A self-consistent description of the electron-phonon system in metals and the problem of lattice stability

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A set of self-consistent equations for the electron and phonon Green functions of a normal metal is derived on the basis of the complete electron-ion Hamiltonian. A qualitative analysis of the obtained equations is carried out. It is shown, in complete agreement with the adiabatic approximation, that the nonadiabatic electron-phonon interaction, which leads to a considerable change in the electronic properties of a metal, cannot be the cause of a lattice instability. The stability of a lattice is determined by its dynamical vibration matrix. The electronic contribution to this vibration matrix is connected not with the electron-phonon coupling constant, but with the unscreened bare electron-ion interaction and the electronic susceptibility. It is shown on the example of the simple isotropic system that the condition for the dynamical stability of the system does not impose any restrictions on the electron-phonon coupling constant, but only leads to some restriction on the ratio of the bare electron-ion interaction to the electron-electron interaction. In particular, for the simple jellium model this condition leads to the absence of the Peierls instability even in the one-dimensional case.

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1. INTRODUCTION

The problem of the self-consistent description of the electron-phonon system in metals is undoubtedly one of the central problems in solid state physics. The establishment of the cause of the instability of a given crystal lattice, the influence on this instability of the electron-phonon interaction, the connection between the electron-phonon coupling constant, which determines the renormalization of the electron mass, and, for example, the value of the lattice-instability temperature, all these problems have, in our opinion, up till now not been satisfactorily solved. The reason for this lies not only in the complexity of the concrete computations of the properties of metals, but also in the absence of a consistent mathematical apparatus in the theory of the electron-ion system of a metal that takes the many-particle nature of such a system into account. Most often, the Hamiltonian used in considering the properties of the electron-phonon system is the Fröhlich Hamiltonian.[1] The properties of the system described by this Hamiltonian have been studied by Migdal.[2] In particular, it is shown in this paper, as well as in the paper[3] by Tyablikov and Tolmachev, that the phonon frequencies become purely imaginary, and, consequently, the lattice becomes unstable when the dimensionless electron-phonon coupling constant $\zeta = g^2 N(0) > 1$. As was shown in an even earlier paper by Fröhlich himself,[4] as well as by Kuper,[5] in a one-dimensional metallic system described by the Fröhlich Hamiltonian, the lattice becomes unstable at an arbitrarily small value of the electron-phonon coupling constant. Although, as has recently been elucidated in quite a number of papers,[6-8] allowance for the Coulomb interaction between the electrons, which is neglected in the Fröhlich model, leads to the establishment of certain conditions on the magnitude of the electron-phonon coupling constant at which a structural transition occurs, the possibility itself of establishing these conditions remains very much debatable.

The point is that the consistent adiabatic approach to the computation of the phonon spectra of an electron-ion system, first proposed by Born and Oppenheimer[9] and developed recently on a rigorous many-particle basis in Brovman and Kagan's papers,[10] shows that the renormalization of the phonon frequencies as a result of the nonadiabatic electron-phonon interaction is small and certainly cannot lead to any lattice instability. In this connection, the attempts undertaken in, for example, Kulik's paper[6] to establish a connection between the conditions for lattice stability and superconductivity on the basis of the assumption that the cause of both of these phenomena is the electron-phonon interaction also seem quite doubtful to us. In fact, lattice instability is possible even in the framework of the adiabatic approximation, and allowance for the nonadiabatic electron-phonon interaction adds little to this phenomenon. The cause, however, of the appearance of superconductivity is precisely the nonadiabatic electron-phonon interaction.

Unfortunately, the mathematical apparatus of the adiabatic approach is very poorly equipped for a self-consistent analysis of the electron and phonon systems. As one of the illustrations of this circumstance, we can cite Chan and Heine's paper,[11] where an incorrect use of the adiabatic approach led to the establishment of a lattice-instability condition containing the nonadiabatic electron-phonon coupling constant.

Recently, there have appeared in the wake of Baym's paper[12] investigations[13,14] in which attempts at a self-consistent description of the electron-phonon system are undertaken with the aid of the Green-function technique. It is absolutely clear that the self-consistent equations for the electron and phonon subsystems will be extremely complex. Unfortunately, in the majority of the indicated papers, these equations are unnecessarily overcomplicated. In Baym's early paper,[12] rigorous sum rules allowing the simplification of these equations were not used. In the recent Cohen and Rajagopal's paper,[14] which is closest in spirit to the present paper, instead of a single permittivity function for the electrons, several types of such functions were introduced. Also absent in these papers are analyses of the equations obtained.

The object of the present paper is to derive self-consistent equations for the electron-phonon system and

investigate on the basis of them the problem of lattice stability. We shall also consider the behavior of the non-adiabatic electron-phonon interaction constant and the possible connection between this constant and lattice instability. In Sec. II we derive the complete set of self-consistent equations describing the electrons and phonons; in the next section we carry out a qualitative analysis of the equations obtained and elucidate a number of their characteristic properties; in the last section of the paper we consider the results obtained from the equations derived and as illustrated by the simple quasi-isotropic system.

2. DERIVATION OF THE SELF-CONSISTENT EQUATIONS DESCRIBING THE ELECTRON-PHONON SYSTEM

Let us begin the analysis of the problem with the consideration of the complete electron-ion Hamiltonian in the harmonic approximation:

$$H = H_e + H_i + H_{ei}. \tag{1}$$

Here

$$H_e = \int d\mathbf{r} \psi^+(\mathbf{r}, t) \left[-\frac{\nabla^2}{2m} - \mu \right] \psi(\mathbf{r}, t) + \frac{1}{2} \int \int d\mathbf{r}\, d\mathbf{r}' \psi^+(\mathbf{r}, t) \psi^+(\mathbf{r}', t')$$

$$\times \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \psi(\mathbf{r}', t') \psi(\mathbf{r}, t), \tag{2}$$

$$H_i = \frac{1}{2} \sum_n M [\dot{u}_n{}^\alpha]^2 + \frac{1}{2} \sum_{n,n'} V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n'}{}^0)$$

$$+ \frac{1}{2} \sum_{n,n'} (u_n{}^\alpha - u_{n'}{}^\alpha) \nabla_\alpha V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n'}{}^0)$$

$$+ \frac{1}{4} \sum_{n,n'} (u_n{}^\alpha - u_{n'}{}^\alpha)(u_n{}^\beta - u_{n'}{}^\beta) \nabla_\alpha \nabla_\beta V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n'}{}^0), \tag{3}$$

$$H_{e-i} = \sum_n \int d\mathbf{r} \psi^+(\mathbf{r}, t) \psi(\mathbf{r}, t) V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0)$$

$$- \sum_n \int d\mathbf{r} \psi^+(\mathbf{r}, t) \psi(\mathbf{r}, t) \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0) u_n{}^\alpha$$

$$+ \frac{1}{2} \sum_n \int d\mathbf{r} \psi^+(\mathbf{r}, t) \psi(\mathbf{r}, t) \nabla_\alpha \nabla_\beta V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0) u_n{}^\alpha u_n{}^\beta. \tag{4}$$

Here, in writing down the Hamiltonian, we used the second-quantization representation for the electrons, $\psi^+(\mathbf{r}, t)$ and $\psi(\mathbf{r}, t)$ are electron creation and annihilation operators, and μ is the chemical potential of the electron system.

The ionic subsystem has been written in first-quantized form with the use of the ion-displacement operators:

$$\mathbf{u}_n = \mathbf{R}_n - \mathbf{R}_n{}^0, \tag{5}$$

where $\mathbf{R}_n{}^0$ is the location of an ion in a perfect periodic lattice, $V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n'}{}^0)$ is the ion-ion interaction potential, and $V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0)$ is the electron-ion interaction potential. A consistent analysis of the problem requires, generally speaking, that we treat the conduction and valence electrons on the same footing. In that case $V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n'}{}^0)$ and $V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0)$ are simply the Coulomb potentials of, respectively, the internuclear and the electron-nuclear interactions. The successes of the pseudopotential theory[15] have shown that a metal can be treated as a degenerate plasma with an electron density determined by the valence electrons, whose interaction with the ions is given by some pseudopotential. In our paper we shall consider this pseudopotential, $V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0)$, to be local and independent of the energy. We shall return to this

question and discuss it more rigorously in a specific computation of the physical properties of metals on the basis of the equations obtained by us.

Let us introduce in the usual manner the temperature Green function for the electrons:

$$G(\mathbf{r}, \tau; \mathbf{r}', \tau') = -i \langle T_\tau \psi(\mathbf{r}, \tau) \psi^+(\mathbf{r}', \tau') \rangle, \tag{6}$$

as well as the Green function for the ion displacements:

$$D_{nn'}^{\alpha\beta}(\tau - \tau') = -i \langle T_\tau u_n{}^\alpha(\tau) - \langle u_n{}^\alpha \rangle; \ u_{n'}{}^\beta - \langle u_{n'}{}^\beta \rangle \rangle,$$

where τ is a fictitious time varying within the limits

$$-i/T \leqslant \tau \leqslant i/T. \tag{7}$$

In a perfect crystal the function $D_{nn'}^{\alpha\beta}(\tau - \tau')$ goes over into the standard phonon Green function if we expand the ion displacement in terms of the phonon operators. We shall not do this, but shall obtain all the equations directly in coordinate space. For the derivation of these equations we shall use the method of functional differentiation. For this purpose, we shall add to the Hamiltonian (1) the external sources

$$H' = \int d\mathbf{r} \psi^+(\mathbf{r}, t) \psi(\mathbf{r}, t) U(\mathbf{r}, t) + \sum_n J_n{}^\alpha(t) u_n{}^\alpha(t). \tag{8}$$

Let us write down the equation for the operators:

$$i \frac{\partial \psi}{\partial \tau} = \frac{\delta H}{\delta \psi^+}, \quad -M \frac{\partial^2 u_n{}^\alpha}{\partial \tau^2} = \frac{\delta H}{\delta u_n{}^\alpha}. \tag{9}$$

Averaging the equations for $u_n{}^\alpha$, and taking into account the fact that

$$\frac{\delta \langle u_n{}^\alpha(\tau) \rangle}{\delta J_{n'}{}^\beta(\tau')} = D_{nn'}^{\alpha\beta}(\tau - \tau'), \tag{10}$$

we obtain the equation for the ion-displacement Green function

$$M \frac{\partial^2}{\partial \tau^2} D_{nn'}^{\alpha\beta}(\tau - \tau') + \frac{\delta}{\delta J_{n'}{}^\beta(\tau')} \int d\mathbf{r} \langle \psi^+(\mathbf{r}, \tau) \psi(\mathbf{r}, \tau) \rangle \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0)$$

$$- \frac{\delta}{\delta J_{n'}{}^\beta(\tau')} \int d\mathbf{r} \langle \psi^+(\mathbf{r}, \tau) \psi(\mathbf{r}, \tau) u_n{}^\gamma(\tau) \rangle \nabla_\alpha \nabla_\gamma V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0) \tag{11}$$

$$+ \sum_{n'' \neq n} \nabla_\alpha \nabla_\gamma V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n''}{}^0) [D_{nn'}^{\gamma\beta}(\tau - \tau') - D_{n''n'}^{\gamma\beta}(\tau - \tau')] = -\delta_{nn'}^{\alpha\beta} \delta(\tau - \tau').$$

In the usual manner, for the electron Green function $G(x, x')$ (here $x = \mathbf{r}, \tau$; $x' = \mathbf{r}', \tau'$), we obtain

$$\left[i \frac{\partial}{\partial \tau} + \left(\frac{\nabla^2}{2m} + \mu \right) - U(x) - \sum_n V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0) \right] G(x, x')$$

$$= \delta(x - x') + i \sum_n \langle T_\tau \psi(x) \psi^+(x') u_n{}^\alpha(\tau) \rangle \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0)$$

$$- \frac{i}{2} \sum_n \langle T_\tau \psi(x) \psi^+(x') u_n{}^\alpha(\tau) u_n{}^\beta(\tau) \rangle \nabla_\alpha \nabla_\beta V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0)$$

$$- i \int d\mathbf{r}_1 \frac{e^2}{|\mathbf{r} - \mathbf{r}_1|} \langle T_\tau \psi^+(\mathbf{r}_1, \tau) \psi(\mathbf{r}_1, \tau) \psi(x) \psi(x') \rangle. \tag{12}$$

By using the rules of functional differentiation, we can rewrite the equations for the Green functions $G(x, x)$ and $D_{nn'}^{\alpha\beta}(\tau - \tau')$ in the form of equations in functional derivatives:

$$M \frac{\partial^2}{\partial \tau^2} D_{nn'}^{\alpha\beta}(\tau - \tau') + \left[\sum_{n'' \neq n} \nabla_\alpha \nabla_\gamma V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n''}{}^0) \right.$$

$$\left. - \int d\mathbf{r} \langle \rho_c(\mathbf{r}, \tau) \rangle \nabla_\alpha \nabla_\gamma V_{ei}(\mathbf{r} - \mathbf{R}_n{}^0) \right] D_{nn'}^{\gamma\beta}(\tau - \tau')$$

$$= -\delta_{nn'}^{\alpha\beta} \delta(\tau - \tau') + \sum_{n'' \neq n} \nabla_\alpha \nabla_\gamma V_{ii}(\mathbf{R}_n{}^0 - \mathbf{R}_{n''}{}^0) D_{n''n'}^{\gamma\beta}(\tau - \tau')$$

E. G. Maksimov

$$+ \int dr \frac{\delta}{\delta J_n'^{\beta}(\tau')} \Big[\langle \rho_e(\mathbf{r}, \tau) \rangle \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n^0)$$
$$+ \frac{\delta}{\delta J_n^{\tau}(\tau)} \langle \rho_e(\mathbf{r}, \tau) \rangle \nabla_\alpha \nabla_\tau V_{ei}(\mathbf{r} - \mathbf{R}_n^0) \Big]. \quad (13)$$

Here $\langle \rho_e(\mathbf{r}, \tau) \rangle$ is the averaged electron-density operator:

$$\langle \rho_e(\mathbf{r}, \tau) \rangle = \langle \psi^+(\mathbf{r}, \tau) \psi(\mathbf{r}, \tau) \rangle,$$

$$\Big[i\frac{\partial}{\partial \tau} + \Big(\frac{\nabla^2}{2m} + \mu\Big) - U(x) - \int dr'' \frac{e^2 \langle \rho_e(\mathbf{r}'', \tau) \rangle}{|\mathbf{r} - \mathbf{r}''|}$$

$$- \sum_n V_{ei}(\mathbf{r} - \mathbf{R}_n^0) + \sum_n \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n^0) \langle u_n^\alpha(\tau) \rangle$$

$$- i\sum_n \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n^0) \frac{\delta}{\delta J_n^\alpha(\tau)}$$

$$- ie^2 \int dr'' \frac{1}{|\mathbf{r} - \mathbf{r}''|} \frac{\delta}{\delta U(\mathbf{r}'', \tau)} \Big] G(x, x') = \delta(x - x'). \quad (14)$$

Introducing in place of the external source U(x) the generalized field $U_{eff}(x)$:

$$U_{eff}(x) = U(x) + e^2 \int dr'' \frac{\langle \rho_e(\mathbf{r}'', \tau) \rangle}{|\mathbf{r} - \mathbf{r}''|}$$

$$+ \sum_n V_{ei}(\mathbf{r} - \mathbf{R}_n^0) - \sum_n \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n^0) \langle u_n^\alpha(\tau) \rangle, \quad (15)$$

we can express the functional derivatives $\delta/\delta U(x)$ and $\delta/\delta J_n^\alpha(\tau)$ in terms of $\delta/\delta U_{eff}(x)$. With that end in view, let us, to begin with, determine the irreducible polarization operator $\Pi(x, x')$ of the electrons:

$$\Pi(x, x') = \frac{\delta \langle \rho_e(x) \rangle}{\delta U_{eff}(x')} = - \int dx_1 dx_2 G(x, x_1) G(x, x_2) \Gamma(x_1, x_2, x'), \quad (16)$$

where $\Gamma(x_1, x_2, x')$ is the irreducible vertex function of the interelectron interaction:

$$\Gamma(x_1, x_2, x') = \frac{\delta G^{-1}(x_1, x_2)}{\delta U_{eff}(x')}. \quad (17)$$

We shall return a little later to the consideration of this function. Using the formula (16) we can determine the permittivity function $\epsilon(x, x')$ and the total electronic susceptibility $\chi(x, x')$:

$$\epsilon^{-1}(x, x') = \delta(x - x') + \int dx_1 \int dr'' \frac{e^2}{|\mathbf{r} - \mathbf{r}''|} \Pi(\mathbf{r}''\tau, x_1) \epsilon^{-1}(x_1, x'), \quad (18)$$

$$\chi(x, x') = \int dx_1 \Pi(x, x_1) \epsilon^{-1}(x_1, x') = \frac{\nabla_x^2}{4\pi e^2}[\epsilon^{-1}(x, x') - \delta(x - x')]. \quad (19)$$

Using the above-introduced functions, we can write

$$\frac{\delta}{\delta J_n'^\beta(\tau')} = \int dx_1 \frac{\delta U_{eff}(x_1)}{\delta J_n'^\beta(\tau')} \frac{\delta}{\delta U_{eff}(x_1)}$$

$$= \sum_{n''} \int dx_1 dx_2 \epsilon^{-1}(x_1, x_2) \nabla_\alpha V_{ei}(\mathbf{r}_2 - \mathbf{R}_{n''}^0) D_{n''n'}^{\alpha\beta}(\tau_2 - \tau') \frac{\delta}{\delta U_{eff}(x_1)}, \quad (20)$$

$$\frac{\delta}{\delta U(x')} = \int dx_1 \frac{\delta U_{eff}(x_1)}{\delta U(x')} \frac{\delta}{\delta U_{eff}(x_1)}$$

$$= \int dx_1 \Big\{ \epsilon^{-1}(x_1, x') - \sum_{n,n'} \int dx_3 dx_4 \epsilon^{-1}(x_1, x_4)$$

$$\times \chi(x', x_3) \nabla_\alpha V_{ei}(\mathbf{r}_4 - \mathbf{R}_n^0) \nabla_\tau V_{ei}(\mathbf{r}_3 - \mathbf{R}_{n'}^0) D_{nn'}^{\alpha\tau}(\tau_3 - \tau_4) \Big\}. \quad (21)$$

Finally, after lengthy, but straightforward calculations, we can reduce the equations for the ion-displacement Green functions and the electron Green function to the following quite standard form:

$$\Big[M\frac{\partial^2}{\partial \tau^2} \delta_{nn''}^{\tau\alpha} + \sum_{n'' \neq n} \Phi_{nn''}^{\alpha\tau} \Big] D_{n''n'}^{\tau\beta}(\tau - \tau') = -\delta_{nn'}^{\alpha\beta} \delta(\tau - \tau'), \quad (22)$$

where $\Phi_{nn''}^{\alpha\gamma}$ is the dynamical vibration matrix, determined by the sum of the ionic and electronic parts:

$$\Phi_{nn''}^{\alpha\tau} = \frac{\partial^2 V_{ii}(\mathbf{R}_n^0 - \mathbf{R}_{n''}^0)}{\partial R_n^\alpha \partial R_{n''}^\tau} - \delta_{nn''} \sum_{n''' \neq n} \frac{\partial^2 V_{ii}(\mathbf{R}_n^0 - \mathbf{R}_{n'''}^0)}{\partial R_n^\alpha \partial R_{n'''}^\tau}$$

$$+ \int dr dx' \chi(\mathbf{r}\tau, x') \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n^0) \nabla_\tau V_{ei}(\mathbf{r}' - \mathbf{R}_{n''}^0)$$

$$- \delta_{nn''} \sum_{n''' \neq n} \int dr dr' \chi(\mathbf{r}\tau, \mathbf{r}'\tau^+) \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_n^0) \nabla_\tau V_{ei}(\mathbf{r}' - \mathbf{R}_{n'''}^0). \quad (23)$$

In writing down the last term, we used the well-known[13] sum rule:

$$\int dr \langle \rho_e(\mathbf{r}, \tau) \rangle \nabla_\alpha \nabla_\tau V_{ei}(\mathbf{r} - \mathbf{R}_n^0) = - \int dr \langle \nabla_\alpha \rho_e(\mathbf{r}, \tau) \rangle \nabla_\tau V_{ei}(\mathbf{r} - \mathbf{R}_n^0)$$

$$= \sum_{n'' \neq n} \int dr dr' \chi(\mathbf{r}\tau, \mathbf{r}'\tau^+) \nabla_\alpha V_{ei}(\mathbf{r} - \mathbf{R}_{n''}^0) \nabla_\tau V_{ei}(\mathbf{r}' - \mathbf{R}_n^0).$$

For the electron Green function we have

$$G^{-1}(x, x') = i\frac{\partial}{\partial \tau} + \Big(\frac{\nabla^2}{2m} + \mu\Big) - U_{eff}(x) - \Sigma(x, x'). \quad (24)$$

When the external source is switched off, i.e., when we set $U(x) = 0$, the quantity $U_{eff}(x)$, as can be seen from the formula (15), goes over into the usual expression for a crystal potential of the Hartree type for conduction electrons. The self-energy part, $\Sigma(x, x')$, is determined by the exchange and correlation of the electrons as a result of the direct Coulomb interaction and the electron-phonon interaction, and is given by the following expression:

$$\Sigma(x, x') = -i \int dx_1 dx_2 \Big\{\Big[\int \frac{dr'' e^2}{|\mathbf{r} - \mathbf{r}''|} \epsilon^{-1}(\mathbf{r}''\tau, x_1)$$

$$+ \sum_{n,n'} \int dx_3 dx_4 \epsilon^{-1}(x, x_3) \nabla_\alpha V_{ei}(\mathbf{r}_3 - \mathbf{R}_n^0) \epsilon^{-1}(x_1, x_4)$$

$$\times \nabla_\beta V_{ei}(\mathbf{r}_4 - \mathbf{R}_{n'}^0) D_{nn'}^{\alpha\beta}(\tau_3 - \tau_4) \Big\} G(x, x_2) \Gamma(x_2, x', x_1). \quad (25)$$

The quantity figuring in the curly brackets in the formula (25) plays the role of an effective interelectron interaction $V_{eff}(x, x')$:

$$V_{eff}(x, x') = \int dr'' \frac{e^2}{|\mathbf{r} - \mathbf{r}''|} \epsilon^{-1}(\mathbf{r}''\tau, x')$$

$$+ \sum_{n,n'} \int dx_1 dx_2 \epsilon^{-1}(x, x_1) \nabla_\alpha V_{ei}(\mathbf{r}_1 - \mathbf{R}_n^0) \epsilon^{-1}(x', x_2)$$

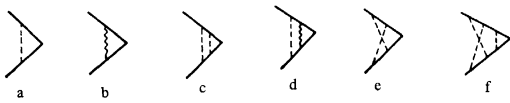$$\times \nabla_\beta V_{ei}(\mathbf{r}_2 - \mathbf{R}_{n'}^0) D_{nn'}^{\alpha\beta}(\tau_1 - \tau_2). \quad (26)$$

The first term in $V_{eff}(x, x')$ is the potential for the screened Coulomb interaction between the electrons and the second term is the potential for the electron-phonon interaction.

3. QUALITATIVE ANALYSIS OF THE SELF-CONSISTENT EQUATIONS

Before proceeding to make an attempt at a consistent solution of the obtained equations, let us discuss some characteristic properties of these equations. Let us point out at once that the main fundamental difficulty in solving these equations lies in the computation of the vertex function $\Gamma(x_2, x', x_1)$. Using the definition (17) and the formula (24), we can write $\Gamma(x_2, x', x_1)$ the following equation:

$$\Gamma(x_2, x', x_1) = \delta(x_2 - x')\delta(x_2 - x_1) - \int dx_3 dx_4 dx_5 dx_6 \cdot$$

$$\cdot \frac{\delta \Sigma(x_2, x')}{\delta G(x_3, x_4)} G(x_3, x_5) \Gamma(x_5, x_6, x_1) G(x_6, x_4).$$

Some simple perturbation-theory diagrams for $\Gamma(x_2, x', x_1)$ are shown in Fig. 1. In these diagrams the wavy line corresponds to the electron-phonon interaction; the dashed line, the screened Coulomb interaction. As has been shown by Migdal,[2] allowance for the phonon corrections to the vertex function leads to quantities smaller than the bare vertex function by a factor of

$\sqrt{m/M}$. Indeed, it is easy to verify that the diagram 1b is smaller than 1a by precisely a factor of $\sqrt{m/M}$. The same is true for the diagrams 1d and 1c. It would seem to follow from this that we can, in computing the vertex function $\Gamma(x_2, x', x_1)$, neglect all the diagrams with phonon lines. It can be shown that this is, in fact, correct when computing the polarization operator $\Pi(x, x')$. At least at temperatures lower than the characteristic phonon frequencies, we should in the formula (16) use in place of the total vertex $\Gamma(x_2, x', x_1)$ the function $\Gamma_0(x_2, x', x_1)$ determined by only the screened Coulomb interaction (the sum of diagrams of the type 1, a), c), f)). In metals the Coulomb interaction virtually does not have any smallness parameter; therefore, there is no consistent procedure that allows us to select the most important diagrams for the computation of $\Gamma_0(x_2, x', x_1)$. In recent years the problem of Coulomb correlations at electron densities corresponding to real metals has been the subject of numerous investigations.[10,16-19] It was elucidated in these papers that the properties of an electron system with respect to the screened Coulomb interaction are, at least if not literally, then numerically, very close to the properties of a tenuous system. In Rice's paper[20] it is also shown that allowance for even the simplest, to all intents and purposes, ladder diagrams with a screened Coulomb interaction leads to quite a good description of many properties of metals.

Returning to the determination of the self-energy part of the electron Green function (formula (25)), we note that in this case the total neglect of the phonon corrections to the vertex function is absolutely inadmissible. In order to understand why this is so, let us schematically rewrite the expression for $\Sigma(x, x')$ in the form of a sum of two terms:

$$\Sigma(x, x') = -i\int \tilde{V}_{ee}G\Gamma - i\int \nabla_\alpha \tilde{V}_{ie}D_{\alpha\beta}\nabla_\beta \tilde{V}_{ie}G\Gamma. \quad (27)$$

Here we have denoted the screened Coulomb interaction by $\tilde{V}_{ee}$ and the screened electron-ion interaction by $\tilde{V}_{ie}$. As is well known, without allowance for the vertex corrections, the second term is smaller than the first by a factor of ω_D/ϵ_F. The necessity of the allowance for the phonon contribution to $\Sigma(x, x')$ is connected with the fact that the second term is not small in comparison with the electron energies near the Fermi surface and rapidly varies in this region, leading to large corrections Δm to the electron mass ($\Delta m \approx \delta\Sigma/\partial\omega$). Since each additional phonon line at the vertex leads to a smallness of the order of $\sqrt{m/M}$, we can neglect in the vertex function in the second term in (27) the phonon corrections and replace it by $\Gamma_0(x_2, x', x_1)$. We cannot do this in the first term.

Let us consider the series of the simplest diagrams arising as a result of the first term in (27) and shown in Fig. 2. It can easily be verified that the diagrams 2b and 2d are not small compared to the phonon contribution arising from the second term. The overall sum of the diagrams arising from the first term with allowance in the vertex function of one phonon line and the second term can be reduced to the skeleton diagrams shown in Fig. 3. In the diagram 3a the circles denote the total

Coulomb vertices Γ_0. Batyev and Pokrovskiĭ[21] have shown that for isotropic systems with a Coulomb interaction the diagram 3b is small compared to the purely Coulomb interaction (arising from the summation of diagrams of the type 2a, 2c, and 2e) and is a constant near the Fermi surface. An analogous conclusion can be drawn about diagrams of the type 3c. Therefore, we can neglect all these diagrams and rewrite Eq. (27) for $\Sigma(x, x')$ in the following form, which formally coincides with the equation obtained by Batyev and Pokrovskiĭ for an isotropic system:

$$\Sigma(x, x') = -i\int \tilde{V}_{ee}G\Gamma_0 - i\int \Gamma_0 \nabla_\alpha \tilde{V}_{ie}D_{\alpha\beta}\Gamma_0 \nabla_\beta \tilde{V}_{ie}G. \quad (28)$$

The dynamics of the lattice is determined by Eqs. (22) and (23). The nonadiabaticity is contained only in the third term of Eq. (23), which determines the dynamical vibration matrix $\Phi_{nn''}^{\alpha\gamma}$. In the framework of the self-consistent approach to the electron-phonon system, the adiabaticity condition reduces to the following approximation for the electronic susceptibility:

$$\chi(x, x') = \delta(\tau - \tau')\chi(r, r'). \quad (29)$$

The characteristic times, τ_e, of the variation of the electronic susceptibility are due to the interelectron correlations. In metals, $\tau_e \approx 1/\epsilon_F$, i.e., they are considerably less than the characteristic phonon times $\tau_{ph} \approx 1/\omega_D$ at which the temporal behavior of $\chi(x, x')$ is important. For such large times τ_{ph}, the relation (29) is valid up to quantities of the order of ω_D/ϵ_F. It should be noted that the deviation from adiabaticity and the nonadiabatic corrections to the phonon frequencies, as well as the attenuation of these frequencies, arise not only because of the electron-phonon interaction, but also because of the purely Coulomb correlations. Indeed, as can be seen from (19) and (23), the nonadiabatic corrections and the deviations from the relation (29) will arise also in the case when the influence of the phonons is neglected in the computation of the electronic susceptibility $\chi(x, x')$. As has been shown by Ipatova and Subashiev,[22] an analogous phenomenon obtains also in the adiabatic approach when the Coulomb correlations are correctly taken into account.

Before proceeding to a concrete investigation of the condition for lattice stability and its connection with the effective interelectron interaction, a problem which is very important, in particular for the superconductivity of metals, we note two conclusions which follow from the equations for the lattice dynamics, (22) and (23), and for the electron self-energy part $\Sigma(x, x')$, (28).

1. The electronic contribution to the lattice dynamics is, as follows from (23), determined by the unscreened electron-ion pseudopotential and the electronic susceptibility. The electron-phonon interaction matrix element determining the phonon contribution to the electron self-energy (the second term in (28)) is connected with the
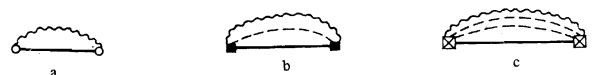

FIG. 2

FIG. 3

E. G. Maksimov

effective screened electron-ion pseudopotential which takes the vertex corrections into account, $\widetilde{\widetilde{V}}_{ie}$:

$$\widetilde{\widetilde{V}}_{ie} = \int \Gamma_0 \varepsilon^{-1} V_{ic}. \qquad (30)$$

If even we assume the unscreened electron-ion pseudopotential to be local, the effective pseudopotential $\widetilde{\widetilde{V}}_{ie}$ will, because of the presence of Γ_0, be nonlocal. As the Yasuhara and Watabe's computations [23] show, this nonlocal nature of $\widetilde{\widetilde{V}}_{ie}$ can be very important for real metals.

2. In the standard Bloch approach to the electron-phonon system, it is assumed that the matrix element of the electron-phonon interaction is determined by the gradient of the total self-consistent crystal potential. As can be shown from Eqs. (24) and (8), this is, in fact, not so; the electron band structure is, in accordance with (24), determined by the following equation:

$$\left[\left(\frac{\nabla^2}{2m} + \mu\right) - U_{eff}(x)\right]\psi_k(r) - \int d^3r' \Sigma(r, r', E_k)\psi_k(r') = E_k\psi_k(r'). \qquad (31)$$

The matrix element of the electron-phonon interaction is determined by the gradient of the effective electron-ion pseudopotential $\widetilde{\widetilde{V}}_{ie}$ (formula (30)). As the computations of Rasolt and Vosko [24] show, the nonlocal potential determining the band structure in Eq. (31) can, generally speaking, be significantly different from $\widetilde{\widetilde{V}}_{ie}$.

4. A CRITERION FOR LATTICE STABILITY AND THE EFFECTIVE INTERELECTRON INTERACTION IN A QUASI-ISOTROPIC MEDIUM

In conclusion of this paper, let us, as an example of the use of the above-obtained self-consistent equations, consider the properties of a quasi-isotropic electron-phonon system. For such a system, we can, on the basis of Eqs. (22) and (23), write

$$D^{-1}(q\lambda, \omega) = D_0^{-1}(q\lambda, \omega) - M(q\lambda, \omega). \qquad (32)$$

The function $D_0(q\lambda, \omega)$ will determine the vibrations of the ionic lattice, and the longitudinal vibrational mode for $q \to 0$ gives the plasma frequency of the ion vibrations:

$$\omega_0(q) = 4\pi N Z^2 e^2/M, \qquad (33)$$

$$D(q\lambda, \omega) = \omega_0^2(q\lambda)/[\omega^2 - \omega_0^2(q\lambda)]. \qquad (34)$$

The mass operator $M(q\lambda, \omega)$ contains the electron contribution to the lattice dynamics and is, in accordance with Eq. (23), equal to

$$M(q\lambda, \omega) = g_0^2(q\lambda)\chi(q, 0), \qquad (35)$$

where $g_0^2(q\lambda)$ is the matrix element of the interaction of the electrons with the plasma oscillations of the ions

$$g_0(q\lambda) = i\sqrt{\frac{N}{M\omega_0^2(q\lambda)}} q^2 V_{ic}^2(q). \qquad (36)$$

In accordance with these equations,

$$D(q\lambda, \omega) = \frac{\omega_0^2(q\lambda)}{\omega^2 - \omega_0^2(q\lambda)[1 - g_0^2(q\lambda)\chi(q, 0)]} \qquad (37)$$

The phonon frequencies are determined by the condition

$$\omega^2(q\lambda) = \omega_0^2(q\lambda)[1 - g_0^2(q\lambda)\chi(q, 0)]. \qquad (38)$$

The condition for dynamical lattice stability, $\omega^2(q\lambda) > 0$, leads to the following inequality:

$$g_0^2(q\lambda)\chi(q, 0) < 1. \qquad (39)$$

If we use for $\chi(q, 0)$ the well-known approximate expression [11]

$$\chi(q, 0) = \frac{\Pi_0(q, 0)}{1 - [V(q) - \frac{1}{2}U]\Pi_0(q, 0)} \qquad (40)$$

where $\Pi_0(q, 0)$ is the standard Lindhard expression for the polarization operator, $V(q)$ is the direct unscreened Coulomb interaction in an isotropic system ($V(q) = 4\pi e^2/q^2$), and U is the exchange interaction, then we obtain the following condition for lattice stability:

$$g_0^2(q\lambda) + \frac{U}{2} - V(q) < \frac{1}{|\Pi_0(q, 0)|}. \qquad (41)$$

This condition is quite similar to the condition obtained in the already mentioned paper by Chan and Heine. [11] However, because of the incorrect use of the adiabatic approximation in their paper, instead of the coupling constant g_0^2 for the interaction of the electrons and phonons with the bare plasma oscillations, into the condition (41) entered the true coupling constant for the interaction with the phonons. The incorrectness of their result is clear even from the fact that at small q the quantity $g_0^2 \approx 1/q^2$, i.e., it behaves just like $V(q)$, whereas the true coupling constant for the interaction with the phonons $g(q\lambda) \to 0$ as $q \to 0$. If we do not use the approximate expression for $\chi(q, 0)$, but express it in terms of $\varepsilon(q, 0)$:

$$\chi(q, 0) = \frac{1}{V(q)}\left(\frac{1}{\varepsilon(q, 0)} - 1\right),$$

then we can write the stability condition in the form

$$\frac{g_0^2(q\lambda)}{V(q)} < \frac{\varepsilon(q, 0)}{\varepsilon(q, 0) - 1}. \qquad (42)$$

It can be seen from (42) that, in contrast to the Fröhlich model, the lattice-stability condition does not impose any limitation on the electron-phonon coupling constant, but only establishes a relation for the ratio of the electron-phonon coupling constant to the Coulomb constant. In the simplest isotropic "jellium" model, as is well known,

$$g_0^2(q\lambda)/V(q) = 1.$$

Since $\varepsilon(q, 0) > 1$ in an electron system, there cannot be any lattice instability in the jellium model—not even in the one-dimensional case. The conclusion about the absence of the Peierls instability in the one-dimensional jellium model was arrived at in [7,8].

The last question that we consider in this paper consists in the following. Does the lattice-stability condition impose any limitations on the effective interelectron interaction $V_{eff}(q, \omega)$ determined by the formula (26)? Let us rewrite this interaction in the form

$$V_{eff}(q, \omega) = \frac{4\pi e^2}{q^2\varepsilon(q, \omega)} + \frac{g_0^2(q\lambda)}{\varepsilon^2(q, 0)}\frac{\omega_0^2(q\lambda)}{\omega^2 - \omega_0^2(q\lambda)} = \frac{4\pi e^2}{q^2\varepsilon_{eff}(q, \omega)}, \qquad (43)$$

where

$$\varepsilon_{eff}(q, \omega) = \varepsilon(q, \omega) - \frac{g_0^2(q\lambda)}{V(q)}\frac{\omega_0^2(q\lambda)}{\omega^2 + \omega_0^2(q\lambda)[g_0^2(q\lambda)/V(q) - 1]}.$$

In Nozières and Pines's book, [24] there is derived virtually for an isotropic medium a stability condition for the system that amounts to the following:

$$\varepsilon_{eff}(q, 0) > 0. \qquad (44)$$

It follows from this condition that the electron-phonon interaction, which is the second term in (43), should be weaker than the direct Coulomb repulsion. Cohen and Anderson [25] and Kirzhnits, Maksimov, and Khomskiĭ [26]

have shown that in such a situation there obtains a very strong limitation on the possible maximum values of the critical superconducting-transition temperature T_c in the isotropic medium. As follows from the analysis carried out in this paper, the lattice-stability condition (42) leads, in fact, only to the following limitation on $\epsilon_{eff}(q, 0)$:

$$\epsilon_{eff}(q, 0)\,[g_0^2(q\lambda)/V(q)-1]<0.$$

At small $q \to 0$, as follows from (42) and from the behavior of $\epsilon(q, 0)$ at small q, we indeed have that $g_0^2(q\lambda)<V(q)$ and $\epsilon_{eff}(q, 0) > 0$. On the other hand, at large values of q, which are the most important in superconductivity, the condition (42) allows us to have $g_0^2(q\lambda)/V(q) > 1$, and in this case $\epsilon_{eff}(q, 0) < 0$. This means that the electron-phonon attraction at large q can be considerably stronger than the Coulomb repulsion and the stability condition does not impose any limitations on the possible values of T_c.

Irrespective of the computations carried out here the very existence of the stability condition introduced by Pines and Nozières[24] arouses, as D. A. Kirzhnits has informed this author, a strong objection from the dynamical point of view.

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