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. The properties of the system described by this Hamiltonian have been studied by Migdal. In particular, it is shown in this paper, as well as in the paper by Tyablikov and Tolmachev, that the phonon frequencies become purely imaginary, and, consequently, the lattice becomes unstable when the dimensionless electron-phonon coupling constant \( \xi = g^2 N(0) > 1 \). As was shown in an even earlier paper by Fröhlich himself, as well as by Kuper, 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, 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 and developed recently on a rigorous many-particle basis in Brovman and Kagan's papers, 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 to establish a connection between the conditions for lattice stability and superconductivity on the basis of the assumption that the cause of both 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, 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 investigations 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, rigorous sum rules allowing the simplification of these equations were not used. In the recent Cohen and Rajagopal's paper, 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 nonadiabatic 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:

\[ H = H_0 + H_I + H_{\text{int}} \]  

(1)

Here

\[ H_0 = \int d\mathbf{r} d\mathbf{r}' \left( -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{\mu}{2} \right) \psi^* (\mathbf{r}, t) \psi (\mathbf{r}', t') \times \frac{e^{i \mathbf{r} \cdot \mathbf{e} \cdot \mathbf{r}'}}{r - r'} \psi^* (\mathbf{r}', t') \psi (\mathbf{r}, t), \]

(2)

\[ H_I = \frac{1}{2} \sum_{\mathbf{R}} \sum_{\mathbf{r}} \sum_{\mathbf{r}'} \left( \Delta_{\mathbf{r} \mathbf{r}'}^2 + \frac{1}{2} \sum_{\mathbf{R}} V_{\mathbf{r} \mathbf{R}} \Delta_{\mathbf{R} \mathbf{R}'} \right) + \sum_{\mathbf{R} \mathbf{r} \mathbf{r}'} V_{\mathbf{r} \mathbf{R}} \Delta_{\mathbf{R} \mathbf{R}'} \Delta_{\mathbf{R} \mathbf{R}'}^* \psi^* (\mathbf{r}, t) \psi (\mathbf{r}', t'), \]

(3)

\[ H_{\text{int}} = \sum_{\mathbf{R}} \int d\mathbf{r} d\mathbf{r}' \psi^* (\mathbf{r}, t) \psi (\mathbf{r}', t) V_{\mathbf{r} \mathbf{R}} \psi^* (\mathbf{r}, t) \psi (\mathbf{r}', t'), \]

(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 \( \mu \) 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:

\[ u_{\mathbf{R}} = -\mathbf{R}, \]

(5)

where \( \mathbf{R} \) is the location of an ion in a perfect periodic lattice, \( V_{\mathbf{r} \mathbf{R}} (\mathbf{R}^a - \mathbf{R}^b) \) is the ion-ion interaction potential, and \( V_{\mathbf{r} \mathbf{R}} (\mathbf{r} - \mathbf{R}^a) \) 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 \( V_{\mathbf{r} \mathbf{R}} (\mathbf{R}^a - \mathbf{R}^b) \) and \( V_{\mathbf{r} \mathbf{R}} (\mathbf{r} - \mathbf{R}^a) \) are simply the Coulomb potentials of, respectively, the internuclear and the electron-nuclear interactions. The successes of the pseudopotential theory 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, \( V_{\mathbf{r} \mathbf{R}} (\mathbf{r} - \mathbf{R}^a) \), 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:

\[ G (x, x') = -i \langle T \psi^* (x, t) \psi^* (x', t') \rangle, \]

(6)

as well as the Green function for the ion displacements:

\[ D_{\mathbf{R} \mathbf{R}'}^2 (t - t') = -i \langle T u_{\mathbf{R}}^* (t) u_{\mathbf{R}'}^* (t') \rangle \]

(7)

where \( \tau \) is a fictitious time varying within the limits

\[ -i T < \tau < i T. \]

In a perfect crystal the function \( D_{\mathbf{R} \mathbf{R}'}^2 (\tau - \tau') \) 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

\[ H' = \int d\mathbf{r} d\mathbf{r}' \psi^* (\mathbf{r}, t) \psi (\mathbf{r}, t) U (\mathbf{r}, t) + \sum_{\mathbf{R}} J_{\mathbf{R}}^* (t) u_{\mathbf{R}}^* (t). \]

(8)

Let us write down the equation for the operators:

\[ M \frac{\partial}{\partial \tau} D_{\mathbf{R} \mathbf{R}'}^2 (\tau - \tau') + \frac{\delta}{\delta J_{\mathbf{R}}^* (\tau')} \int d\mathbf{r} d\mathbf{r}' \psi^* (\mathbf{r}, t) \psi (\mathbf{r}, t) V_{\mathbf{r} \mathbf{R}} u_{\mathbf{R}}^* (\mathbf{r}) \psi^* (\mathbf{r}, t) \psi (\mathbf{r}, t) V_{\mathbf{r} \mathbf{R}} u_{\mathbf{R}}^* (\mathbf{r}) = -M \frac{\delta}{\delta J_{\mathbf{R}}^* (\tau')} \int d\mathbf{r} d\mathbf{r}' \psi^* (\mathbf{r}, t) \psi (\mathbf{r}, t) V_{\mathbf{r} \mathbf{R}} u_{\mathbf{R}}^* (\mathbf{r}) \psi^* (\mathbf{r}, t) \psi (\mathbf{r}, t) V_{\mathbf{r} \mathbf{R}} u_{\mathbf{R}}^* (\mathbf{r}) \]

(9)

(10)

In the usual manner, for the electron Green function \( G (x, x') \) (here \( x = \mathbf{r}, t; x' = \mathbf{r}', t' \)), we obtain

\[ \left( \frac{i}{\hbar} + \frac{\mathbf{V}}{2m_e} + \mu \right) G (x, x') = \delta (x - x') + \int d\mathbf{r} \psi (\mathbf{r}, t) \psi^* (\mathbf{r}, t) \psi^* (x') \psi (x'). \]

(11)

\[ -\delta (x - x') + \int d\mathbf{r} \psi (\mathbf{r}, t) \psi^* (\mathbf{r}, t) \psi^* (x') \psi (x'). \]

By using the rules of functional differentiation, we can rewrite the equations for the Green functions \( G (x, x') \) and \( D_{\mathbf{R} \mathbf{R}'}^2 (\tau - \tau') \) in the form of equations in functional derivatives:

\[ M \frac{\partial^2}{\partial \tau^2} D_{\mathbf{R} \mathbf{R}'}^2 (\tau - \tau') + \left( \sum_{\mathbf{R}} V_{\mathbf{R}} u_{\mathbf{R}}^* (\mathbf{R}, t) \right) \int d\mathbf{r} \psi^* (\mathbf{r}, t) \psi^* (\mathbf{r}, t) \psi^* (x') \psi (x'). \]

(12)
Here \( \langle \rho (x, \tau) \rangle \) is the averaged electronic-density operator:
\[
\langle \rho (x, \tau) \rangle = \langle \psi^\dagger (x, \tau) \psi (x, \tau) \rangle ,
\]
\[
\frac{\partial}{\partial \tau} \left( \frac{\hbar^2}{2m} \right) \rho (x, \tau) = - \int d\tau ' \frac{\hbar^2}{2m} \frac{\partial^2 \rho (x, \tau ')}{\partial x^2}.
\]

At the energy gap we can reduce the equations for the ion-displacement phonon interaction. Let us, to begin with, determine the irreducible polarization operator \( \Pi (x,x ') \):
\[
\Pi (x,x ') = \frac{\delta \rho (x,x ')}{\delta \rho (x,x ')} = \int dx dx ' G(x,x') G(x,x2) \Gamma (x,x,x ').
\]

where \( \Gamma (x,x,x ') \) is the irreducible vertex function of the interelectron interaction:
\[
\Gamma (x,x,z) = \frac{\delta G^{-1}(x,z)}{\delta U_{eff}(x,z)}.
\]

We shall return a little later to the consideration of this function. Using the formula (16) we can determine the permittivity function \( \varepsilon (x,x') \) and the total electronic susceptibility \( \chi (x,x') \):
\[
\varepsilon^{-1}(x,x') = \delta(x-x') + \int dx dx ' \frac{\varepsilon^2}{\varepsilon^2 - \varepsilon^2 \varepsilon '}(x,x') \chi (x,x'),
\]
\[
\chi (x,x') = \int dx \Pi (x,x') \varepsilon^{-1}(x,x') \frac{\varepsilon^2}{\varepsilon^2 - \varepsilon^2 \varepsilon '}(x,x') - \delta(x-x').
\]

Using the above-introduced functions, we can write
\[
\frac{\partial}{\partial \tau} \rho (x,x') = \int dx dx ' \frac{\partial}{\partial \tau} U_{eff}(x,x') \frac{\partial}{\partial \tau} \rho (x,x'),
\]
\[
\frac{\partial}{\partial \tau} \rho (x,x') \frac{\partial}{\partial \tau} \rho (x,x') = \int dx dx ' \frac{\partial}{\partial \tau} U_{eff}(x,x') \frac{\partial}{\partial \tau} \rho (x,x'),
\]
\[
\chi (x,x') = \int dx \Pi (x,x') \varepsilon^{-1}(x,x') \frac{\varepsilon^2}{\varepsilon^2 - \varepsilon^2 \varepsilon '}(x,x') - \delta(x-x').
\]

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:
\[
\left[ M \frac{\partial^2}{\partial \tau^2} + \Phi_{\alpha \alpha'}^{(2)} \right] \Phi_{\alpha \alpha'}^{(2)} (t-\tau') \rho (x,x') = - \delta_{\alpha \alpha'} \delta (t-\tau'),
\]

where \( \Phi_{\alpha \alpha'}^{(2)} \) is the dynamical vibration matrix, determined by the sum of the ionic and electronic parts:
\[
\Phi_{\alpha \alpha'}^{(2)} = \frac{\partial}{\partial \tau} V_{\alpha \alpha'}^{(2)} (r-R_{\alpha}, r') \frac{\partial}{\partial \tau} V_{\alpha \alpha'}^{(2)} (r-R_{\alpha}, r').
\]
of the electron Green function (formula (25)), we note that
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ally rewrite the expression for the first term can be reduced to the skeleton diagrams shown in Fig. 3. In the diagram 3a the circles denote the total

\[ \sqrt{m/M} \]. 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 1e. It would seem
to follow from this that we can, in computing the vertex
function \( \Gamma(x_1, x_2, x_3) \), neglect the diagrams with pho-
non 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 pho-
non frequencies, we should in the formula (16) use in
place of the total vertex \( \Gamma(x_1, x_2, x_3) \) the function
\( \Gamma_0(x_1, x_2, x_3) \) 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 consist-
ent procedure that allows us to select the most impor-
tant diagrams for the computation of \( \Gamma_0(x_1, x_2, x_3) \).
In recent years the problem of Coulomb correlations at
electron densities corresponding to real metals has been
the subject of numerous investigations.\(^{16,18-19}\) It was
elucidated in these papers that the properties of an elec-
tron system with respect to the screened Coulomb interac-
tion 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 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 corre-
tions to the vertex function is absolutely inadmissible.
In order to understand why this is so, let us schemati-
cally rewrite the expression for \( \Sigma(x, x') \) in the form of
a sum of two terms:

\[ \Sigma(x, x') = -i \int \Gamma_0, G \Gamma_0 - \int V \Gamma_0, D \nu \Gamma_0 \nu' \Gamma_0^* \Gamma_0. \]  

(27)

Here we have denoted the screened Coulomb interaction
by \( V_{\text{se}} \) and the screened electron-ion interaction by \( V_{\text{ie}} \).
As is well known, without allowance for the vertex cor-
tections, the second term is smaller than the first by a
factor of \( \omega_D/\varepsilon_F \). 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 \( \Delta \)
to the electron mass (\( \Delta m = \partial E/\partial \omega \)). Since each addi-
tional phonon line at the vertex leads to a smallness of
the order of \( \sqrt{m/M} \), we can neglect in the vertex func-
tion in the second term in (27) the phonon corrections
and replace it by \( \Gamma_0(x_1, x_2, x_3) \). 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 contribu-
tion 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

\[ \chi(x, x') = \psi_0 (r, x') \chi(r, r'). \]  

(29)

The characteristic times, \( \tau_p \), of the variation of the
electron susceptibility are due to the interelectron corre-
lations. In metals, \( \tau_p \approx 1/\varepsilon_F \), 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 \( \tau_{ph} \), the relation (29) is valid up to quan-
tities of the order of \( \omega_D/\varepsilon_F \). It should be noted that the
deviation from adiabaticity and the nonadiabatic corre-
tions to the phonon frequencies, as well as the attenua-
tion 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,\(^{21}\) an anal-
ogous 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, we shall be concerned
with the problem of adiabaticity. As has been shown
by Ipatova and Subashiev, the nonadiabatic corrections
are responsible for the deviations from the relation (29)
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 suscepti-

\[ \chi(x, x') = \psi_0 (r, x') \chi(r, r'). \]

FIG. 3

\[ \chi(x, x') = \psi_0 (r, x') \chi(r, r'). \]

FIG. 2

\[ \chi(x, x') = \psi_0 (r, x') \chi(r, r'). \]
effective screened electron-ion pseudopotential which takes the vertex corrections into account, $\tilde{V}_{1e}$:

$$\tilde{V}_e = \int \Gamma e^{-V}$$

(30)

If even we assume the unscreened electron-ion pseudopotential to be local, the effective pseudopotential $V_{1e}$ will, because of the presence of $\Gamma$, be nonlocal. As the Yasuhara and Watabe’s computations show, the nonlocal nature of $\tilde{V}_{1e}$ 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:

$$\left( \frac{V_{1e}}{2m} + \mu \right) - U_{\alpha r}(q) \phi(r) - \int d'r' \Sigma(r, r', E_0) \phi(r') = E \phi(r')$$

(31)

The matrix element of the electron-phonon interaction is determined by the gradient of the effective electron-ion pseudopotential $\tilde{V}_{1e}$ (formula (30)). As the computations of Rasolt and Voisko show, the nonlocal potential to be local, the effective pseudopotential $V_{1e}$ (formula (30)).

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

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

(32)

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

$$\omega_0(q) = (N e^2 q^2 / M)^{1/2}$$

(33)

$$D(q, \omega) = \omega^2 - \omega_0^2(q) [1 - g^2(q) \chi(q, 0)]$$

(34)

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

$$M(q, \omega) = g^2(q) \chi(q, 0)$$

(35)

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

$$g(q) = \int \frac{N}{M e^2 q^2} q' V(q')$$

(36)

In accordance with these equations,

$$D(q, \omega) = \omega^2 - \omega_0^2(q) [1 - g^2(q) \chi(q, 0)]$$

(37)

The phonon frequencies are determined by the condition

$$\omega(q) = \omega_0(q) [1 - g^{-1}(q) \chi(q, 0)]$$

(38)

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

$$g^{-1}(q) \chi(q, 0) < 1$$

(39)

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

$$\chi(q, 0) = 1 - \frac{\Pi_0(q, 0)}{|\Pi(q, 0)|}$$

(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:

$$g^{-1}(q) + \frac{U}{2} - V(q) < \frac{1}{|\Pi(q, 0)|}$$

(41)

This condition is quite similar to the condition obtained in the already mentioned paper by Chan and Heine.

However, because of the incorrect use of the adiabatic approximation in their paper, instead of the coupling constant $g^2$ 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 $g^2 \approx 1 / q^2$, i.e., it behaves just like $V(q)$, whereas the true coupling constant for the interaction with the phonons $g(q) \rightarrow 0$ as $q \rightarrow 0$.

If we do not use the approximate expression for $\chi(q, 0)$, but express it in terms of $\epsilon(q, 0)$:

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

then we can write the stability condition in the form

$$g^{-1}(q) + \frac{U}{2} - V(q) < \frac{1}{|\Pi(q, 0)|}$$

(41)

It can be seen from (42) that, in contrast to the Frohlich model, the lattice-stability condition does not impose any limitation on the effective 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,

$$g^{-1}(q) / V(q) < 1$$

Since $\epsilon(q, 0) > 1$ 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 [11].

The last question that we consider in this paper consists in the following. Does the lattice-stability condition impose any limitations on the effective electron-electron interaction $V_{1e}(q, 0)$ determined by the formula (26)? Let us rewrite this interaction in the form

$$V_{1e}(q, \omega) = \frac{4 \pi e^2}{\omega^2 - \omega_0^2(q) [1 - g^{-1}(q) \chi(q, 0)]} \left( \frac{\Pi_0(q, 0)}{|\Pi(q, 0)|} \right)^{-1}$$

(43)

where

$$\epsilon_{1e}(q, \omega) = \epsilon(q, \omega) - g^{-1}(q) V(q) \omega^2 - \omega_0^2(q) [1 - g^{-1}(q) \chi(q, 0)]$$

(34)

In Nozières and Pines’s book, for an isotropic medium a stability condition for the system that amounts to the following:

$$\epsilon_{1e}(q, 0) > 0$$

(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 and Kirzhnitz, Maksimov, and Khomskii;

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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 $\epsilon_{\text{eff}}(q, 0)$:

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

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 $\epsilon_{\text{eff}}(q, 0) > 0$. 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 $\epsilon_{\text{eff}}(q, 0) < 0$. 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\textsuperscript{[22]} arouses, as D. A. Kirzhnits has informed this author, a strong objection from the dynamical point of view.

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\textsuperscript{[1]}  H. Frölich, Phys. Rev. 79, 845 (1950).
\textsuperscript{[3]}  S. V. Tyablikov and V. V. Tolmachev, Zh. Eksp. Teor. Fiz. 34, 1254 (1958) [Sov. Phys.-JETP 6, 867 (1958)].
\textsuperscript{[9]}  M. Born and R. Oppenheimer, Ann. der Phys. 84, 457 (1928).
\textsuperscript{[20]}  M. Rice, Ann. Phys. 31, 100 (1965).

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