determines the self-trapping barriers characteristic for changing defects, metastable bound electron states, and therefore specific long-lasting nonequilibrium effects. Finally, in all the models examined above (3.1), (3.3)–(3.6), and (3.8) we are talking about bound, self-trapped, one-electron states with spin $\sigma = 1/2$.

c) Two-electron bound self-trapped states

When the inequalities (2.43) hold, the ground state of a changing defect can only be a two-electron singlet self-trapped state with a negative correlation energy $U < 0$. Thus in the model (3.4) the energy of the two-electron self-trapped state $E_2(q) \simeq (1/2)kq^2 + 2\varepsilon_1(q) + U_c(q)$ is minimum,

$$E_2 = E_2(q_2) \equiv \min E_2(q) \simeq 2\varepsilon_1^0 + W_2^{(JT)} + U_c)$$

with

$$q_2 \approx 2q_1 \approx 2\lambda_{JT}/k, \quad W_2^{(JT)} \approx 4W_1^{(JT)} \approx -2\lambda_{JT}^2/k,$$

and such a state is the ground state when $E_2 < 2E_1 < 0$, i.e.,

$$U = E_2 - 2E_1 \simeq U_c - \frac{\lambda_{JT}^2}{k} < 0. \tag{3.9}$$

($|U| < 0.3$ eV for typical values $|W_1^{(JT)}| \lesssim 0.3$ eV and $U_c \lesssim 0.3$ eV).[89,90] The ground bound two-electron state of a defect is spinless (at least when the populated term is orbitally nondegenerate) and, generally speaking, is separated by a self-trapping barrier from metastable one-electron bound and Bloch states; such different states and the long-lasting nonequilibrium effects can therefore exist even here, especially at low temperatures T. Under equilibrium conditions the two-electron self-trapped states are stable only when $E_2 < 2\zeta$, while when $E_2 > 2\zeta$ such states are not populated.

An example of a defect with a singlet two-electron ground state (V^0) with $E_2/2 < \zeta$ or a V^{2+} state with $E_2/2 > \zeta$ is a vacancy in p–Si (see above). For this defect $U < 0$ and $|U| \simeq 0.1$ eV with $U_c \simeq 0.25$ eV and $q_2 \simeq 2q_1 \simeq 0.3$ Å.[89,90] In this case, the single-electron state V^+ is metastable, as demonstrated in experiments on photo-induced EPR.[90] These experiments and investigations of the electron structure of a vacancy in p–Si showed, within the framework of the method of dielectric capacitive spectroscopy, for all practical purposes unequivocally that such a defect is a center with $U < 0$, described by the model (3.4) and (3.9).

Similar singlet two-electron self-localized states with $U<0$ can also be characteristic for the models (3.5), (3.6), and (see Ref. 93b) (3.8), with realistic $|U| \lesssim 0.3$ eV or even (in the same models) $2|U| \lesssim E_g \lesssim 1-2$ eV (see Sec. 5). From this viewpoint, such a state can be a ground state for a changing diamagnetic defect in $Pb_{1-\bar{c}}Sn_{\bar{c}}Te$ (In,Ga) also, in agreement with a recent hypothesis.[95]

We also assume that the interstitial boron atom B_i in the p–Si crystal, which has, depending on the position of ζ, one of two stable states, B_i^- or B_i^+,[90] i.e., it is a center with $U<0$, can be described as a changing defect of the off-center type in the model (3.5), whose stable state B_i^- corresponds to a filled singlet two-electron ground state (on the reference B_i^+ ion) with $U<0$ (see Sec. 5).

4. SELF-TRAPPED ELECTRON STATES IN A DISORDERED SYSTEM

In disordered systems both polaron self-trapped states and new types of self-trapped states, which do not occur in regular systems and are determined by the nonlinear response of the medium, can exist. The latter includes fluctuons, which we shall study in this section, and two-electron states with a negative correlation energy, which are studied in Sec. 5.

a) Characteristic features of polaron self-trapped states

These features are determined by the characteristic features of the "bare" (in the absence of electron-induced deformation of the structure) one-electron energy spectrum E.[96–100] Thus in 1D and 2D (in the absence of magnetic fields) systems all states are trapped in the sense that the conductivity $\sigma=0$ with $T=\omega=0$.[96,97,103] In a 3D system near the mobility threshold $E_1^* \equiv E_c^* (E_2^* \equiv E_v^*)$, separating the mobility gap (region of trapped states) from the conduction (valence) "band", the amplitudes of the untrapped states when $E_c^* < E < E_{uv}^*$ ($E_{uv}^* < E < E_v^*$) and weakly localized states when $E_{lc}^* < E < E_c^*$ ($E_v^* < E < E_{lv}^*$) are substantially inhomogeneous, fluctuating over distances ρ of the order of $\rho_1(E) \gg \rho_1(E_u^*) \approx a$, $\rho_2(E) \gg \rho_2(E_l^*) \approx a$ (they are almost homogeneous when $\rho \gg a$ for $E > E_{uc}^*$ or $E < E_{uv}^*$, or have a radius $\approx a$ for $E < E_{lc}^*$ or $E > E_{lv}^*$).

It was recently shown[101] that in a 3D system even a weak electron-phonon (short-range) coupling ($\Lambda < 1$) transforms the inhomogeneous (metastable) states mentioned above into stable polaron self-trapped states. The latter have a large radius ρ_p, $\rho_\alpha(E) \lesssim \rho_p \approx \rho_p^{(c)} \sim a\Lambda^{-1} \gg a$ when $\Lambda < 1$ ($\alpha = 1,2$), since $\rho_\alpha(E) \gtrsim \rho_0(\Lambda) \sim 3a\Lambda^{-1}$.[160] In this case the mobility threshold is displaced, $E_1^* \equiv E_c(\Lambda=0) \to E_c \equiv E_c(\Lambda)$ for $\rho_1(E_c) = \rho_0(\Lambda)$ and $E_c^* < E_c < E_{uc}^*$, while the conductivity $\sigma(E) \equiv \sigma(E|T=\omega=0)$ as $E \to E_C \pm 0$ undergoes a jump $\Delta\sigma = A_c \Lambda^\delta$ with $A_c = 0.05e^2/\pi^2\hbar a$ and $\delta = 2/3$. As Λ increases, ρ_p continuously decreases and $\Delta\sigma$ increases. In the presence of strong coupling, $\Lambda \gtrsim \Lambda_c$ ($1 < \Lambda_c < 10$; see Sec. 2d), all such self-trapped states are small polarons and $E_c \simeq E_{uc}^*$ (compare the phenomenological model,[102] in accordance with which the important current carriers in a glassy semiconductor are small polarons), while $\Delta\sigma$ is close to the Mott minimum metallic conductivity $\sigma_M \approx 0.25e^2/\pi^2\hbar a$ (see Refs. 96 and 97). This situation differs significantly from that described in Sec. 2d for self-trapping in a crystal (for a discussion of Anderson localization of small polarons in a 3D system see, for example, Refs. 103, 21, 96). According to Ref. 101, the effects under study occur at least as soon as the interelectron correlations are no longer important and for very low T (and these effects are negligible for very small $\Lambda \ll 1$).

The motion of localized polarons (in the gap) is determined by thermally activated hopping. The effective activation energy of such hopping $\mathscr{E}_a(T, \Lambda)$ is virtually independent of T, $\mathscr{E}_a(T, \Lambda) \simeq \mathscr{E}_a(\Lambda) \geqslant \mathscr{E}_a(0)$, for high $T \gtrsim T_0$, but $\mathscr{E}_a(T, \Lambda) \propto T^\varkappa$ for lower temperatures T. In the latter region $\varkappa \equiv \varkappa(\Lambda) \simeq \varkappa(0)$ for very low T ($\to 0$) or $\Lambda \ll 1$ (for example, $\varkappa(0) = 4^{-1}$ [96] or $\varkappa(0) = 1/2$ with $d = 3$[98]), but $\varkappa < \varkappa(0)$ for $\Lambda > 1$ and intermediate values of T ($\varkappa = 1/7$ instead of $\varkappa = 1/4$ with $d = 3$ or $\varkappa < 1/2$ instead of $\varkappa = 1/2$), due to the contribution of the polaron effect and multiphonon processes.[21,104]

b) Fluctuons. Basic relations

In a system in which the important interaction with the medium is short-ranged, self-trapped states with large radius ($\rho_f \gg a$)—fluctuons—appear.[15,16,23] Unlike polarons, they are determined by the nonlinear response of the medium and can exist in a system with any dimensionality, including 3D systems. In the latter, fluctuon states can be both untrapped and trapped (in the mobility gap), while in 2D (in the absence of magnetic fields, see above) and 1D systems they are trapped in the sense indicated above.

Let a spatial fluctuation—a deviation $\delta\eta \equiv \eta - \bar{\eta}$ of the macroscopic parameter $\eta(\mathbf{r})$ from the average value $\bar{\eta}$, which in the absence of an electron decays over a characteristic time τ_R—appear in the system. Such a fluctuation with appropriate sign and magnitude of $\delta\eta$ can lead to the formation of a quite wide and deep potential well for the electron, which is required (at least, in 3D systems) for the existence of a bound state of the electron with a radius $\rho_f \gg a$ with quite a low-lying discrete energy $\varepsilon_1 < 0$, $|\varepsilon_1| \gg T$. The field of such a bound electron maintains the stationary nature of the fluctuations. The self-consistent self-trapped state—the fluctuon—which appears can be viewed as a thermodynamically stable bound state of the electron and the fluctuations. Examples of such systems are solid and liquid solutions of the type $X_{\bar{c}}Y_{1-\bar{c}}$ ($0 \leqslant \bar{c} \leqslant 1$) and magnetic materials, in which the spins $\uparrow$ and $\downarrow$ play the role of the X and Y atoms: in the former $\eta(\mathbf{r}) \equiv c(\mathbf{r}) \equiv c(\leqslant 1)$—is the local concentration of X atoms, and in the latter $\eta(\mathbf{r}) \equiv M_z(\mathbf{r})/M^0$, $|\eta(\mathbf{r})| \leqslant 1$ ($M_z(\mathbf{r})$ is the local magnetization and $M^0 \equiv M_0(0)$, $M_0(T)$ is its equilibrium value). Unlike polarons, fluctuons exist in a bounded range of temperatures, which need not include low temperatures T, and must correspond to a minimum of the thermodynamic potential of the system Φ.

There are two approaches to the study of such electron states. In one approach the states of an electron in a random field of fixed, randomly distributed atoms is studied.[16] Actually, the fluctuation levels E of the electron—the ground

states in potential wells created by suitable, optimal, local fluctuations of the atomic (spin) configuration—are important (at least, below the mobility threshold E_c in the mobility gap). Such an optimal fluctuation with radius $R_f(E)$ is macroscopic, $R_f(E) \gg a$, in the often encountered case of wide-band electrons with

$$D \gg |A_0| \gg T, \tag{4.1}$$

in which electron trapping on a separate atom (spin) is not realized in a 3D system; $A_0 (\gtrless 0)$ is the electron-atom (spin) coupling constant. In the case (4.1), which we shall have in mind primarily below, in the macroscopic approximation the level E corresponds to the probability $p_f(E) \equiv \exp\{-\Delta S[R_f(E)]\}$ for the realization of the optimal fluctuation; its radius $R_f(E)$, in its turn, is determined by the radius $\rho_f(E)$ of the ground state of the electron in the fluctuation potential well ($a \ll \rho_f(E) \lesssim R_f(E), \rho_f(E) \ll 1$). For a fixed temperature T it is possible to find the energy E for which the quantity

$$\Delta F(E) = -T \ln p(E) = E - T \ln p_f(E) \tag{4.2}$$

is maximum, as soon as the distribution of the electrons over the fluctuation levels is determined by the function $p(E) = p_f(E)\exp(-E/T)$. The state $\psi_T^{(0)}(E)$ with the energy E, at a given temperature, is most probable, as is the corresponding stationary fluctuation of the composition $\delta c_T^{(0)}(E)(\delta\eta_T^{(0)}(E))$, and in this sense it is a self-consistent stable self-trapped state. According to this model, the required condition for realizing the self-trapped states

$$\tau_R \gg \tau_e \tag{4.3}$$

means that the electron in the fluctuation potential well over its lifetime τ_e does not have enough time to cause a corresponding rearrangement of the atoms.

Another approach,[15,23] which is widely used to study fluctuations in the same case (4.1), consists of a significant generalization of Pekar's approach (2.13)–(2.14). In this approach the problem of finding the thermodynamically stable fluctuons of the self-trapped states $\psi_T^{(0)}$ reduces to the solution of the problem of finding the minimum thermodynamic potential of a system containing a "stationary" self-trapped electron (with a fixed center of inertia), i.e., of the corresponding functional $\Phi[\psi,\eta]$:

$$\begin{aligned}
&\min_{\{\psi,\eta\}}\Phi[\psi,\eta] = \min_{\{\psi\}}\Phi[\psi] = \Phi_T^{(0)}\\
&\text{with } \psi = \psi_T^{(0)} \text{ and } \eta = \eta_T^{(0)} \equiv \eta[\psi_T^{(0)}],\\
&\text{где } \Phi[\psi,\eta] = E_e[\psi,\eta] + R(\eta),\\
&E_e[\psi,\eta] = K_e[\psi] + V[\psi,\eta],\\
&V[\psi,\eta] = \int d\mathbf{r}\,|\psi(\mathbf{r})|^2 V(\mathbf{r},\eta),\\
&\Phi[\psi] \equiv \min_{\{\eta\}}\Phi[\psi,\eta].
\end{aligned} \tag{4.4}$$

where $\Phi[\psi,\eta] = E_e[\psi,\eta] + R(\eta)$, $E_e[\psi,\eta] = K_e[\psi] + V[\psi,\eta]$, $V[\psi,\eta] = \int d\mathbf{r}|\psi(\mathbf{r})|^2 V(\mathbf{r},\eta)$, $\Phi[\psi] \equiv \min_{\{\eta\}} \times \Phi[\psi,\eta]$.

The expression for $V(\mathbf{r},\eta)$, the potential energy of the electron in the region of the fluctuation $\eta(\mathbf{r})$, is usually approximated in the form[23]

$$V(\mathbf{r},\eta) = -A_0\delta\eta(\mathbf{r}) \equiv -A_0(\eta(\mathbf{r}) - \bar{\eta}), \quad A_0 \gtrless 0, \tag{4.5}$$

and the relation for the minimum work required for a reversible creation of the fluctuation $\eta(\mathbf{r})$ has the form

$$R(\eta) = \int d\mathbf{r}\left[\varphi(\eta(\mathbf{r})) - \varphi(\eta_0) + \frac{1}{2}P_0(\nabla\eta)^2\right] \equiv R_1 > 0, \tag{4.6}$$

or

$$R = R_1 + R_2, \quad R_2 = \int d\mathbf{r}\,(c(\mathbf{r}) - \bar{c})\left(-\frac{\partial\varphi(c(\mathbf{r}))}{\partial c}\right); \tag{4.7}$$

where $\varphi(\eta)$ is the density of the thermodynamic potential, while R_2 takes into account the conservation of the total number of atoms. The fluctuon exists when

$$\Phi_T^{(0)} < 0, \quad |\Phi_T^{(0)}| \gg T. \tag{4.8}$$

The condition that $\Phi[\psi,\eta]$ has a minimum with respect to η, with the state ψ fixed, determines the distribution $\eta[\psi]$ in the effective field $(-A_0|\psi|^2)$ of the self-trapped electron. Ultimately, the functional $\Phi[\psi]$, which determines the ground fluctuation state $\psi_T^{(0)}$, has the form

$$\Phi[\psi] = K_e[\psi] - A_0\int d\mathbf{r}\,|\psi(\mathbf{r})|^2\delta\eta[\psi(\mathbf{r})] + R\{\eta[\psi(\mathbf{r})]\}. \tag{4.9}$$

In the approach under discussion,[15] the self-consistent self-trapped state is formed with the self-trapped electron adiabatically following the slow changes of the fluctuations, while over its lifetime τ_e the self-trapped electron has time to cause a corresponding redistribution of the atoms (spins)

$$\tau_R \ll \tau_e. \tag{4.10}$$

However, Euler's equations for the extremal problem for the functionals (4.2) and (4.9), determining the self-trapped state, the energy of the electron ε_1, and correspondingly the thermodynamic potential of the system, coincide in both approaches, because the stationary characteristics of the self-trapped state should not depend on the kinetics of its formation, i.e., on the value of τ_R/τ_e. The ground state of the fluctuon (as also of a large polaron) corresponds to a spherically symmetrical wave function (the s state) $\psi_T^{(0)}(\mathbf{r})$.

In the case (4.10) the motion of the fluctuon, at least, corresponding to the untrapped "bare" one-electron state in the 3D system, is essentially linked to a specific mechanism, determined by the diffusion of atoms (spins) and the displacement of the electron and the accompanying stationary fluctuation corresponding to the diffusion.[23] This mechanism (instead of the direct electron hops) could be important also for fluctuons, corresponding to the trapped states of the 3D system, and also to states of 2D and 1D systems. At the same time, the mobility of the fluctuon, associated with thermally activated transitions of atoms (spins) during their diffusion, can be estimated as[15,105]

$$\mu_f \approx |e|\, D_T\, (Tn_f)^{-1} \ll |e| D_T T^{-1}$$

$$\text{for} \quad n_f \equiv \beta_d \rho_f^d v_0^{-1} \approx \left(\frac{\rho_f}{a}\right)^d \gg 1 \quad (\mu_f \to 0 \text{ for } T \to 0); \tag{4.11}$$

where n_f is the number of atoms (spins) in a macroscopic fluctuation, accompanying the electron; D_T is the coefficient of atomic ($D_T^{(a)}$) or spin ($D_T^{(\sigma)}$) diffusion ($D_T \to 0$ as $T \to 0$); $\beta_d = \text{const} \sim 1$. In any case, the displacement in an elementary act is small, $L_f \lesssim L_D\, n_f^{-1/2} \ll \rho_f$, where the characteristic diffusion length is $L_D < \rho_f$. In addition, since the contribution of the translational motion of N_f fluctuons to the thermodynamic potential $\Phi(N_f)$ of a degenerate gas is determined by the number of permutations over N_0 possible positions, a relation exists between N_f and the number N_e of non-self-trapped (band) electrons in Ref. 15:

$$N_f N_e^{-1} = \frac{\alpha_f}{v_0}\left(\frac{2\pi\hbar^2}{mT}\right)^{d/2} \exp\left(-\frac{\Phi_T^{(0)}}{T}\right) \gg 1$$

$$\text{for} \quad |\Phi_T^{(0)}| \gg T,\ \alpha_f \sim 1. \tag{4.12}$$

On the other hand, in the case (4.3), which most likely corresponds to the trapped electron states of a system with arbitrary dimensionality, the formula (4.12) is adequate only for $N_e\, N_0^{-1} < p_0$ (p_0 is the concentration of entrained optimal fluctuations), while the motion of the fluctuon is most likely determined by electron hops, not necessarily associated with the diffusion of atoms (spins), $\mu_f \to 0$ as $T \to 0$.

The formation of fluctuons must be more efficient in a system in which the fluctuations $\delta\eta$ lead to a relatively small value of $R(\eta)$. This occurs primarily near second-order phase transitions and critical points of the system.[15,106] In the general case a fluctuon forms in the presence of a nonlinear response of the medium—the stationary distribution $\eta_T^{(0)}(\mathbf{r})$ in the region of the fluctuation self-trapped state is related nonlinearly to the field of the electron $-A_0|\psi|^2$. This is observed most clearly for a fluctuon in an ideal system, in which, by definition, there are no direct couplings between atoms (spins), so that only indirect couplings, determined by the self-trapped electron, exist near the fluctuon.

c) A fluctuon in an ideal system

For an ideal solution $X_{\bar{c}}\, Y_{1-\bar{c}}$ with $A_0 > 0$ the substantially nonlinear relationship between $\eta_T^{(0)}$ and $|\psi(\mathbf{r})|^2$ has the form[15]

$$\eta_T^{(0)}(\mathbf{r}) = \bar{\eta}\left\{\alpha_1 + \alpha_2 \exp\left[-A_0 \frac{v_0}{T}|\psi(\mathbf{r})|^2\right]\right\} \equiv \eta_T^{(0)}[\psi(\mathbf{r})], \tag{4.13}$$

where

$$\varphi(\eta) \equiv \varphi(c) = (T/v_0)\,[c \ln c + (1-c)\ln(1-c)]$$

and $\alpha_1 = \bar{\eta} \equiv \bar{c}$,

while for $A_0 < 0$ it is necessary to make the substitution $\bar{c} \rightleftarrows 1 - \bar{c}$ in (4.13). The same relation is also valid for ideal paramagnets with an atomic spin $S_a = 1/2$ with the substitution

$$\bar{c} \to S_a = \frac{1}{2}, \quad A_0 \to 2A_0 \text{ and with } \eta \equiv \frac{M_z}{M_0} \tag{4.14}$$

(and for estimates in the general case of an ideal paramagnet—with $\bar{c} \to S_a \geqslant 1/2$ and $A_0 \to A_0 S_a^{-1}$.

The analysis of the extremal problem for the functional $\Phi[\psi,\eta]$ in a 3D system showed that the fluctuon in an ideal system exists at all sufficiently low temperatures $0 < T < \theta^*$.[15,23] In this case, according to Ref. 23,

$$n_f \equiv \frac{4\pi}{3}\rho_f^3 v_0^{-1} = \gamma_1\left(\frac{D}{T}\right)^{3/5} \gg 1$$

$$\text{for} \quad T \ll \theta^* \quad \left(\text{and } \bar{c} \approx \frac{1}{2}\right), \tag{4.15}$$

$$\theta^* = \gamma_2 |A_0| \left|\frac{A_0}{D}\right|^{3/2} \ll |A_0|, \quad n_f(\theta^*) = \gamma_3 \left|\frac{D}{A_0}\right|^{3/2} \gg 1, \tag{4.16}$$

where $\gamma_i = \text{const}$ (more precisely, $\gamma_1 \simeq 1/3$, $\gamma_2 \simeq 1/20$ and $\gamma_3 \simeq 3$). In the ideal system studied $\varepsilon_1 \simeq -0.12|A_0|$ and $T = \theta^*, \bar{c} \approx 1/2$, so that for (4.1) and $T \ll \theta^*$ the inequalities $D \gg |A_0| \gg 20T$, $|\varepsilon_1| \gg T$, and also $|\Phi_T^{(0)}| \gg T$ hold automatically, in accordance with the criterion (4.8). A characteristic feature of a fluctuon in an ideal system is the sharp change in $c_T^{(0)}(\mathbf{r})$ in the region of the self-trapped electron (see (4.14)): At the center when $A_0 < 0$ $c_T^{(0)}(0) \ll \bar{c}$, while the potential energy has the smallest possible value ($A_0\bar{c}$), to which ε_1 and $\Phi_T^{(0)}$ tend.[15] It is precisely the nonlinear response of the medium, i.e., the nonlinear dependence of the quantity $\delta c_T^{(0)}(\mathbf{r}) \equiv c_T^{(0)}(\mathbf{r}) - \bar{c}$ on the field of the electron $-A_0|\psi|^2$, leading to its saturation, with $\delta c_T^{(0)} \approx -\bar{c}$ for $r \ll \rho_f$, that produces for (4.1) the macroscopic dimensions of the fluctuon. It is this that strongly distinguishes a fluctuon from a small polaron, which in the presence of short-range electron-phonon coupling arises in the case of a linear response of the medium only as a result of an increase in the depth (but not width) of the potential well in the case of quite strong coupling. Like a small polaron, however, in a 3D system the fluctuon is separated from the Bloch states of the electron in the band by a self-trapping barrier, whose height $H_b^{(f)} \sim 5|D/A_0|^{3/2}T^2|A_0|$ ($T \ll \theta^*$ and $\bar{c} \approx 1/2$) can be significant for $D \gg |A_0| \gg 20T$ decreasing as T decreases. For a fluctuon in 1D and 2D systems the presence of a self-trapping barrier is not characteristic. This follows explicitly from the results of Ref. 16, where the electron states, similar to the states of the fluctuon type in the solution $X_{\bar{c}}\, Y_{1-\bar{c}}$ with $\bar{c} \ll 1$ (or $1 - \bar{c} \ll 1$) both in 3D and in 1D and 2D systems, were studied in detail.

Fluctuons exist in a ferromagnet only at quite high temperatures $T > \theta_1^*$, and in addition $0 < \theta_1^* < T_c$ (T_c is the Curie point, see Ref. 23 and below). Fluctuon self-trapped states can also exist as stable states of an electron in an antiferromagnetic crystal not only at temperatures $T \gtrsim T_N$ but also at temperatures $T \ll T_N$, when the system is ordered, in this case the self-trapped state of the electron is identical to the spin polaron (2.44) discussed in Sec. 2g.[26,27]

The transition of the electrons into the fluctuon state occurs at $T = \theta_0^* \approx \theta^*$ in a narrow range $\delta T \approx 2\theta^* n_f^{-1} \ll \theta^*$, reminiscent of a diffuse first-order phase transition.[15,16,23] At the same time the electron properties of the system must change substantially; in particular, the electron heat capacity must have a peak at $T \approx \theta^*$, $C_f N_f^{-1} \sim n_f^2 \gg 1$(see Ref. 23). The effect of the fluctuons formed on the properties of a semiconductor was studied in a number of works (see, for example, Refs. 15, 23, and 107). Thus the magnetic properties (magnetic susceptibility, etc.) of a semiconductor in the region of existence of stable fluctuons differ substantially from the properties in the alternative region, since the moment of the fluctuon is anomalously large $m_f \approx n_f \mu_B \gg \mu_B$.

The mobility μ_f and the effective mass M_f of a fluctuon in 3D system were studied in Ref. 105 and it was shown that M_f is large, $M_f \gg m$, and μ_f is small, $\mu_f \ll \mu_0 \sim 1$ cm^2/V·s, and there is no direct coupling between them; in addition, $\mu_f \to 0$ as $T \to 0$($\mu_f \propto \exp(-E_a/T)$) in the solutions $X_{\bar{c}} Y_{1-\bar{c}}$ or $\mu_f \propto T^{1/10}$ when $T \lesssim \theta^*$ in paramagnetic materials. The coexistence of stable fluctuons and metastable band electrons with $\mu_e \gg \mu_f$ could be manifested in the strong growth of the mobility accompanying an increase in T ($\lesssim \theta^*$).

d) Other fluctuon effects

Self-trapped electron states, reminiscent of fluctuons, also appear in the paramagentic phase of a Hubbard semiconductor. In this case, an effective exchange coupling between a conduction electron and the core electrons arises due to the Hubbard interelectron interactions and the well-known symmetry properties of multielectron states. Such self-trapped states (in particular, for magnetic ^{3}He atoms in an ^{4}He crystal[110]) and their properties have been studied in a number of works (see, for example, Refs. 17, 110–113). The effect of a direct interaction between atoms (spins) on the properties of fluctuons leads primarily to the appearance of a finite lower boundary θ_1^* of the region of their existence (see, for example, Refs. 114–116). Thus in a paramagnetic material this region encompasses the point T_c of the magnetic phase transition, $\theta_1^* < T < \theta^*$ for $\theta^* > T_c$ and $0 < \theta_1^* < T_c$. (In the fluctuon group the indirect interaction between atoms or spins, caused by the self-trapped electron, is usually greater than their direct interaction; see, for example, Refs. 23 and 114.) Fluctuon states can also form on defects and impurity centers.[117] The characteristic features of self-trapped states with an arbitrary value of $D/|_1 A_0|$, the properties of fluctuons with a multiellipsoidal anisotropic (nondegenerate) electronic band, and other problems in the theory of fluctuon self-trapped states were studied in a number of recent works (see, for example, Ref. 118).

As the number $N_f a^3$ of current carriers increases, thermodynamically stable complexes consisting of ν electrons ($\nu \geqslant 2$) in a common fluctuon potential well[15,23] and, for not very large values of N_f, an equilibrium heterogeneous structure, containing small ($\sim 10^2$–10^3 Å) metallic particles ($\nu \gtrsim 10^2 - 10^3$) and having specific properties, appear.[119,23] A heterogeneous equilibrium structure of a ferroelectric crystal can appear near the point of a phase-transition.[120] Such a structure can also exist in magnetic semiconductors.[121,122]

5. SELF-TRAPPED STATES IN AMORPHOUS SYSTEMS—TWO-ELECTRON CENTERS WITH NEGATIVE CORRELATION ENERGY

The specific features of electron states in a mobility gap (not very close to the electron mobility threshold, see Sec. 4a) in 3D amorphous, actually glassy semiconductors (GS) are manifested in the coexistence of different properties, such as the stabilization (pinning) of the electronic Fermi level ζ near the center of the gap and, on the other hand, the virtual absence of paramagnetism, which within the framework of the theory of one-electron trapped states are actually incompatible.[96] In this connection, it was postulated in Ref. 68 that states in the gap are two-electron states with total spin $\sigma = 0$ and negative correlation energy $U < 0$ with very large $|U| \approx E_g/2 \sim 1$ eV (E_g is the gap width). In two very different models such states were actually apparently associated with anomalously weak intrinsic valence bonds of an "ideal" (ideal, continuous, random network of atoms) covalent glass[68,123] or the ground state of pairs of oppositely charged defects in the structure of the glass.[96,124] Chalcogenide glasses—the amorphous alloys $a - As_{\bar{c}} C_{1-\bar{c}}$, $a - Ge_{\bar{c}} C_{1-\bar{c}}$ with $0 \leqslant \bar{c} \leqslant 1/2$, etc. (C is the chalcogen atom: S, Se, Te), in which the energy gap is small, $E_g \approx 2 - 1$ eV, are typical examples of GS, amorphous systems with predominantly covalent bonds and low average coordination number $\bar{z}$, $2 \leqslant \bar{z} < 3$ (see Ref. 96).

a) Self-trapped states in the mobility gap. General relations

According to a recently developed theory,[17,125,126] important electron states in the mobility gap in a GS are self-trapped states of charge carriers ("excess" electrons, holes) with anomalously large self-trapping energy $|W|$ of the order of the atomic energy $\varepsilon_0 \equiv \hbar^2/2m_0 a^2$ (~ 1 eV); in addition, self-trapping occurs primarily in the starting, ideal, continuous, random network of atoms with the intrinsic structure of such an amorphous system (i.e., it is not necessarily associated with any defect in the structure, when such a defect can be uniquely identified). Another feature of this self-trapping is that the two-electron and/or two-hole singlet self-trapped states with a negative correlation energy $U < 0$ with anomalously large $|U| \sim \varepsilon_0$ and with a charge (relative to the center) $e_{\mp}^* = \mp 2|e|$, characterizing a pair of identical charge carriers, are actually stable; the single-particle self-trapped states can only be metastable. In the theory under study such large values of $|W|$ and $|U|$ appear because of the following factors.

In an amorphous system fluctuations of the "short-range order" generate a finite concentration $c_a \ll 1$ of "atoms" (separate atoms and/or groups consisting of a large number of atoms) in relatively easily movable, "soft" local atomic configurations, on which the electron self-trapping under study is realizable.[17,126] The local potential of such an "atom," along at least one of the modes of motion (x), is substantially anharmonic: large displacements of the "atom" $\delta u \equiv u - u^{(0)} \equiv a_0(x - x^{(0)})$ give rise to anomalously small changes in the potential energy of the system.

$$|V(x)| \ll A \equiv \frac{1}{2} k^{(0)} a_0^2 \approx \frac{1}{2} M_a \omega_D^2 a_0^2 \approx 10-30 \text{ eV}$$

$$\text{for} \quad |x| \lesssim 1. \tag{5.1}$$

In (5.1) $V(x^{(0)}) \equiv 0 \equiv x^{(0)}$; M_a is the mass of the "atom"; a_0 is a typical atomic radius ($a_0 \sim 1$ Å); A and $k^{(0)}$ are the usual scales of the atomic (elastic) binding energy and of the quasielastic constants k in solids, excluding, apparently, molecular crystals, etc. Such anharmonic atomic potentials with anomalously small quasielastic constants $k \ll k^{(0)}$ (large local susceptibility of the "soft" configuration with respect to deformation, $\chi \simeq k^{-1} \gg (k^{(0)})^{-1}$), called in this connection critical, can in the general case be approximated for significant $|x| \lesssim 1$, by a unimodal potential of the type[17,126]

$$V(x) \approx A(\eta x^2 + tx^3 + x^4), \tag{5.2}$$

where $|\eta| \ll 1, t^2 \ll 1$ and $\partial V/\partial x = 0$ with $x = x^{(0)} = 0$. Indeed, according to Ref. 127, typical (i.e., most probable) critical potentials are precisely unimodal. The obvious meaning of the mode x and of the parameters of the fluctuations of "short-range order" and asymmetry of the environment (η, t) (in this theory, in this sense microscopic) is determined by the specific structure of the amorphous system. Thus it could be that $\eta \equiv (\Omega_c - \Omega) a_0^{-3}$ or, in the simplest model (Fig. 2a) $\eta \equiv r_c - r$ with a one-dimensional displacement of the "atom"; Ω is the volume per atom and $R \equiv a_0 r$ is the distance between atoms (-1) and (1), while Ω_c and R_c are their critical values, characteristic for the system.[17,127] In the (η, t) plane the potential (5.2) has one or two wells with $\eta \gtrless \eta^{(0)} \equiv 9t^2/32$; in addition $k \ll k^{(0)}$ with $|\eta| \ll 1$ and $\eta^{(0)} \ll 1$* (Fig. 2b).[7] The existence of critical potentials is linked at least to the fact that for very large $\Omega \gg \Omega_c$ the atomic potentials must not be single-well potentials (see Ref. 17). Since the main parameter of the theory $c_a \ll 1$, it is plausible to assume that the form of the density distribution determining it $F(\eta, t) = F(\eta, -t) \equiv N(\eta) g(t|\eta)$ corresponds to $N(\eta)$ and $g(t) \equiv g(t|0)$ shown schematically in Fig. 3. In this case the potentials (5.2) correspond to a small region of the rapidly decreasing tail of $N(\eta)$, while the usual single-well potentials ($k \simeq k^{(0)}$) for most of the atoms correspond to a peak with a width $\Delta\eta < 1$ near $\eta = \bar{\eta} \sim 1$ and $F(\eta, t) \simeq$ const for $|\eta| \lesssim \eta_c$ and $|t| \lesssim t_c$ and typical decay scales $\eta_c \lesssim 0.1$, $t_c \lesssim 0.1$.[17]

From this point of view, glasses are distinguished from amorphous materials by the fact that in glasses c_a is highest, $c_a \lesssim 0.1$, making them in this sense systems with a large anharmonicity.[17] This fact already determines the fundamental difference between glasses and the corresponding crystals, which is manifested in the universal anomalies of the heat capacity C_T and other properties for $T \ll \omega_0$ (see Refs. 130–131). The latter are determined by specific low-energy excitations with energy $\mathscr{E} \ll \omega_D$, corresponding in this theory to excited states of anharmonic oscillators (5.2) (see Ref. 17). They include two-level systems in double-well atomic potentials (the tunneling states in the potentials with small asymmetry, etc.) with almost uniform density of states $\rho(\mathscr{E}) \simeq$ const (with $\mathscr{E} \ll w \lesssim 0.1\omega_D \approx 10$–$30$ K),[17,127] whose existence was previously postulated in Ref. 130 and which determine the anomalies in the properties of glasses ($C_T \propto T$, etc.) for very low $T \lesssim 1\text{K} \ll w$. Another branch of the excitations of the system of oscillators (5.2) corresponds to atomic quasilocal vibrations with characteristic energy

$$w \approx A\eta_L^2 \ll \omega_D \left(\eta_L \equiv \left(\frac{\hbar^2}{2M_a a_0^2 A}\right)^{1/3}\right)$$

and a narrow band—a "peak"—and a state density $\rho(\mathscr{E})$, determined by the logarithmic singularity at $\mathscr{E} \simeq w$ (see Refs. 17 and 132, and also Ref. 133). According to Refs. 17 and 132, such vibrational excitations can determine the anomalies in the properties of glasses ("hump" in $C_T(T)$, plateau in the thermal conductivity, etc.) at moderately low temperatures T, $5\text{K} \lesssim T \lesssim 20$–$30\text{K}$.

The self-trapped state under study appears as a result of the interaction of electrons, having a "bare" (in the absence of deformation of the medium, at $x = 0$) one-electron trapped state ψ_q primarily of a small size $\rho_q \simeq a$ and the term $E \equiv E_q \equiv E_q(x = 0)$, with an "atom" in the starting critical potential (5.2) in the region of localization of ψ_q; in a three-dimensional system E_q must not lie too close to the mobility threshold, for example, at $E_q \lesssim E_{1c}^* < E_c^*$; see Sec. 4a. In other words, self-trapping is realized on a bare "soft" atomic configuration primarily of a small size ($\simeq a$), and we shall assume this in what follows. At the same time the electron-atom interaction constant $Q_q \simeq Q_0 \equiv Q_q(a)$, as usual, is significant, $Q_0 \sim \varepsilon_0$ ($Q_0 \sim 1$–3 eV, etc.). With an n-fold ($n = 1,2$) population of the term E_q this interaction can cause large displacements of the "atom" (deformation of the medium) $|x| \lesssim 1$ and a strong lowering of the term, $|\delta E_q(x)| \equiv |E_q - E_q| \lesssim Q_0$. At the same time a self-trapped state with significant equilibrium displacement x_n and self-trapping energy $W_n < 0$ can appear. The total change in the energy of the system is described by a relation of the form (see Refs. 17 and 126)

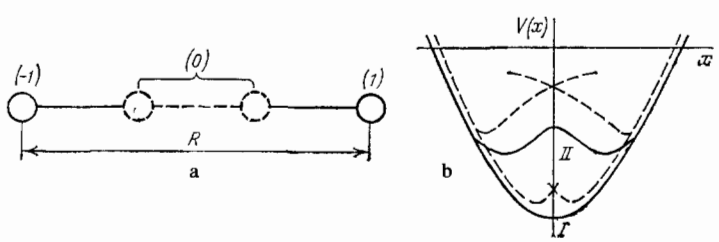

FIG. 2. Simplest model of an atomic subsystem with a critical potential: single-well with $\eta > 9t^2/32$ (I) or double-well with $\eta < 9t^2/32$ (II).

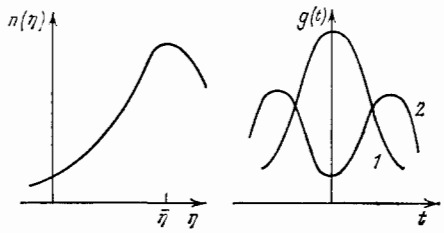

FIG. 3. Characteristic form of the density distributions $N(\eta)$ and $g(t) = g(-t)$ [two possible types of $g(t)$].

$$\varepsilon_n \equiv \min \varepsilon_n(x) \equiv \varepsilon_n(x_n) \equiv W_n(x_n) + U_c(x_n)\delta_{n,2}, \quad (5.3)$$

with $\varepsilon_n(x) = V(x) + n\delta E_q(x) + U_c(x)\delta_{n,2} \equiv W_n(x) + U_c(x)\delta_{n,2}$; $V(x) \equiv W_0(x)$. In (5.3) $\varepsilon_n(x)$ is the energy functional of the system being minimized (analog of (2.13) in Pekar's problem), $U_c(x)$ is the energy of the effective Hubbard interelectron repulsion and $W_n(x)$ is the adiabatic potential of the system. Here the adiabatic approximation is indeed applicable for states ψ_q in the gap, when the following inequalities actually hold:

$$\omega_D \ll Q_0 \ll A. \quad (5.4)$$

The two-electron self-trapped state ($n = 2$) with charge $e^*_- = -2|e|$ is stable (ground state), as soon as the correlation energy of the electron pair is negative[8]

$$U = \varepsilon_2 - 2\varepsilon_1 = W_2 - 2W_1 + U_c < 0, \quad (5.5)$$

i.e., interelectron attraction occurs (at the same time, evidently, there is a repulsion between the electron and the hole).

As is evident from what follows, for typical $U_c \lesssim 0.3$ eV (see Ref. 73) and $Q_0 \approx 1$–3 eV in semiconductors the inequality (5.5) is satisfied in GS, and in addition U is large, $|U| \sim \varepsilon_0 \sim 1$ eV.[9] Such a strong interelectron attraction actually occurs due to the strong rearrangement of the "soft" local configuration with the largest possible (for fixed $Q_q \approx Q_0$) values $|x_2| \approx x_{max} \equiv \max|x_2| \sim 1$, $|W_2| \approx W_{max} \equiv \max|W_2| \sim Q_0$ and $|U| \approx U_{max} \equiv \max|U| \sim Q_0$. It is also evident from what was said above that in GS a relationship must exist between the manifestations of such self-trapped states and the universal low-temperature anomalies in the properties (C_T, etc.); some aspects of this relationship are noted below.

For such large W_{max} the interband interaction, i.e., and mixing of the states ψ_p of the "foreign" band (valence band for the electron) to the given state ψ_q of the tail of its "own" band becomes significant here, in contrast to the usual situation for polarons and fluctuons (see Secs. 2–4).[17] The change in the term $E_q(x)$ and the state $\psi_q(x)$ accompanying deformation of the medium ($x \equiv 0$) is determined by the Schrödinger equation usual in such a two-band system (see Ref. 134)

$$\{E_q(x) - [E_q + J_{qq}(x)]\}\psi_q(x) = \hat{I}\psi_q(x) \equiv \sum_p I_{qp}(x)\psi_p. \quad (5.6)$$

Here $J_{qq}(x)$ determines the displacement of the term in the absence of other states, $|J_{qq}(x)| \lesssim Q_q \approx Q_0$, $I_{qp}(0) \equiv I_{qq}(x) \equiv J_{qq}(0) \equiv 0$; the transition matrix elements $I_{qp}(x)$ between ψ_q and the "foreign" states ψ_p describe the perturbing interband interactions, $|I_{qp}(x)| \ll Q_0$. The contribution of the latter, as usual, is important only when $E_q(x)$ approaches the terms E_q, $|E_q(x) - E_q| \lesssim |I_{qp}(x)|$. Perturbation theory for close-lying levels, describing their repulsion, leads to the resulting terms $E_q(x)$ (and $E_p(x)$), corresponding to "two-band" states—superpositions of the form $\psi_q(x) = c_q(x)\psi_q + \Sigma_q c_{qp}(x)\psi$ with $|c_{qp}(x)|^2 \lesssim 1$ (see Refs. 134 and 135). This general quantum phenomenon of repulsion of interacting close-lying levels, which are displaced toward one another as an external parameter x varies and could intersect ($E_q(x) \equiv E_p(x)$ at $x = x_0$), has been studied for many systems, in particular, for molecular terms and for a discrete term in the interband gap (see Refs. 136 and 137). The phenomenon is significant here, because in an amorphous system with a significant probability the quantity

$$\Delta_q^2 \equiv \Delta_q^2(x_0) \equiv \sum_p |I_{qp}(x_0)|^2 \approx \int dE_p\, g_0(E_p)|I_{qp}(x_0)|^2, \quad (5.7)$$

determining the splitting of the terms in the case of their repulsion, is finite (not exponentially small), as is the largest part of the matrix elements $I_{qp}(x)$ and $\Delta_q(x)$, due to the contribution of random fields.[10] In (5.7) $g_0(E)$ is the one-electron density of "bare" states of the two-band spectrum of the system. Actually the energy splitting, characterizing the repulsion of the $E_q(x)$ term, is determined by the contribution of weakly localized ($\rho_p \gg a$) states ψ_p near the mobility threshold of the "foreign" band E^*_S; their overlapping with ψ_q, like $g_0(E_p)$ in the gap, is significant, while the terms satisfy $E_p(x) \approx E^*_S$. (A quantitative theory of this effect in an amorphous system, taking into account the appropriate manifestation of the probability distribution of the random fields and analytically describing the behavior of the term $E_q(x)$ in the region of the splitting, is still not available.)

b) Two-electron self-trapped states. Structural rearrangements

The energy of the system E_n, containing n ($= 1,2$) self-trapped electrons, obtained by minimizing $\varepsilon_n(x)$ from (5.3), is described by the expression

$$E_n = nE_q + W_n + U_c\delta_{n,2} + \text{const}; \quad (5.8)$$

taking into account the effect (5.7) leads to an upper limit on $|W_n|$ and on the equilibrium displacement $|x_n|$ [see (5.13)]. Here $W_n \equiv W_n(x_n)$, and the expression for $W_n(x)$ can be represented in the form (5.2) with a renormalization of η and t:

$$\eta \to \eta_n \equiv (\eta + nq^{(2)})[1 + 3\lambda_n^{-1}(\varkappa_n^2 + 2\varkappa_n)],$$
$$t \to t_n \equiv (t + nq^{(3)})(1 + \varkappa_n), \quad (5.9)$$

in addition, generally speaking, $W_n(0) \equiv P_n(\eta,t) \neq 0$ for $n = 1,2$, with $W_0(0) \equiv V(0) \equiv 0$. Here $|q^{(j)}| \equiv A^{-1}|d^j J_{qq}(x)/dx^j|_{x=0} \lesssim Q_0 A^{-1} \ll 1$, and $\varkappa_n$ is the root (which vanishes at $n = 0$) of the equation $\varkappa^3 + 3\varkappa^2 + \lambda_n\varkappa$

$+\rho_n = 0$; $\lambda_n = 8(\eta + nq^{(2)})(t + nq^{(3)})^{-2}$, $\rho_n \equiv 16nq^{(1)} \times (t + nq^{(3)})^{-3}$. As a result, $W_n(x)$ is the critical potential also when $n = 1$ and 2 also (i.e., $|\eta_n| \ll 1$ and $t_n^2 \ll 1$).

The self-trapped states studied have the following features (in particular, compared with the small polarons and bipolarons in crystals)[17]: (1) the self-trapped states are determined, generally speaking, by the nonlinear coupling of the electron with the "critical" mode (x) of atomic displacements(not with phonons, tunneling states, or other excitations of the medium); (2) the spectrum

$$W_n = W_n^{(H)}(K) = -\frac{Q_0^2 n^2}{2R_0|K|}, \qquad U = U^{(H)}(K) = U_c - \frac{Q_0^2}{R_0|K|}, \tag{5.10}$$

corresponds to almost harmonic atomic displacements with $A \gg |K| > K^* = p_1 Q_0^2/^3 A^{1/3} R_0^{-1}$, $2p_1 \approx 1$, $R_0 = 2-3$, while with $|K| < K^*$ the quantities "saturate" taking on the largest (with the given value of Q_0) moduli, corresponding to anharmonic displacements, which can be significant when $E_g \gtrsim W_{max} \equiv \max|W_n^{(A\Gamma)}|$:

$$W_n = W_n^{(AH)} \equiv -\max|W_n| \approx W_n^{(H)}(K^*), \qquad |W_2^{(AH)}| \simeq \varepsilon_g(Q_0) \equiv 2p_1 Q_0 \left(\frac{Q_0}{A}\right)^{1/3}, \qquad U = U^{(A\Gamma)} \equiv -\max|U| \equiv -U_{max} \approx U_c - \frac{1}{2}|W_2^{(AH)}|. \tag{5.11}$$

Such "saturation" is characteristic for self-trapping accompanying a nonlinear response of the medium (compare Sec. 4b).

The general combined criteria for the stability of the two-electron state (as the ground state, when $U < 0$) have the form[17,18,134]:

$$2U_0 < \varepsilon_g(Q_0), \quad |K| < K^{**} \approx \frac{Q_0^2}{R_0 U_c} \quad \text{for} \quad 1 \gg Q_0 A^{-1} > f(\eta, t), \tag{5.12}$$

where $K \equiv A(\eta - 3t^2/8)$ for example, $f \approx |t||K|$. For GS, with typical values $U_c \lesssim 0.3$ eV, $Q_0 \approx 1$–3 eV, $A \approx 10$–30 eV, the criteria (5.12) are, of course, satisfied (in the corresponding region of the (η, t) plane). Moreover, for values of E_g which are typical for GS, 2 eV $\gtrsim E_g > 1$ eV, and Q_0, most likely, $\varepsilon_g(Q_0) \gtrsim E_g$. In this case, the effect (5.7) is significant; it determines the characteristic (largest for given Q_0) value of the self-trapping energy W_{max}, so that in the theory under study, for $U < 0$, the relation[17]

$$W_{max} = \max|W_2| \simeq E_g, \quad \text{i.e.} \quad 2U_{max} \simeq E_g \tag{5.13}$$

(up to terms $\lesssim 0.1\, E_g$), characteristic for GS with $W_{max}/2 \simeq U_{max} \gg U_c$ [the effect (5.7) is not significant and $E_g \gg W_{max} \simeq 2U_{max}$ when $E_g \gg \varepsilon_g(Q_0)$, as most likely happens in oxide and other glasses of the type a–SiO_2 with $E_g \approx 5$–10 eV $\gg Q_0 \approx 1$–3 eV] must hold. The relation (5.13) characterizes self-trapping in the intrinsic structure of the glass, since E_g is an important parameter of the glass.[11)]

The stable self-trapped pair states correspond to the ground state of the system, and a significant fraction of them (~ 1) has large binding energies of the order of the atomic energy ε_0, $U_{max} \leqslant E_g/2$. These self-trapped pair states, described by the formulas (5.8)–(5.13), are singlet states; the orbital states of both electrons in the pair are the same, $\Psi_{\uparrow\downarrow}(1.2) = \psi_q(1)\psi_q(2)(\varphi\uparrow(1)\varphi\downarrow(2) - \varphi\uparrow(2)\varphi\downarrow(1))$ (analogous to a Cooper pair[75] and a weak covalent bond—an electron pair with $U < 0$ in the mobility gap in the model[68]). The corresponding correlation effect (with given Q_0, U_c, and A) is characterized by the largest gain in energy $|W_2(\uparrow\downarrow)| \approx W_{max} \leqslant E_g$ (this occurs in GS as a result of the fact that $W_{max} \gg 2U_c$ and that the "bare" term localized in the given small region is most likely orbitally nondegenerate). In this case, the triplet self-trapped pair states correspond to excitations with a large creation energy per particle $\varepsilon_{ex} \lesssim U_{max}/2$.

In this connection, we note one of the most important features of the system under study. Generally speaking, high-energy ($\varepsilon_{ex} \gtrsim U_{max}/2$) excited states of self-trapped pairs in a gap are metastable, with lifetimes $\tau \gg \omega_D^{-1}$, in the sense that they substantially include significant metastable structural changes (large atomic displacements, $\Delta x \lesssim 1$, in the critical potential) compared with the configuration of the ground state, which is unstable in the presence of such excitations. Such structural changes are realized when the local relaxation corresponds to the appearance of the appropriate barriers of the adiabatic potential, separating the configuration of the ground and excited states (see below; compare the model in Ref. 68). Thus the form of the adiabatic potential $W_n(x)$ can change substantially, while remaining critical (see (5.9)), together with the number ν_n of potential wells and the potential can acquire or lose the barrier as a result of a change in the number of electrons n ($= 2,1,0$), depending on the value and sign of $q^{(j)}$ ($j = 1,2,3$), in other words, on the type of electron orbital $\psi_q^{(e)}$—nonbinding, antibinding, etc. (or $\psi_q^{(h)}$—binding, nonbinding, etc., for holes), i.e., on the type of "bare" local chemical bond. For example, the single-well potential $W_{n=2}(x)$ can transform into a double-well potential $W_{n=0}(x) \equiv V(x)$ [see (5.2)] accompanying the removal of an electron pair, with the possible appearance of tunneling states (with a seemingly stretched bond) as soon as in (5.9) η_2 is large enough, $(9/32)t_2^2 < \eta_2 \ll 1$ for $\eta < 9t^2/32$.

c) Basic effects of self-trapped electron pairs

For the main self-trapped pairs in the intrinsic structure of the glass—electron ($\alpha = 1$) and hole ($\alpha = 2$)—in the mobility gap the density of states $g_2(E_2/2) = \Sigma_{\alpha=1,2} g_2^{(\alpha)}(E_2/2)$ (per carrier), formally defined in Refs. 17 and 134 by a convolution of the density distributions $g_0^{(\alpha)}\{(1/2)[E_2 + (-)^\alpha (W_2^{(\alpha)}(\eta,t) + U_c^{(\alpha)})]\}$ with $F(\eta,t)$, can be approximated by a structure consisting of two almost flat bands with widths $\lesssim E_g/2$ (and, generally speaking, two possible narrower "peaks") with large $g_2(E_2/2) \lesssim 10^{20}/\text{cm}^3$ eV and a power-law drop-off to the region of overlapping around the Fermi level (per particle) ζ. Actually, a redistribution of charge occurs with charge flowing from the band created in the gap by the valence band over into another band, arising from the conduction band, with the for-

mation of real electron $(2e)_0$ (and hole) pairs in the ground state of the system below and above ζ, respectively; for such real pairs a high concentration $c_2 \lesssim 10^{-3} - 10^{-2}$ and effective "peaks" in the density of states of large magnitude $\lesssim 10^{19}$–10^{20} cm^3 eV and widths $\sim w_0 < E_g/4$ are characteristic; w_0 is the scale of the drop-off in $g_0(E)$. (This is what was contemplated in Refs. 17 and 134). This behavior of $g_2(E_2/2)$ on the whole determines, together with the characteristic (for GS), "symmetry" of the electron and hole self-trapped pairs ($U^{(1)}_{max} \simeq U^{(2)}_{max}$), the electron structure of the mobility gap with almost symmetrical "peaks" in the density of states of real singlet pairs and the stabilization of ζ by these states around the center of the gap,[17]

$$\zeta - E_2^* \simeq E_1^* - \zeta \approx \frac{E_g}{2}. \quad (5.14)$$

At the same time the concentration c_1 of single-particle charge carriers ("excess" electrons, holes), corresponding to singly filled states with $U > 0$, is very low, $c_1 \ll c_2$. In practice such systems (GS) are diamagnetic and are transparent to light with $\hbar\omega < E_g$, since the spectrum of single-particle excitations (1_{ex}, for example, $(1e)_{ex}$) has two gaps: a thermal gap with width $\varepsilon_{th} \simeq E_g/2$, determining the corresponding conduction activation energy, and an optical gap $\varepsilon_{opt} \simeq E_g$ for thermal and Franck-Condon decay of self-trapped pairs, respectively. The spectrum of two-particle excitations (2_{ex}, for example, $(2e)_{ex}$) does not have gaps (as in the BCS model[75] and in the model of the electron spectrum of GS in Ref. 68). It is possible to separate in it, at least, excitations with high ($\varepsilon^{(2)}_{ex} \gtrsim U_{max}/2$) and low ($\varepsilon^{(2)}_{ex} \ll U_{max}/2$) energies; the latter could contribute to the anomalies in the heat capacity and other properties of GS for $T \lesssim 1$K (see, however, Refs. 17 and 68 and Sec. 6).

The high-energy two-particle and single-particle excitations, including metastable structural changes (see above) and characterized by wide, not necessarily monotonic, spectra of lifetimes τ, play, from this point of view, the role of intrinsic metastable centers of nonequilibrium (photoinduced, etc.) phenomena,[17,134] such as luminescence ((2_{ex}), with an adiabatic potential of the type illustrated by curves (0) and (1) in Figs. 1a and b, nonradiative processes—recombination ((1_{ex}) etc.) and capture of current carriers (1_{ex}, 2_{ex}, and, for example, $(2e)_0$), and long-lived structural changes (with adiabatic potentials, similar to curves (0) and (1) in Figs. 1c and d).

For amorphous systems, for which (5.13) holds, in the theory under study the following relations have been obtained[17]:

$$E_{opt} \simeq \varepsilon_{opt} \simeq 2\varepsilon^*_{opt} \simeq 2\varepsilon_{th} \simeq 2E_L \simeq E_X(L) \simeq E_g, \quad (5.14)$$

and, in addition, $E_x(L) \lesssim E_g$, $2W_\sigma \simeq E_x(\mathrm{PC}) \simeq E_g$; these relations have indeed been found experimentally for GS. In (5.14) E_{opt} and W_σ are the width of the main optical gap and the conduction activation energy (taking into account the decay of the self-trapped pairs and generation of ordinary electron-hole pairs), ε^*_{opt} and E_L are the characteristic energies of the weak photoinduced absorption and luminescence, and $E_x(L)$ and $E_x(\mathrm{PC})$ are the threshold energies for excitation of luminescence and photoconductivity (for oxide and similar glasses with $E_g \gg \{Q_0, W_{max}\}$, the relations (5.14), generally speaking, do not hold and the role of self-trapped pairs is much less significant than in GS). Several new electron effects and their correlation with the low-temperature anomalies in the properties of the glasses, determined by the existence of a common factor—the critical atomic potentials, can be interpreted and predicted within the framework of this theory. They include (see Refs. 17, 134, and 138–142) the following effects observed in GS: narrowing of the optical gap accompanying photostructural changes, as a result of new electron transitions with lower energy ($< E_g$); enormous Stokes shift ($\approx E_g/2$); long-time relaxations of electron distributions, manifested, in particular, in the photoconductivity; "fatigue" (attenuation) of luminescence in the case of continuous prolonged illumination, due to competing nonradiative processes involved in structural changes; and, an anomalous dependence of the parameter of the luminescence intensity on T, $I_L(T) \propto \exp(-T/T_A)$ with $T_A \approx w \approx 10$–30 K for $T_A \lesssim T < \omega_D/2$. It can also be expected that $dI_L/dT \approx 0$ for $T \ll w$ and that a contribution can occur to the Urbach absorption tail—with adiabatic potentials of the type illustrated by curves (0) and (1) in Fig. 1d, in accordance with the models in Refs. 143 and 144. Here it should also be expected[17,34] that the anomalies in the properties of GS (at temperatures $T \lesssim 1$K) should be attenuated (or amplified) in the case of photoexcitation of self-trapped pairs (compare the experimental results in Ref. 145), and also the effects of self-trapped pairs and anomalies in the properties should be suppressed in GS and a-Si:H or amplified in a-Si, respectively, when the density of the material increases or decreases (compare the experiment in Ref. 146).

6. CONCLUSIONS

The review presented here indicates that the phenomenon of self-trapping of electrons and holes is quite general and important, at least, in nonmetallic (especially amorphous) solids (and in some liquids, see Refs. 147 and 148). This phenomenon determines many types of real current carriers and is linked to the electron-induced metastable states and instabilities of atomic configurations, including those which destroy the symmetry and lead to the formation of defects (structural changes).[12)]

There are a number of important problems in the theory of self-trapped electron and hole states. These concern, in particular, the characteristic features of Anderson trapping and Mott conductivity, the role of multielectron effects and nonlinear couplings between the electrons and the medium, the structure of the excited states of electron self-trapped pairs, and self-trapping in metals. It is of interest to analyze further the problems involving the general correlation between the excitation of self-trapped electron and hole pairs and restructuring of the chemical bonds (in accordance with the idea of commonality between the covalent bond and the self-trapped electron pairs[68]) and the role of self-trapped pairs in the anomalies in the properties of GS at low temperatures T and low ω (see Ref. 149).

One can hope that the investigations of these and other problems in the theory of self-trapped states, confronted

with experimental studies of kinetic, optical, and other effects induced by light and other forms of radiation, will lead to new results in the physics of semiconductors and ionic crystals (and, possibly, narrow-band metals).[13)]

The author had the invaluable opportunity to discuss a number of problems in the theory of self-trapping with I. M. Lifshitz. These discussions stimulated the writing of this review. The author also thanks Yu. M. Kagan, M. I. Kaganov, M. A. Krivoglaz, L. P. Pitaevskiĭ, and V. Ya. Frenkel' for very useful discussions.

[1)]The following discussion of self-trapped electron states under the corresponding equivalent conditions is equally applicable to self-trapped hole states and in some respects to self-trapped states of other quasiparticles (excitons, etc.).

[2)]Important specific aspects of the theory of self-trapped excitons (structure of the spectrum, coexistence of free and self-trapped excitons, etc.) are in many respects different; together with the general aspects of the theory of self-trapped states in crystals, they are studied in an excellent review[22] and are not discussed here.

[3)]The notation $\hbar \equiv 1$ is mainly used here and below.

[4)]The finite mobility of a small bipolaron in a crystal is determined by the small effective tunneling amplitude, which for low-temperature coherent transport is characterized by the quantity $\sim \Delta^2 |U|^{-1} \ll \Delta$ with $\Delta \ll U$ [see (2.28)]; see Refs. 72 and 150 as well as Ref. 71. The possibility of such bipolar transport within the framework of the phenomenological Hubbard Hamiltonian with a negative correlation energy $U<0$ was pointed out previously in Ref. 151. In Ref. 151 and even earlier in Ref. 152a (see also Ref. 152b) it was concluded that charge ordering of electron pairs with $U<0$ trapped on lattice sites is possible in crystals (see also Refs. 70–72). A theory of superconductivity in narrow-band superconductors, which is determined by the condensate of small bipolarons and is similar to the superconductivity in a system with spatially nonoverlapping electron "quasimolecules" studied a long time ago,[155] was developed in a number of recent works (see Refs. 72a, 150, 153, 154). We also note that for sufficiently strong electron-phonon coupling a system of many small polarons is capable of passing into a dielectric state (see Refs. 72, 150–154).

[5)]For $D \ll |A_0| S_a$ and $T_N \ll |A_0| S_a$ such a self-trapped state does not appear either at $T=0$,[27,81] or at finite T.[82]

[6)]This effect was not previously taken into account and does not occur in ferro or paramagnetic materials, in which the change in the mobility due to the presence of the magnetic structure is determined only by the weakly T-dependent average equilibrium value $\langle \cos^2(\theta_0/2) \rangle$, where θ_0 is the angle between the electron spin and the spin of the magnetic atoms (see, for example, Ref. 21).

[7)]The formula (5.2) is similar to the expression for the thermodynamic potential in Landau's theory of critical phenomena.[128] The relationship between the breakdown of long-range order in the crystal and the increase in the volume (with $T=$ const) and the appearance of non-single-well (double-well, etc.) atomic potentials in it was pointed out by Frenkel' in a discussion of the nature of melting.[129]

[8)]In what follows, the discussion of electron self-trapped states is also applicable, with obvious modifications, to self-trapped hole states (for the latter, evidently, $U = 2\varepsilon_1 - \varepsilon_2$).

[9)]Generally speaking, within the framework of the theory of mobility-gap states studied here it is possible to obtain in an analogous manner the main characteristics and relations for electron (hole) pairs whose charge $|e^*_{\mp}|$ differs from that studied above $|e^*_{\mp}| = 2|e|$, corresponding to self-trapping on a neutral (with charge $q^* = 0$), bare, "soft" atomic configuration of an ideal glass (see Refs. 17 and 126). Thus, if it is assumed that $q^* = 2|e|$ ("depleted covalent bond") or $q^* = -|e|$ ("charged broken bond"), then the self-trapped pair of electrons or holes can correspond to $e^*_- = 0$ (possibly, an intrinsic weak covalent bond; compare Ref. 68) or $q^*_+ = |e|$ (possibly, a center, similar to the defect 0^+ in the Street-Mott-Kastner-Adler-Fritsche model; see Ref. 96). The experimental data apparently play a decisive role in the determination of the type of dominating self-trapped pairs and their charge (see below).

[10)]For a discrete term E_q of a defect in a crystal, evidently, it can happen that $I_{qp}(x) \equiv 0$ with an appropriate symmetry of the states ψ_q and band ψ_p.

[11)]The relation (5.13) and the relations (5.14) and (5.15) following from it, which adequately describe the experimental data for GS, are obtained in an obvious manner in the theory under study for self-trapped states of pairs of the same types of charge carriers—both "excess" electrons and holes with charge $e^*_{\mp} = \mp 2|e|$ (in the starting, ideal, continuous, random, network of atoms; see above). In this connection it may be assumed that such self-trapped states are significant, if not determining, for the mobility gap in GS; see footnote 9) (the concentration of self-trapped pairs with charge $\mp |e|$, c, from the point of view studied here, is relatively low, since the concentration of broken bonds $c_{oc} \ll c_a$[17]).

[12)]The relationship between self-trapping of charge carriers (and excitons) and appearance of instabilities of atomic configurations which lead to the creation and transformation of structural defects of solids, was recently discussed in Refs. 22, 42b, 43, 44, 156, and 157 for dielectrics, in Refs. 141, 157, and 158 for crystalline semiconductors, and (see Sec. 5c above) in Refs. 134, 141, and 157 for glassy semiconductors.

[13)]New papers appeared after this paper was submitted for publication. The conditions for the existence of small bipolarons in crystals are analyzed in a recent work[159] within the framework of a theory of polarons based on the use of scale transformations [see (2.21)].[5,25,22] A similar analysis is given for disordered systems in Ref. 160, which generalizes Ref. 101.

The superconducting properties of systems whose ground state is a Bose condensate of small strongly-coupled bipolarons ($|U| \gg \Delta$, $U<0$) were studied in a recently published paper.[161] It was shown that the magnetic and critical properties of such a model differ radically from those of the usual superconductors described by the BCS model. The possibilities of the realization of a bipolaron model of superconductivity are discussed (see Refs. 71, 72 and the remarks in footnote[4)]).

A series of papers continuing the experimental and theoretical study of the properties of the alloys $Pb_{1-c} - Sn_c - Te$(In) (see Secs. 3b and c), in which electron self-trapping and metastable electron states (see Ref. 37 and the references cited therein) play an important role, also appeared recently.

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