Electron–phonon system with strong coupling and violation of the Migdal–Éliashberg theory

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It is shown that the traditional theory of electron–phonon interaction is not correct in the case of strong electron–phonon coupling ($\lambda \gtrsim 1$). The ground state described by that theory is unstable to infinitesimal perturbations that violate the translational invariance of the crystal.

INTRODUCTION

Modern theory of strong-coupling superconductors is based in the Éliashberg equations,[1] which are obtained by a natural generalization of the theory of electron–phonon interaction in a normal[2] metal (see, e.g., Ref. 3, pp. 390 and 236 of the Russian original). It is customarily assumed that these equations are valid in the presence of a small adiabatic parameter

$$\omega/D \ll 1, \tag{1}$$

where ω and D are respectively the characteristic phonon frequency and the characteristic kinetic energy of the electrons. (In metals as well as in intermetallic compounds, including high-temperature metal-oxide superconductors, the electron bands have a half-width $D \sim 1$ eV and this ensures smallness of the adiabatic parameter (1).)

On the other hand, as noted in Refs. 4–7, the traditional theory of electron–phonon interaction in metals takes no account of the lattice local instability that leads to known polaron effect, viz., electron self-trapping and polaron narrowing of the electron band. A consistent analysis of the multipolaron problem, based on the known methods of the small-radius-polaron (SRP) theory,[8] leads to a picture that differs qualitatively from the classical (BCS) picture of either the normal or the superconducting state of electrons that interact strongly with phonons.[7] This last circumstance is particularly vital for the interpretation of the properties of the new metal-oxide high-temperature superconductors.[9,10] The polaron effect comes into play in the case of strong electron–phonon interaction, when the depth E_p of the polaron well (the polaron shift of the atomic level)[8] exceeds the half-width D of the electron band:

$$E_p/D \geqslant 1. \tag{2}$$

For the usual Fröhlich electron–phonon interaction, the ratio E_p/D coincides with the known electron–phonon coupling constant Λ.[7] The traditional superconductivity theory turns out therefore to be incorrect already for

$$\lambda \geqslant 1, \tag{3}$$

notwithstanding the adiabaticity of the initial renormalized electron band (1).

Polaron effects in a many-electron system have been heretofore[4–7] considered by using the formalism of single-particle SRP theory,[8] which takes correct account of both local violation of translational invariance (discreteness of the lattice) and the phonon corrections to the vertex part.

Of undisputed interest is a formulation, for metals and superconductors, of a consistent electron–phonon strong interaction theory that takes the polaron effect into account, using the Green's function (GF) formalism that is universally accepted in traditional superconductivity theory.[1–3]

We formulate in the present paper, for the electron and phonon GF of a normal metal with a Fröhlich electron–phonon interaction, equations that make it possible to take the polaron effect into account. We show that from among the three basic assumptions of the classical theory,[1–3], viz.: 1) initial translational invariance of the Green's function

$$G(\mathbf{x}, \mathbf{x}', \tau) \equiv G(\mathbf{x}-\mathbf{x}', \tau); \tag{4}$$

2) neglect of phonon corrections to the vertex part, and 3) neglect of the finite width of the electron band, as manifested by the assumption that the single-particle density of the electron states is constant:

$$N(\varepsilon) \approx N(0), \tag{5}$$

the first assumption is incorrect if $\lambda \gtrsim 1$. The last approximation, as shown in Ref. 11, is incorrect for very large λ:

$$\lambda \gtrsim D/\omega \gg 1. \tag{6}$$

It appears that allowance for the phonon corrections to the vertex part can lead, even in the presence of polaron narrowing of the band, only to quantitative corrections which do not alter the qualitative picture of the energy spectrum.

1. EQUATIONS FOR GF, WITH ACCOUNT TAKEN OF LOCAL INSTABILITY OF THE LATTICE

The reason for the absence of a polaron effect in the usual theory of electron–phonon interaction in metals is that the electron GF (4) is assumed beforehand (prior to solving the equation) to depend, in view of the translational invariance of the crystal, only on the coordinate difference, so that it is possible to change over the equations for the Fourier transform $G(\mathbf{p}, \omega)$. This excludes automatically the possibility of local violation of the translational invariance due to lattice deformation near the electron site. To enable the electrons to become attuned to one another in a minimum-energy state we introduce in the Hamiltonian, following Refs. 12–15, an infinitesimal translationally invariant potential of the "sources"; this potential can be set equal to zero only after the calculation of the GF. It is well known here[12–14] that a premature vanishing of this potential can lead to finite differences in the result, i.e., in the GF, the energy spectrum,

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or thermodynamic and other properties. In our case this is the result of instability of the initial electron band to polaron collapse.[11]

It is important that even for infinitesimal but nonzero sources the average ion deviations $\langle \hat{\mathbf{u}}_n(\tau)\rangle$ from the equilibrium positions R_n^0 differ from zero and are not infinitesimally small. This circumstance was disregarded in the traditional theory of electron–phonon interaction. Furthermore, even in Refs. 15 and 16, in which the general form of the GF contained $\langle \hat{\mathbf{u}}_n(\tau)\rangle$ explicitly, it was assumed that $\langle \hat{\mathbf{u}}_n(\tau)\rangle \neq 0$ corresponds only to an imperfect crystal and does not hold for a perfect one.

We write the Hamiltonian of the electron–phonon system, omitting for simplicity the Coulomb interaction, in the form

$$\hat{H}=\hat{H}_e+\hat{H}_i+\hat{H}_{ei}+\int U(\mathbf{r},t)\psi^+(\mathbf{r},t)\psi(\mathbf{r},t)\,d\mathbf{r} + \sum_{n\alpha} J_n^{\alpha}(t)\hat{u}_n^{\alpha}(t). \tag{7}$$

The contributions $\hat{H}_e$ and $\hat{H}_i$ to the Hamiltonian, corresponding to the electron and ion subsystems, and that to the electron–ion interaction, are given by

$$\hat{H}_e=\int d\mathbf{r}\psi^+(\mathbf{r},t)\left[-\frac{\nabla^2}{2m}-\mu\right]\psi(\mathbf{r},t) - \sum_{n\varkappa}\int \psi^+(\mathbf{r},t)\psi(\mathbf{r},t)\,\Phi(\mathbf{r}-\mathbf{R}_{n\varkappa}^0)\,d\mathbf{r}; \tag{8}$$

$$\hat{H}_i=\frac{1}{2}\sum_{n\varkappa\alpha} M_{\varkappa}[\hat{\mathbf{u}}_n^{\alpha}]^2+\frac{1}{2}\sum_{\substack{nn'\\ \varkappa\varkappa'}} V(\mathbf{R}_{n\varkappa}^0-\mathbf{R}_{n'\varkappa'}^0) + \frac{1}{2}\sum_{\substack{nn'\\ \varkappa\varkappa'}} (\hat{u}_{n\varkappa}^{\alpha}-\hat{u}_{n'\varkappa'}^{\alpha})\nabla_{\alpha}V(R_{n\varkappa}^0-R_{n'\varkappa'}^0); \tag{9}$$

$$\hat{H}_{ei}=\sum_{n\varkappa}\int \psi^+(\mathbf{r},t)\psi(\mathbf{r},t)\,\hat{u}_{n\varkappa}^{\alpha}\nabla_{\alpha}\Phi(\mathbf{r}-\mathbf{R}_{n\varkappa})\,d\mathbf{r}. \tag{10}$$

Here $\hat{u}_{n\varkappa}^{\alpha}$ is the ion-displacement operator, and $V(R_{n\varkappa}^0-R_{n'\varkappa'}^0)$ and $\Phi(\mathbf{r}-R_{n\varkappa}^0)$ are the potentials of the ion–ion and electron–ion interactions. The last two terms of (7) are the aforementioned potentials of the external sources. Terms quadratic in $\hat{u}_{nx}^{\alpha}$ are assumed to be present in (9) and (10), but are not written out explicitly.

Using (7), we obtain in standard fashion the equations for the electron and phonon temperature GF[12,13,15]:

$$\delta(\mathbf{r},\mathbf{r}')\delta(\tau,\tau')=\int\left[\left(i\frac{\partial}{\partial\tau}+\left(\frac{\nabla_{\mathbf{r}}^2}{2m}+\mu\right)-U+\sum_{n\varkappa}\Phi(\mathbf{r}-\mathbf{R}_{n\varkappa}^0) - \sum_{n\varkappa}\nabla_{\alpha}\Phi(\mathbf{r}-\mathbf{R}_{n\varkappa}^0)\langle\hat{u}_n^{\alpha}(\tau)\rangle\right)\delta_{\mathbf{rr}''}\delta_{\tau\tau''} - \Sigma(\mathbf{r},\mathbf{r}'',\tau-\tau'')\right]G(\mathbf{r}'',\mathbf{r}',\tau''-\tau')\,d\mathbf{r}''. \tag{11}$$

The self-energy part Σ in (11) is given by

$$\Sigma(\mathbf{r}'',\mathbf{r}',\tau''-\tau') = i\sum_{\substack{nn'\\ \varkappa\varkappa'}}\nabla_{\alpha}\Phi(\mathbf{r}''-\mathbf{R}_{n\varkappa}^0)\nabla_{\beta}\Phi(\mathbf{r}'-\mathbf{R}_{n'\varkappa'}^0) \times D_{nn'\varkappa\varkappa'}^{\alpha\beta}(\tau''-\tau')G(\mathbf{r}'',\mathbf{r}',\tau''-\tau'),$$

where $D_{nn'\varkappa\varkappa'}^{\alpha\beta}(\tau)$ is the temperature GF for the ion displacements:

$$D_{nn'\varkappa\varkappa'}^{\alpha\beta}(\tau)=-i\langle T_{\tau}(\hat{u}_{n\varkappa}^{\alpha}-\langle\hat{u}_{n\varkappa}^{\alpha}\rangle),(\hat{u}_{n'\varkappa'}^{\beta}(\tau)-\langle\hat{u}_{n'\varkappa'}^{\beta}\rangle)\rangle. \tag{12}$$

The expansion of the ion-displacement operator in terms of the phonon operators is

$$\hat{u}_{n\varkappa}^{\alpha}=\langle\hat{u}_{n\varkappa}^{\alpha}\rangle+\sum_{\mathbf{q}j}\frac{e^{\alpha}(\mathbf{q}j|\varkappa)}{[2NM_{\varkappa}\omega_j(\mathbf{q})]^{1/2}}\exp(i\mathbf{q}R_{n\varkappa}^0)(\hat{b}_{\mathbf{q}j}+\hat{b}_{-\mathbf{q}j}^+). \tag{13}$$

Here $e^{\alpha}(\mathbf{q}j|\varkappa)$ is the polarization vector for an ion $\varkappa$ with a radius vector $\rho_{\varkappa}$ in a unit cell, $M_{\varkappa}$ is the ion mass, and $\omega_j(\mathbf{q})$, $\hat{b}_{\mathbf{q}j}^+$, $\hat{b}_{\mathbf{q}j}$ are respectively the frequency and the creation and annihilation operators of a phonon with polarization j. Substitution of (13) in (12) yields

$$D_{nn'\varkappa\varkappa'}^{\alpha\beta}(\tau)=\sum_{\mathbf{q}j}\frac{e^{\alpha*}(\mathbf{q}j|\varkappa')e^{\beta}(\mathbf{q}j|\varkappa')}{N(M_{\varkappa}M_{\varkappa'})^{1/2}\omega_j(\mathbf{q})}\exp[i\mathbf{q}(\mathbf{R}_n^0-\mathbf{R}_{n'}^0)] \times\exp[i\mathbf{q}(\rho_{\varkappa}-\rho_{\varkappa'})]T\sum_{p}D_j(\mathbf{q},\omega_p)\exp(-i\omega_p\tau),$$

$$\omega_p=\pi nT,\ n=0,\pm1,\pm2\ldots, \tag{14}$$

where $D_j(\mathbf{q},\omega_p)$ is the temperature GF of the phonons of branch j in the momentum representation.

To calculate $\langle\hat{u}_n^{\alpha}(\tau)\rangle$ we average the equation for $\hat{u}_n^{\alpha}(\tau)$:

$$-M_{\varkappa}\frac{\partial^2\hat{u}_{n\varkappa}^{\alpha}(\tau)}{\partial\tau^2}=\frac{\delta\hat{H}}{\delta\hat{u}_{n\varkappa}^{\alpha}}. \tag{15}$$

As a result we have

$$\langle\hat{u}_{n'}^{\beta}\rangle=\sum_{n}\int d\mathbf{r}\rho_e(\mathbf{r},\tau)\nabla_{\alpha}\Phi(\mathbf{r}-\mathbf{R}_n^0)D_{nn'}^{\alpha\beta}(\omega_p=0). \tag{16}$$

Here $\rho_e(\mathbf{r},\tau)$ is the coordinate-dependent electron density in the crystal. Substituting (16) in (11), we add the increment to the mean field:

$$-\sum_{n'}\nabla_{\beta}\Phi(\mathbf{r}-\mathbf{R}_{n'}^0)\langle\hat{u}_{n'}^{\beta}(\tau)\rangle = -\sum_{nn}\int d\mathbf{r}'\rho_e(\mathbf{r}',\tau)\nabla_{\alpha}\Phi(\mathbf{r}-\mathbf{R}_n^0)\nabla_{\beta}\Phi(\mathbf{r}-\mathbf{R}_{n'}^0)D_{nn'}^{\alpha\beta}(\omega_p=0), \tag{17}$$

applied to the electron by the polarization (by the shift of the equilibrium positions) of the ions surrounding the given electron.

Since the sources violate translational invariance, we expand the electron field operators $\psi(\mathbf{r},\tau)$ in terms of functions $\varphi_m(\mathbf{r})\equiv\varphi(\mathbf{r}-\mathbf{R}_m)$, that are centered on the lattice sites—in analogy with Wannier functions. The exact form of the functions $\varphi_m(\mathbf{r})$ will be determined later by a variational procedure. We have

$$\psi(\mathbf{r},\tau)=\sum_m \hat{a}_m(\tau)\varphi_m(\mathbf{r}). \tag{18}$$

The fact that only one wave function corresponds to the site $\mathbf{R}_m^0$, rather than a complete and orthonormalized set of functions $\varphi_{m,n}(\mathbf{r})$, is equivalent to the single-band approximation.

Substituting (18) in (7)–(10), we separate from the interaction Hamiltonian $\hat{H}_{ei}$ (10) the term $\tilde{H}_{ei}$ that leaves the electron on one site:

$$\hat{\tilde{H}}_{ei}=\sum_m \tilde{H}_m \hat{a}_m^+ \hat{a}_m, \tag{19}$$

where

$$\tilde{H}_m=\int d^3\mathbf{r}\varphi_m^*(\mathbf{r})\varphi_m(\mathbf{r})\sum_n \hat{u}_n^\alpha \nabla_\alpha \Phi(\mathbf{r}-\mathbf{R}_n^0). \tag{20}$$

We neglect hereafter the difference between $\hat{\tilde{H}}_{ei}$ and $\hat{H}_{ei}$, assuming $\hat{H}=\hat{H}_0+\hat{\tilde{H}}_{ei}$ with $\hat{H}_0\equiv\hat{H}_e+\hat{H}_i$.

It is easy to show, by changing to the momentum representation, that allowance for the terms $(\hat{H}_{ei}-\hat{\tilde{H}}_{ei})$ means departure from the framework of a Fröhlich interaction Hamiltonian with a constant that depends only on the phonon momentum.[1]

We rewrite the electron GF in the form

$$\mathcal{G}(\mathbf{x},\mathbf{x}',\tau)=\sum_{mm'}\varphi_m(\mathbf{x})\varphi_{m'}^*(\mathbf{x}')\mathcal{G}_{mm'}(\tau),$$

$$\mathcal{G}_{mm'}(\tau)=-\sum_{mm'}e^{\Omega/T}\,\mathrm{Sp}\left\{\exp\left(-\frac{\hat{H}_0-\mu\hat{N}}{T}\right)\right.$$

$$\left.\times T_\tau\left(\hat{a}_m(\tau_1)\hat{a}_{m'}^*(\tau_2)\mathfrak{S}\left(\frac{1}{T}\right)\right)\right\}, \tag{21}$$

$$e^{-\Omega/T}=\mathrm{Sp}\left\{T\exp\left(-\frac{\hat{H}_0-\mu\hat{N}}{T}\right)\hat{\mathfrak{S}}\left(\frac{1}{T}\right)\right\}, \tag{22}$$

$$\mathfrak{S}\left(\frac{1}{T}\right)=\exp\left\{-\int_0^{1/T}\hat{\tilde{H}}_{ei}(\tau')\,d\tau'\right\}, \tag{23}$$

$$\hat{\tilde{H}}_{ei}(\tau)=\exp[\tau(\hat{H}_0-\mu\hat{N})]\,\hat{\tilde{H}}_{ei}\exp[-\tau(\hat{H}_0-\mu\hat{N})]. \tag{24}$$

Substituting in (17) the explicit expression for $\hat{u}_n^\alpha$ and integrating, we obtain $\mathfrak{S}(1/T)=\exp(-\tilde{S})$, where

$$\hat{\tilde{S}}=\sum_m\int d^3\mathbf{r}\varphi_m^*(\mathbf{r})\left[\sum_n \hat{\tilde{u}}_n^\alpha\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)\right]\varphi_m(\mathbf{r})\hat{a}_m^+\hat{a}_m. \tag{25}$$

Here

$$\hat{\tilde{u}}_n^\alpha=\sum_{\mathbf{q}j\varkappa}\frac{\exp(i\mathbf{q}\mathbf{R}_n^0)}{[2NM_\varkappa\omega_j(\mathbf{q})]^{1/2}\omega_j(\mathbf{q})}e^\alpha(\mathbf{q}j|\varkappa)(\hat{b}_{\mathbf{q}j}-\hat{b}_{-\mathbf{q}j}^+). \tag{26}$$

i.e., $\hat{\tilde{u}}_n^\alpha$ differs from $\hat{u}_n^\alpha$ by the presence of an extra factor $\omega_j(\mathbf{q})$ in the denominator in the summation over $\mathbf{q}$ and j, and by the sign of $\hat{b}_{-\mathbf{q}j}$. The operator $\hat{\tilde{S}}$ is dimensionless. Note now that by using an identity transformation of the GF $\mathcal{G}_{mm'}(\tau>0)$ we can rewrite (21) in the form

$$\mathcal{G}_{mm'}(\tau>0)=-e^{-\Omega/T}\,\mathrm{Sp}\{\mathfrak{S}^{+1}(1/T)e^{-\hat{H}/T}\mathfrak{S}^{-1}(1/T)\mathfrak{S}(1/T)$$
$$\times\hat{a}_m(\tau_1)\mathfrak{S}^{-1}(1/T)\mathfrak{S}(1/T)\hat{a}_{m'}^+(\tau_2)\mathfrak{S}^{+1}(1/T)\} \tag{27}$$

and arrive at the expression

$$\mathcal{G}(\tau>0)$$
$$=-e^{-\Omega/T}\,\mathrm{Sp}\left\{\exp\left(-\frac{\hat{H}-\mu\hat{N}}{T}\right)\hat{\tilde{a}}_m(\tau_1)\right.$$
$$\left.\times\exp(\hat{\tilde{S}}_m)\hat{\tilde{a}}_{m'}^+(\tau_2)\exp(-\hat{\tilde{S}}_{m'})\right\}. \tag{28}$$

where

$$\hat{\tilde{H}}=\mathfrak{S}^{-1}(1/T)\hat{H}\mathfrak{S}^{-1}(1/T),$$
$$\hat{\tilde{a}}_m(\tau)=\exp[\tau(\hat{\tilde{H}}-\mu\hat{N})]\hat{a}_m\exp[-\tau(\hat{\tilde{H}}-\mu\hat{N})].$$

We have then in (28)

$$\exp\left(-\frac{\hat{\tilde{H}}-\mu\hat{N}}{T}\right)=\mathfrak{S}^{+1}\left(\frac{1}{T}\right)\exp\left(-\frac{\hat{H}_0-\mu\hat{N}}{T}\right)$$
$$\equiv\exp\left(-\frac{\hat{\tilde{H}}_e-\mu\hat{N}}{T}\right)\mathfrak{S}^{+1}\left(\frac{1}{T}\right)\exp\left(-\frac{\hat{H}_i}{T}\right). \tag{29}$$

Here

$$\hat{\tilde{H}}_e=\mathfrak{S}(1/T)\hat{H}_e\mathfrak{S}^{-1}(1/T). \tag{30}$$

2. ELECTRON GREEN'S FUNCTION AND ENERGY SPECTRUM

Finding the electron energy spectrum calls for an analytic continuation of the temperature GF into the region of real t. To this end, we find the explicit form of the correlator $\langle\hat{\tilde{a}}_m(\tau_1)\hat{\tilde{a}}_{m'}^+(\tau_2)\rangle$ in expression (28) for the GF.

Direct calculations using Eq. (29) lead to the basic property of the transformed part H_i+H_{ei} of the Hamiltonian H: this part of the Hamiltonian was diagonalized with respect to the electron and phonon variables, namely

$$\mathfrak{S}^{+1}\left(\frac{1}{T}\right)\exp\left(-\frac{\hat{H}}{T}\right)=\exp\left[-\frac{1}{T}\left(\hat{H}_i+\sum_m\hat{a}_m^+\hat{a}_m E_p\right)\right], \tag{31}$$

where

$$E_p=\left\langle m\left|\frac{\nabla_{\mathbf{r}}^2}{2m}+\mu+\sum_n\Phi(\mathbf{r}-\mathbf{R}_n^0)\right|m\right\rangle$$
$$-\langle m|\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)|m\rangle\langle\hat{u}_n^\alpha\rangle$$
$$-\sum_{j\mathbf{q}}\hbar\omega_j(\mathbf{q})|\pi_{\mathbf{q}}|^2; \tag{32}$$
$$\pi_{\mathbf{q}}=\sum_n\exp(i\mathbf{q}\mathbf{R}_n^0)\langle u_n^\alpha\rangle i\mathbf{q}_\alpha.$$

We now uncouple (28) and assume that

$$\mathcal{G}_{mm'}(\tau>0)=\langle\hat{\tilde{a}}_m\hat{\tilde{a}}_{m'}^+\rangle\langle\exp(\hat{\tilde{S}}_m)\exp(-\hat{\tilde{S}}_{m'})\rangle$$
$$\equiv\langle\hat{\tilde{a}}_m(\tau_1)\hat{\tilde{a}}_{m'}^+(\tau_2)\rangle\exp[-\langle(\hat{\tilde{S}}_m-\hat{\tilde{S}}_{m'})^2\rangle/2]. \tag{33}$$

Averaging over the ion operators in the second factor of (33) leads to the expression

$$\exp(-g_{mm'}^2)\equiv\exp[-\langle(\hat{\tilde{S}}_m-\hat{\tilde{S}}_{m'})^2\rangle/2], \tag{34}$$

where

$$g^2_{mm'}=\sum_{qj}\sum_{nn'}\sum_{\alpha\beta m''}\int\frac{d\omega\,\mathrm{Im}\,D_{qj}^{\alpha\beta}(\omega)}{\omega^2}\langle m|\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)|m\rangle$$
$$\times\langle\langle m''|\nabla_\beta\Phi(\mathbf{r}'-\mathbf{R}_{n'}^0)|m''\rangle\cos[\mathbf{q}(\mathbf{R}_n^0-\mathbf{R}_{n'}^0)](\delta_{mm''}-\delta_{m''m'}).$$

We see that $g^2_{mm'}$ vanishes if $m'=m$. For $m'\neq m$ Eq. (34) is a rigorous generalized expression for the polaron factor (see, e.g., Refs. 4 and 8).

Multiplying (11) from the left by $\varphi_m^*(\mathbf{r})$ and from the right by $\varphi_{m'}(\mathbf{r}')$ and integrating with respect to $\mathbf{r}$ and $\mathbf{r}'$, we obtain after changing to the ω representation in imaginary time ($m'\neq m$)

$$S^0_{mm'}=(i\omega_p+H_{emm})G_{mm'}(\omega_p)+H_{emm'}G_{m'm'}(\omega_p)$$
$$-\sum_n\langle m|\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)|m\rangle$$
$$\times\langle\langle u_n^\alpha(\tau)\rangle G_{mm'}(\omega_p)-\sum_n\langle m|\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)|m'\rangle$$
$$\times\langle\hat{u}_n^\alpha\rangle G_{m'm'}(\omega_p)$$
$$-2i\sum_{nn'}\sum_{\substack{dd'\\rr'}}\langle d|\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)|m\rangle\langle r|\nabla_\beta\Phi(\mathbf{r}''-\mathbf{R}_{n'}^0)|d'\rangle\cdot$$
$$\sum_s D_{nn'}^{\alpha\beta}(\omega_p-\omega_s)G_{dd'}(\omega_s)G_{rr'}(\omega_p)S^0_{m'r'}. \qquad (35)$$

Here

$$H_{emm'}=\left\langle m\left|\frac{\nabla_{\mathbf{r}}^2}{2m}+\mu+\sum_n\Phi(\mathbf{r}-\mathbf{R}_n^0)\right|m'\right\rangle, \qquad (36)$$

$$S^{\mathbf{q}}_{mm'}=\langle m|\exp(i\mathbf{q}\mathbf{r})|m'\rangle. \qquad (37)$$

For $m'=m$, the analogous equation is

$$1=\left[i\omega_p+H_{emm}-\sum_n\langle m|\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)|m\rangle\langle u_n^\alpha\rangle\right]G_{mm}(\omega_p)$$
$$-i\sum_{nn'}\langle m|\nabla_\alpha\Phi(\mathbf{r}'-\mathbf{R}_n^0)|m\rangle\langle m|\nabla_\beta\Phi(\mathbf{r}''-\mathbf{R}_{n'}^0|m\rangle$$
$$\times D^{\alpha\beta}_{nn'}(\omega_s)G_{mm}(\omega_p-\omega_s)G_{mm}(\omega_p). \qquad (38)$$

We substitute in (38) the spectral representation for the GF of the electrons and phonons in the form

$$G_{mm'}(\omega_n)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}dz'\frac{a_{mm'}(z')}{i\omega_n-z'}, \qquad (39)$$

$$D_j(\mathbf{q},\omega_n)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}dz'\frac{b_j(\mathbf{q},z')}{i\omega_n-z'} \qquad (40)$$

and recognize that in the case of undamped phonons

$$b_j(\mathbf{q},z')=2\pi[\delta(z'-\omega_j(\mathbf{q}))-\delta(z'+\omega_j(\mathbf{q}))]. \qquad (41)$$

In (39) we have

$$a_{mm'}(z')=-2\,\mathrm{Im}\,G_{Rmm'}(z'), \qquad (42)$$

where $G_{Rmm'}(z')$ is the retarded GF of the electrons. The poles of the electron GF, neglecting the damping of the electronic states, allow us to express $a_{mm'}(z')$ in the form

$$a_{mm'}(z')=-2A_{mm'}\delta(z-h_{mm}). \qquad (43)$$

Substituting (39) and (40) in (38), we sum over n and n' and obtain as a result in the zeroth approximation with respect to the overlap integral $S^{\mathbf{q}}_{mm'}$, recognizing that $h_{mm'}\sim S^{\mathbf{q}}_{mm'}$, the expression

$$G_{mm}^{-1}(\omega_p)=\Big\{i\omega_p+H_{emm}-\sum_{nn'}\langle m|\nabla_\alpha\Phi(\mathbf{r}-\mathbf{R}_n^0)|m\rangle$$
$$\times\int_{+\infty}d\mathbf{r}\rho_e(\mathbf{r},\tau)\nabla_\beta\Phi(\mathbf{r}-\mathbf{R}_n^0)D^{\alpha\beta}_{nn'}(\omega_p=0)$$
$$+\frac{i}{2}\frac{1}{2\pi}\sum_{\mathbf{q}j\varkappa}\int_{-\infty}d\omega\frac{\mathrm{th}(\omega/2T)+\mathrm{cth}(\Delta/2T)}{i\omega_p-\omega-\Delta}b_j(\mathbf{q},\omega) \qquad (44)$$
$$\times A_{mm}\sum_{nn'}\langle m|\nabla_\alpha\Phi(\mathbf{r}'-\mathbf{R}_n^0)|m\rangle\langle m|\nabla_\beta\Phi(\mathbf{r}''-\mathbf{R}_{n'}^0)|m\rangle$$
$$\times\frac{e^{\alpha*}(qj|\varkappa)e^{\beta}(qj|\varkappa')}{N(M_\varkappa M_{\varkappa'})^{1/2}\omega_j(q)}\exp[iq(\rho_\varkappa-\rho_{\varkappa'})].$$

Following an obvious analytic continuation in ω and putting $\omega=h_{mn}\equiv E_p$ we obtain an explicit expression for E_p in the form

$$E_p\approx+H_{emm}-\sum_{\mathbf{q}j\varkappa}\frac{|g_{j\varkappa}(\mathbf{q})|^2}{\omega_{\mathbf{q}j}}|S^{\mathbf{q}}_{mm}|^2. \qquad (45)$$

Here

$$g_{j\varkappa}(\mathbf{q})=-\frac{\exp(iq\rho_\varkappa)}{[2NM_\varkappa\omega_j(\mathbf{q})]^{1/2}}\langle p|e(\mathbf{q}j|\varkappa)\nabla\Phi_\varkappa(\mathbf{r})|p'\rangle \qquad (46)$$

is the matrix element of the electron–phonon interaction. Equation (45) was obtained under the assumption that $E_p\gg T$. In the calculation of (45) we took also into account the symmetry change of a crystal by an infinitesimal source, which lowers the total symmetry of the crystal. Expression (45) was obtained with account taken of the lowering of the crystal symmetry by the sources to the site symmetry. In this case $A_{mm}\neq N_{el}/N$, i.e., the filling of the sites of the perturbed crystal is not uniform. Recognizing the smallness of the overlap integral, so that $A_{m_0m'}\sim A_{m_0m_0}|S^0_{m_0m'}|^2$, and normalizing the GF to an electron number equal to unity, we obtain $A_{m_0m_0}\sim 1$, accurate to the small quantity $|S^0_{m_0m'}|^2$. The exact form of the function $\varphi_m(\mathbf{r})$ can now be obtained by minimizing E_p with respect to φ.

Substituting the explicit form of $G_{mm}(\omega_p)$ in (35), we have for $G^{(0)}_{mm'}(\omega_p)$:

$$G^{(0)}_{mm'}(\omega_p)=\frac{S^0_{mm'}}{i\omega_p-h_{mm}}-\frac{H_{mm'}}{(i\omega_p-h_{mm})^2}. \qquad (47)$$

Here

$$H_{mm'}=\sum_{qj}\frac{(2\,\mathrm{Re}\,S^q_{m'm})S^0_{mm'}+S^0_{m'm}|S^{\mathbf{q}}_{mm}|^2}{\omega_j(\mathbf{q})}|g_j(\mathbf{q})|^2+H_{emm'}. \qquad (48)$$

Solving (35), which reduces to an integral equation, by an iteration using $G^0_{mm'}$ and G_{mm} to first order in the overlap integral $S^q_{mm'}$ and to arbitrary order in G_{mm}, we arrive, as can be easily checked by direct calculations, at a representa-

tion of the factor $\exp(-g^2_{mm'})$ in expression (33) for $G_{mm'}$, so that

$$G_{mm'}(\omega_p)=\frac{S^0_{mm'}\exp(-\theta_{mm'})}{i\omega_p-h_{mm}}-\frac{H_{mm'}\exp(-\theta_{mm'})}{(i\omega_p-h_{mm})^2} \quad (49)$$

in full agreement with (33).

Carrying out the obvious analytic continuation of $G_{mm}(\omega_p)$ (44) and $G_{mm'}(\omega_p)$ (44) into the regions of real frequencies ω, we calculate the electron dispersion law in the band $\varepsilon(\mathbf{k})$, assuming the potentials of the sources to be zero, and restoring by the same token the total symmetry of the crystal. We have

$$\varepsilon(\mathbf{p})=-\left[-2i\lim_{t\to 0}\int_{-\infty}^{+\infty}d\omega\sum_{m'}G_{mm'}(\omega)\exp(i\mathbf{pR}_{mm'})\,\omega\right]$$
$$\times\left[-2i\lim_{t\to 0}\int_{-\infty}^{+\infty}d\omega\sum_{m'}G_{mm'}(\omega)\exp(i\mathbf{pR}_{mm'})\right]^{-1}. \quad (50)$$

Calculating the intervals with respect to ω in (50), we obtain

$$\varepsilon(\mathbf{p})=\frac{\sum_{m'}H_{mm'}\exp(-g^2_{mm'})\exp(i\mathbf{pR}_{mm'})}{\sum_{m'}S^0_{mm'}\exp(-g^2_{mm'})\exp(i\mathbf{pR}_{mm'})}. \quad (51)$$

The dispersion law obtained for the electrons in the band is polaron-like, and the structure $H_{mm'}$ [Eq. (48)] coincides with the structure of an analogous expression obtained long ago by Tyablikov.[17]

CONCLUSION

A consistent analysis, with allowance for the local lattice deformation ($\langle u_n\rangle\neq 0$), leads to a polaron effect in the electron GF. The spectrum (51) corresponds to an exponentially narrow polaron band of width

$$W=D\exp(-g^2), \quad (52)$$

where g^2 is the value of $g^2_{mm'}$ for the nearest neighbors. Obviously, narrowing of the band (52) changes qualitatively the cooperative properties (superconducting and others) of the system if the adiabatic regime is disturbed, i.e., if inequality (6) is satisfied:

$$W\leqslant\omega. \quad (53)$$

Recognizing that $\lambda\simeq g^2\omega/D$ (Refs. 4 and 7), we obtain from (53) the following condition for the electron–phonon coupling constant at which polaron effects become significant:

$$\lambda\gtrsim(\omega/D)\ln(D/\omega). \quad (54)$$

If the adiabatic condition (1) is met, the left-hand side of inequality (54) turns out to be less than unity! It must be noted here, however, that the inequality (54) that determines the limits of applicability of traditional electron–phonon interaction theory is not rigorously exact, in view of the approximate character of the uncoupling (33). A more rigorous analysis, which is possible in the small-radius-polaron theory, shows (see Refs. 8 and 18) that polaron collapse of the band sets in at

$$\lambda\geqslant(2z)^{-1/2}, \quad (55)$$

where z is the coordination number of the lattice; this agrees with the physical condition (2). The transition from a Bloch wide-band electron to a small-radius polaron localized in a narrow band can be jumplike.

The analysis in the present paper, as in the initial ones,[1,2] does not include in explicit form effects of Coulomb interaction of the carriers. Allowance for this interaction influence very little the polaron-formation effects considered here. Indeed, in the case of a small-radius polaron the wave function $|m>$ of a polaron localized on site m decreases rapidly outside the limits of the given unit cell. In the polaron factor $g^2_{mm'}$, the only quantity that depends substantially on the electron density is the electron-ion interaction potential $\Phi(\mathbf{r}-\mathbf{R}^0_n)$, which is screened by free carriers.

The Coulomb interaction of the carriers will influence also the effective electron–electron attraction potential, causing it to decrease by a quantity $\langle m|v_{\text{coul}}|m'\rangle$, where m and m' denote neighboring sites or one and the same site.

This effect was investigated for interacting polarons in Refs. 4–6, and will be treated by us in the GF formalism in a separate paper.

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[1)] In simple metals the interaction $\widehat{\tilde{H}}_{ei}$ (crystal field) may turn out to be screened by free electrons, and at the same time $\tilde{H}-\hat{H}_{ei}$ is small to the extent that the overlap integrals of the atomic wave functions are small. It seems that $\widehat{\tilde{H}}_{ei}$ will be decisive in metal oxides with relatively low carrier density.

[1]G. M. Eliashberg, Zh. Eksp. Theor. Fiz. **38**, 966 (1960) [Sov. Phys. JETP **11**, 696 (1960)].
[2]A. B. Migdal, *ibid.* **34**, 1438 (1958) [7, 996 (1958)].
[3]A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, *Quantum Field-Theoretical Methods in Statistical Physics*, Pergamon, 1965 (p. 444 of Russian original).
[4]A. S. Alexandrov and V. Ranninger, Phys. Rev. B **23**, 1796 (1981).
[5]A. S. Alexandrov, V. Ranninger, and V. Robashkevich, *ibid.* B **33**, 4526 (1986).
[6]A. S. Aleksnadrov, Zh. Fiz. Khim. **57**, 273 (1983).
[7]A. S. Aleksandrov, Dokl. Akad. Nauk SSSR **293**, 835 (1987) [Sov. Phys. Doklady **32**, 286 (1987)].
[8]*Polarons* [in Russian], Yu. A. Firsov, ed., Nauka, 1975.
[9]A. S. Aleksandrov, Pis'ma Zh. Eksp. Teor. Fiz. **46**, Supplement, p. 128 [JETP Lett. **46**, Supplement, p. S107].
[10]A. S. Alexandrov, Phys. Rev. B **38**, 925 (1988)].
[11]A. S. Aleksandrov, V. N. Grebenev, and E. A. Mazur, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 357 (1987) [JETP Lett. **45**, 455 (1987)].
[12]G. Baym, Ann. Phys. (N. Y.) **14**, 1 (1961).
[13]E. S. Fradkin, Trudy FIAN **29**, 7 (1965).
[14]N. N. Bogolyubov, ed., *Statistical Physics and Quantum Field Theory* [in Russian], Nauka, 1973, pp. 7–80.
[15]E. G. Maksimov, Zh. Eksp. Teor. Fiz. **69**, 2236 (1975) [Sov. Phys. JETP **42**, 1138 (1975)].
[16]A. K. Rajagopal and M. H. Cohen, Sol. St. Phys. **1**, 9 (1972).
[17]S. V. Tyablikov, Zh. Eksp. Teor. Fiz. **23**, 381 (1952).
[18]A. S. Aleksandrov and A. B. Krebs, Moscow Engineering-Physics Preprint, 1988.

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