

The Description of Superconductivity in Terms of Dielectric Response Function

D. A. Kirzhnits, E. G. Maksimov, and D. I. Khomskii

P. N. Lebedev Physical Institute, Moscow, USSR

(Received May 30, 1972)

A critical temperature T_c of a superconducting transition is calculated for a rather general form of the electron–electron interaction. It is shown that even if both the energy and momentum dependence of the interaction is included, the equation determining T_c coincides formally with the corresponding equation of the BCS theory. The kernel of this equation is a smooth real function of its variables; it is expressed through $\rho(\mathbf{k}, E)$, the spectral density of the inverse dielectric function of the system. The expression for T_c is written in terms of $\rho(\mathbf{k}, E)$; this enables us to analyze the dependence of the critical temperature on the properties of the metal in a normal state. Some simple models illustrating the results are considered, and a discussion of the limits on T_c is given.

1. INTRODUCTION

Since 1957 the theory of superconductivity has made great progress in the description of this phenomenon. A simple approach starting from the work by Bardeen, Cooper, and Schrieffer¹ (BCS) proved rather effective. In this approach the pairing interaction is taken to be instantaneously (frequency independent) attractive in a narrow region near the Fermi surface. The success of so simple a model may seem at first rather surprising; in fact, the actual electron–electron interaction in a metal has a strong and non-monotonous energy dependence (resonances in the region of the absorption lines), and it has a nonzero imaginary part, the Coulomb “tail” stretches far from the Fermi level. Also, the interaction depends in general on two variables—the frequency and the momentum.*

Moreover, from the condition of the stability of the system one may conclude that the interaction on the Fermi surface cannot be attractive.²

*In contrast to the BCS model, the actual interaction is local in coordinate space (due to the screening of the Coulomb interaction at distances of interatomic order); due to a large difference between the phonon and electron frequencies, the interaction is greatly retarded.

The further steps in the development of the theory of superconductivity were aimed mainly at a correct account of these factors.

This trend was initiated by Bogoliubov's paper³ and proved rather successful⁴⁻⁷ for the description of a superconducting state including the strong coupling superconductors. The corresponding equations, however, turned out to be rather different in form from the BCS ones; as a result the simplicity of the latter was lost. In particular, the kernel of the corresponding integral equation was complex and depended on two variables—the frequency and the momentum. The derivation of these equations required rather complicated investigations of the analytic properties of the corresponding quantities. Finally, certain difficulties arose in the attempts to correctly describe the Coulomb interaction.^{8,9}

The main purpose of the present paper is to make the equations of the theory of superconductivity for a general form of the interaction as close to the usual BCS equations as possible. We shall consider a wide class of interactions with space and time dispersion, damping, etc. Our second purpose is to try to get a consistent description of the Coulomb interaction without its replacement by a constant, as is usually done. And, finally, we tried to express the superconducting characteristics (particularly the critical temperature) through the quantities which can be obtained from an experimental study of a normal metal.

Our approach is based on the description of the electron–electron interaction in terms of the effective dielectric response function $\varepsilon_{\text{eff}}(\mathbf{q}, \omega)$. The effective interaction depends in general on two variables—the total and the transferred four momenta. In many cases, however (for example, for a purely phonon interaction, in a highly compressed substance, etc.), the most important is the dependence of the interaction on the momentum transfer \mathbf{q}, ω . Restricting our consideration to this case we may write the effective interaction in the form

$$V(\mathbf{q}, \omega) = 4\pi e^2 / q^2 \varepsilon_{\text{eff}}(\mathbf{q}, \omega) \quad (1)$$

The function $1/\varepsilon_{\text{eff}}(\mathbf{q}, \omega)$ is the “charge-to-charge” linear response function, and it is just this quantity that enters the electron scattering in a metal.*

As a response function $1/\varepsilon$ satisfies the causality principle; therefore, we can write for it the spectral representation of the Kramers–Kronig type:

$$1/\varepsilon(\mathbf{q}, \omega) = 1 - \int_0^\infty [dE^2 \rho(\mathbf{q}, E) / (E^2 - \omega^2 - i\delta)] \quad (2)$$

The positive spectral density

$$\rho(\mathbf{q}, E) = -(1/\pi) \text{Im} [1/\varepsilon(\mathbf{q}, E)]$$

*We shall deal further only with the dielectric constant defined by (1) and, therefore, the subscript eff will be omitted.

is directly connected with the form factor $S(q, E)$ for the electron scattering in the metal

$$S(\mathbf{q}, E) = (q^2/4\pi e^2)\rho(\mathbf{q}, E)$$

The stability condition implies² that $1/\varepsilon(\mathbf{q}, 0) \geq 0$; hence, according to (1), $V(\mathbf{q}, 0) \geq 0$.

Our formalism is based on the use of the spectral representation (2) and corresponding representations for other quantities. We have thus managed to simplify the calculations considerably; they are reduced to simple and, to a great extent, automatic operations. In such a way we obtain finally the equation directly for the spectral densities. It is this equation that is very similar in form to the usual BCS equation.

It is essential that the kernel of this equation is determined not by the initial interaction (1) or (15) but by some new "pairing" interaction (14) which has already all the properties of the BCS model interaction. The "pairing" interaction is expressed directly through the spectral density ρ of the inverse dielectric function (2). All the quantities entering the final expression for T_c can be expressed through the ρ [see (38) and (39)]. The dependence of a critical temperature on different characteristics of the initial system (energy of the eigenmodes, their damping, the coupling strength, etc.) can be investigated in the general form within the framework of this approach.

Besides the above-mentioned neglect of the dependence of the interaction on the total four momenta there are two other restrictions imposed. First of all we consider only the "homogeneous system"; the influence of the lattice periodicity is taken into account only to the extent that it may be included into $\varepsilon(\mathbf{q}, \omega)$ of the form (2). The second restriction is the use of the weak-coupling approximation. Some relations for a general case are given in the first version of the present paper.¹⁰ The details of some of the calculations can also be found there.

2. DERIVATION OF MAIN RELATIONS

Restricting ourselves to the calculation of a critical temperature, we shall use the technique of the temperature Green functions at $T = T_c$. Introducing in the usual way the electron Green function G and the condensate function F , we shall take the G function in the following form*:

$$G(\mathbf{k}, i\omega_n) = 1/(i\omega_n - \xi_k) \quad (3)$$

*The results obtained below are also valid for a more general form of the G function, namely, for the quasiparticle approximation $G(\mathbf{k}, i\omega_n) = z_k/(i\omega_n - \xi_k)$. It should be noted that the possibility of using the quasiparticle approximation for the electrons in a wide energy range can be justified only for a weak interaction. When the interaction is strong, the G function has a quasiparticle character only in the immediate vicinity of ε_F , and the analysis of the effect of the quasiparticle damping on T_c requires an additional investigation.

where $\xi_k = (\mathbf{k}^2/2m) - \varepsilon_F$, and ε_F is the Fermi energy. At $T = T_c$ the condensate function F satisfies the well-known equation

$$F(\mathbf{p}, i\omega_n) = -G(\mathbf{p}, i\omega_n)G(-\mathbf{p}, -i\omega_n)T_c \sum_{\mathbf{m}} \int [d^3k/(2\pi)^3] \\ \times V(\mathbf{p} - \mathbf{k}, i\omega_n - i\omega_m)F(\mathbf{k}, i\omega_m) \quad (4)$$

from which T_c can be determined.

Then, in contrast to the usual method⁴ we use the spectral representation for V and F in order to make an explicit summation in frequencies in (4). The temperature analog of relation (2) may be written for the V function as

$$V(\mathbf{q}, i\omega_n) = \frac{4\pi e^2}{q^2} \left[1 - \int_0^\infty \frac{dE^2 \rho(\mathbf{q}, E)}{\omega_n^2 + E^2} \right] \quad (5)$$

The spectral representation of the F function is given by

$$F(\mathbf{p}, i\omega_n) = \int_{-\infty}^{+\infty} [f(\mathbf{p}, x) dx] / (i\omega_n - x) \quad (6)$$

The spectral density $f(\mathbf{p}, x)$ may be shown to have the following property:

$$f(\mathbf{p}, x) = -f(\mathbf{p}, -x)$$

Substitution of (5-6) into (4) and summation in frequencies with the aid of the formula

$$T_c \sum_n f(\omega_n) = \frac{1}{2} \sum_i \tan \frac{\omega_i}{2T_c} \text{Res}_i f \quad \omega_n = (2n + 1)\pi T_c$$

where ω_i are the poles of the function $f(\omega)$, leads to the following equation for $f(\mathbf{p}, x)$:

$$f(\mathbf{p}, x) = - \int [d^3k/(2\pi)^3] \int_0^\infty dy \tanh(y/2T_c) K(\mathbf{p}, \mathbf{k}, x, y) f(\mathbf{k}, y) \quad (7)$$

where

$$K(\mathbf{p}, \mathbf{k}, x, y) = \frac{4\pi e^2}{(\mathbf{p} - \mathbf{k})^2} \left\{ \frac{\delta(x - |\xi_p|)}{2|\xi_p|} \left[1 - \int_0^\infty dE \rho(\mathbf{p} - \mathbf{k}, E) \right. \right. \\ \times \left. \left. \left(\frac{1}{E + x + y} + \frac{1}{E + y - x} \right) \right] \right. \\ \left. + P \frac{1}{x^2 - \xi_p^2} \rho(\mathbf{p} - \mathbf{k}, x - y) \theta(x - y) \right\} \quad (8)$$

Using the explicit expression of the F function in terms of the anomalous self-energy part⁴ $\Delta(\mathbf{k}, \omega)$, one can write down the expression for $f(\mathbf{p}, x)$ in the following form.*

$$f(\mathbf{p}, x) = \frac{\text{Re } \Delta(\mathbf{p}, x)}{2|\xi_p|} \delta(x - |\xi_p|) + \frac{1}{\pi} \text{Im } \Delta(\mathbf{p}, x) P \frac{1}{x^2 - \xi_p^2} \quad (9)$$

Equation (7) is an integral equation over two variables. If the interaction is localized near the Fermi surface, then, as is well known, $\int d^3k/(2\pi)^3 \times [\rho(\mathbf{p} - \mathbf{k}, E)/(\mathbf{p} - \mathbf{k})^2]$ does not depend on \mathbf{p} , and, consequently, $\Delta(\mathbf{p}, \omega)$ is independent of \mathbf{p} . Integrating (7) over \mathbf{p} and using (8) and (9) we get in this case a usual "one-dimensional" Eliashberg equation for $\text{Re } \Delta(\omega)$.

When the Coulomb interaction is taken into account we cannot neglect the spatial dependence of all the quantities. Nevertheless, in the case of weak coupling Eq. (7) can be similarly reduced to a "one-dimensional" form.

To do this we introduce the function

$$\Phi(\mathbf{p}) = 2|\xi_p| \int_0^\infty f(\mathbf{p}, x) dx \quad (10)$$

Integrating both sides of (7) over x we have

$$\begin{aligned} \Phi(\mathbf{p}) = & - \int \frac{d^3k}{(2\pi)^3} \frac{4\pi e^2}{(\mathbf{p} - \mathbf{k})^2} \int_0^\infty dy \tanh \frac{y}{2T_c} f(\mathbf{k}, y) \\ & \times \left[1 - 2 \int_0^\infty \frac{dE \rho(\mathbf{p} - \mathbf{k}, E)}{E + y + |\xi_p|} \right] \end{aligned} \quad (11)$$

On the right-hand side of (11) we shall take the term singular at $T_c \rightarrow 0$ by adding and subtracting in the integral the quantity

$$\tanh \frac{|\xi_k|}{2T_c} \left[1 - 2 \int_0^\infty \frac{dE \rho(\mathbf{p} - \mathbf{k}, E)}{E + |\xi_k| + |\xi_p|} \right]$$

Taking into account (10) we obtain

$$\Phi(\mathbf{p}) = - \int \frac{d^3k}{(2\pi)^3} \frac{4\pi e^2}{(\mathbf{p} - \mathbf{k})^2} \frac{\tanh(\xi_k/2T_c)}{2\xi_k} \left[1 - 2 \int_0^\infty \frac{dE \rho(\mathbf{p} - \mathbf{k}, E)}{E + |\xi_k| + |\xi_p|} \right] \Phi(\mathbf{k}) \quad (12)$$

where on the right-hand side we have omitted the term regular in T_c :

$$\begin{aligned} & - \int \frac{d^3k}{(2\pi)^3} \frac{4\pi e^2}{(\mathbf{p} - \mathbf{k})^2} \int_0^\infty dy f(\mathbf{k}, y) \left\{ \tanh \frac{y}{2T_c} \left[1 - 2 \int_0^\infty \frac{dE \rho(\mathbf{p} - \mathbf{k}, E)}{E + y + |\xi_p|} \right] \right. \\ & \quad \left. - (y \rightarrow |\xi_k|) \right\} \end{aligned}$$

*It is easy to see that Eq. (7) with the kernel $\mathbf{K}(\mathbf{p}, \mathbf{k}, x, y)$ corresponds to a general form (9) of the spectral density.

It can be shown that this term leads only to a numerical factor of the order of unity in the preexponential factor in the expression for T_c .¹⁰

It is essential that as seen from (9) and (10) the function Φ , defined by Eq. (12), practically coincides with the real part of the energy gap $\text{Re } \Delta(\omega = \xi_p)$. The difference between these quantities is always small near the Fermi surface, and therefore in Eq. (12) it makes a contribution nonsingular with respect to T_c .

In subsequent calculations it is convenient using the isotropy of the problem to change the argument from the momentum to $\xi(p)$. We introduce the level density $N(\xi) = d^3p/d\xi$ and the designations

$$\mu(\xi, \xi') = N(\xi) \overline{\frac{4\pi e^2}{(\mathbf{p} - \mathbf{k})^2}} \quad v(\xi, \xi', E) = N(\xi) \overline{\frac{4\pi e^2 \rho(\mathbf{p} - \mathbf{k}, E)}{(\mathbf{p} - \mathbf{k})^2}}$$

where the line means the averaging over the angle between the vectors \mathbf{p} and \mathbf{k} . Changing from the variable $\cos \theta$ to $\mathbf{q}^2 = (\mathbf{p} - \mathbf{k})^2 = \mathbf{p}^2 - 2p_k \cos \theta + \mathbf{k}^2$ we have

$$\mu(\xi, \xi') = \frac{4\pi e^2 N(\xi)}{p(\xi)p(\xi')} \ln \frac{p(\xi) + p(\xi')}{|p(\xi) - p(\xi')|}$$

$$v(\xi, \xi') = \frac{4\pi e^2 N(\xi)}{p(\xi)p(\xi')} \int_{|p(\xi) - p(\xi')|}^{p(\xi) + p(\xi')} \frac{dq}{q} \rho(q, E)$$

Here $p(\xi) = \sqrt{2m(\xi + \varepsilon_F)}$. Equation (12) can be finally rewritten in the following form

$$\Phi(\xi) = - \int_{-\infty}^{+\infty} d\xi' [\tanh(\xi'/2T_c)/2\xi'] K(\xi, \xi') \Phi(\xi') \quad (13)$$

$$K(\xi, \xi') = \mu(\xi, \xi') - 2 \int_0^{\infty} [dE v(\xi, \xi', E)/(E + |\xi| + |\xi'|)] \quad (14)$$

Equation (12) or (13) is the basic integral equation determining T_c . It is obtained in the weak-coupling approximation with arbitrary suppositions of the space and time dependence of the interaction.

Equation (13) for the function $\Phi(\xi) = \text{Re } \Delta(\omega = |\xi|)$ coincides in its form with the BCS equation. In this equation the frequency and the momentum are not independent variables but are connected by the relation $\omega = |\xi_p|$. This answers the question in the language of which variable (energy or momentum) the superconductivity equation should be formulated.

The kernel $K(\xi, \xi')$ of Eq. (13) is expressed directly through the spectral density of the initial interaction $\rho = -(1/\pi) \text{Im } (1/\varepsilon)$. It is essential that K differs from the initial interaction (1). To make this difference more evident

we shall write the latter in new terms:

$$V(\xi, \xi', \omega - \omega') = \mu(\xi, \xi') - \int_0^\infty \{dE^2 v(\xi, \xi', E)/[E^2 - (\omega - \omega')^2 - i\delta]\} \quad (15)$$

The main difference of K from V is that in K only the “positive-frequency” part of the initial interaction remains. Due to this fact the kernel K becomes a smooth, real function of its arguments. Under the change from V to K the resonances vanish, and we get the smooth “steps” instead. There is another interesting feature in K : in contrast to V the kernel K depends not on the difference $\omega - \omega'$ but falls off separately in each variable. These features are typical of the usual BCS approximation. The argument presented above may be, therefore, considered to be the basis for the usual scheme for a wide class of interactions.

It is also clear from what has been said that some attempts to “improve” the BCS scheme are incorrect. For example, in the paper by Hurault¹¹ the resonances in the initial interaction are replaced by narrow peaks localized far from the Fermi surface.

The physical origin of the difference of K from V (isolation of the positive-frequency part) may be explained as follows. While the initial interaction corresponds to an exchange of a phonon, the “pairing” interaction corresponds to a simultaneous creation from a vacuum of two electrons and a phonon (or the corresponding annihilation). This is particularly clear in a method of compensation³ of a dangerous diagram.

The analogy of Eq. (13) with the usual BCS equation can be made complete, if we reduce it to the form where the kernel is localized near the Fermi surface. As is known³ this corresponds to the effective suppression of the long-range (Coulomb) part of the interaction and to an introduction of the Coulomb pseudopotential.^{3,5,10} It is of importance that the resulting interaction can already have a character of the attraction on the Fermi surface $\xi = \xi' = 0$ in spite of the condition $V(q, 0) \geq 0$ (see above). We shall not make this transformation now and shall return to this problem later.

3. CALCULATION OF A CRITICAL TEMPERATURE

Let us consider Eq. (13) which determines T_c . As in the usual BCS model T_c contains a small exponential factor and preexponent.

In the latter we will ignore the factors of the order of unity.

Equation (13) contains a logarithmic singularity in T_c at $T_c \rightarrow 0$. It is sufficient that the logarithmic and the T_c -independent terms be kept in this equation. Substituting in (13) the identity

$$K(\xi, \xi')\Phi(\xi') = K(\xi, 0)\Phi(0) + [K(\xi, \xi')\Phi(\xi') - K(\xi, 0)\Phi(0)]$$

and introducing the new function $\chi(\xi) = \Phi(\xi)/\Phi(0) \ln(T_c/\theta)$, where θ is as yet an arbitrary frequency (of the order of mean phonon frequencies), we have

$$T_c \cong \theta \exp(1/\chi(0)) \quad (16)$$

$$\chi(\xi) = K(\xi, 0) + \hat{A}_{\xi'}[K(\xi, \xi')\chi(\xi')] \quad (17)$$

Here the following designation is introduced:

$$\hat{A}_x f(x) = \frac{1}{2} \int_{-\infty}^{+\infty} dx \ln(|x|/\theta) (d/d|x|) f(x)$$

Let us divide the kernel $K(\xi, \xi')$ into the part K_{ph} localized near the Fermi surface and the long-range part K_c :

$$K(\xi, \xi') = K_{\text{ph}}(\xi, \xi') + K_c(\xi, \xi') \quad (18)$$

The possibility of such a representation of $K(\xi, \xi')$ and the physical meaning of K_{ph} and K_c are discussed in the next section.

Correspondingly, $\chi = \chi_{\text{ph}} + \chi_c$, where χ_c is introduced by the condition

$$\chi_c(\xi) = K_c(\xi, 0) + \hat{A}_{\xi'}[K_c(\xi, \xi')\chi_c(\xi')] \quad (19)$$

Designating

$$\hat{A}_{\xi'}[K_c(0, \xi')\chi_c(\xi')] \equiv -K_c(0, 0) \ln(\bar{\xi}/\theta)\chi_c(0)$$

where

$$\ln \bar{\xi} = -[1/2K_c(0, 0)\chi_c(0)] \int_{-\infty}^{+\infty} d\xi \ln |\xi| (d/d|\xi|) [K_c(0, \xi)\chi_c(\xi)] \quad (20)$$

we have

$$\chi_c(0) = K_c(0, 0)/[1 + K_c(0, 0) \ln(\bar{\xi}/\theta)] \quad (21)$$

As is shown below $\bar{\xi} \approx \varepsilon_F$ and $\ln(\bar{\xi}/\theta)$ is large and, therefore, $\chi_c(0)$ is small. It follows from the previous expressions that

$$\begin{aligned} \chi_{\text{ph}}(\xi) &= K_{\text{ph}}(\xi, 0) + K_c(\xi, 0)\hat{A}_{\xi'}\chi_{\text{ph}}(\xi') + \hat{A}_{\xi'}K_{\text{ph}}(\xi, \xi')\chi_c(0) \\ &+ \hat{A}_{\xi'}[K_{\text{ph}}(\xi, \xi')\chi_{\text{ph}}(\xi')] \end{aligned}$$

Applying the operation $\hat{A}_{\xi'}$ to this relation and introducing

$$\hat{A}_{\xi}K_c(\xi, 0) \equiv -K_c(0, 0) \ln(\bar{\xi}/\theta)$$

where $\bar{\xi} \approx \xi$, we have

$$\hat{A}_{\xi}\chi_{\text{ph}}(\xi) = \frac{\hat{A}_{\xi}K_{\text{ph}}(\xi, 0)}{1 + K_c(0, 0) \ln(\bar{\xi}/\theta)}$$

Hence,

$$\chi_{\text{ph}}(0) = K_{\text{ph}}(0, 0) + \frac{K_c(0, 0)\hat{A}_\xi[K_{\text{ph}}(\xi, 0) + K_{\text{ph}}(0, \xi)]}{1 + K_c(0, 0) \ln(\xi/\theta)} + \hat{A}_\xi[K_{\text{ph}}(0, \xi)K_{\text{ph}}(\xi, 0)]$$

The condition

$$\hat{A}_\xi K_{\text{ph}}(0, \xi) = 0$$

will determine the value of θ :

$$\ln \theta = -[1/2K_{\text{ph}}(0, 0)] \int_{-\infty}^{+\infty} d\xi \ln |\xi|(d/d|\xi|) K_{\text{ph}}(0, \xi) \quad (22)$$

Then, finally, we have

$$T_c \equiv \theta e^{-1/g} \quad g = - \left[K_{\text{ph}}(0, 0) + \frac{K_c(0, 0)}{1 + K_c(0, 0) \ln(\xi/\theta)} \right] \quad (23)$$

From the right-hand side we discard the factor

$$\exp \{ -\hat{A}_\xi [K_{\text{ph}}(0, \xi)K_{\text{ph}}(\xi, 0)]/g^2 \}$$

which is of the order of unity, as is easily seen by substituting the formulas for $K_c(\xi, \xi')$ and $K_{\text{ph}}(\xi, \xi')$ obtained in the next section.

4. THE CHOICE OF THE EFFECTIVE INTERACTION

Up to now we have made no special assumptions concerning the form of the effective interaction (1), but considered it in a general form. Now we somewhat specialize the form of this function. We are considering the systems where besides purely Coulomb interaction between the conduction electrons there is an additional interaction caused by the phonons, excitons, and so on.*

We shall limit ourselves to the longitudinal excitations. Their frequencies $\omega_v(\mathbf{q})$ and dampings $\Gamma_v(\mathbf{q})$ are given by the equation $\varepsilon(\mathbf{q}, \omega_v + i\Gamma_v) = 0$. Suppose that the phonon frequencies are small compared to the electron plasma frequency $\omega_e = (4p_F^3 e^2/3\pi m)^{1/2}$ and the Fermi energy ε_F : $\theta \ll (\omega_e, \varepsilon_F)$.

Here θ is the effective phonon frequency introduced in the previous section.

Let us discuss now the form of the spectral density and the effective interaction, taking the dielectric function in the form

$$\varepsilon(\mathbf{q}, \omega) = \varepsilon_c(\mathbf{q}, \omega) + \varepsilon_{\text{ph}}(\mathbf{q}, \omega) - 1 \quad (24)$$

$$\varepsilon_c = 1 + 4\pi\alpha_c \quad \varepsilon_{\text{ph}} = 1 + 4\pi\alpha_{\text{ph}}$$

*We shall speak for brevity only of the phonons.

Here α_c is the part of polarizability entirely connected with the conduction electrons, and α_{ph} is the remaining polarizability describing both a purely phonon effect and the effect of the interference of phonon excitations with the conduction electrons. Using relation (1) one may rewrite similarly the effective interaction:

$$V(\mathbf{q}, \omega) = V_c(\mathbf{q}, \omega) + V_{\text{ph}}(\mathbf{q}, \omega)$$

$$V_c(\mathbf{q}, \omega) = 4\pi e^2/q^2 \varepsilon_c(\mathbf{q}, \omega) \quad V_{\text{ph}} = (4\pi e^2/q^2)[1/\varepsilon(\mathbf{q}, \omega)] - [1/\varepsilon_c(\mathbf{q}, \omega)] \quad (25)$$

The kernel $K(\xi, \xi')$ of the integral equation (13) may be rewritten in the same way. It is evident from (25) that V_{ph} and therefore K_{ph} falls off at characteristic phonon frequencies.

The quantities V_c and V_{ph} may be represented separately in the spectral form. For the Coulomb interaction we have

$$V_c(\mathbf{q}, \omega) = (4\pi e^2/q^2) \left[1 - \int_0^\infty \frac{dE^2 \rho_c(\mathbf{q}, E)}{E^2 - \omega^2 - i\delta} \right] \quad (26)$$

where

$$\rho_c(\mathbf{q}, \omega) = -(1/\pi) \text{Im} [1/\varepsilon_c(\mathbf{q}, \omega)]$$

Similarly

$$V_{\text{ph}}(\mathbf{q}, \omega) = -(4\pi e^2/q^2) \int_0^\infty [dE^2 \rho_{\text{ph}}(\mathbf{q}, E)/(E^2 - \omega^2 - i\delta)] \quad (27)$$

where

$$\rho_{\text{ph}}(\mathbf{q}, E) = \rho - \rho_c = -(1/\pi) \text{Im} [1/\varepsilon(\mathbf{q}, E)] - [1/\varepsilon_c(\mathbf{q}, E)]$$

To calculate the Coulomb part of the effective interaction V_c or, more precisely, $K_c(\xi, \xi')$, one can use the following simple interpolation formula for $\rho_c(\mathbf{q}, E)$:

$$\rho_c(\mathbf{q}, E) = \omega_e^2 \delta[E^2 - \omega_{\text{pi}}^2(\mathbf{q})] \quad (28)$$

where

$$\omega_{\text{pi}}^2(\mathbf{q}) = \omega_e^2 \{1 + [q^2/\kappa^2(q)]\}$$

$$\kappa^2(q) = (\kappa^2/2) \{1 + [(p_F/q) - (q^2/4p_F^2)]\} \ln |(2p_F + q)/(2p_F - q)|$$

$\kappa(0) = \kappa = \sqrt{3}\omega_e/V_F$ is the Debye momentum, and $V_F = p_F/m$ is the velocity on the Fermi surface. Expression (28) for the spectral density of the Coulomb interaction represents correctly the complete screening of the interaction at $E \ll qV_F$ and a plasma character of the Coulomb system in the other limiting case $E \gg qV_F$. At arbitrary E and q , (28) does not describe some details

of the properties of the Coulomb system. However, the calculations of Ref. 12 show that the use of (28) for $\rho_c(\mathbf{q}, E)$ gives quite satisfactory results for many physical characteristics of the electron system.

For $|\xi|, |\xi'| \ll \varepsilon_F$ with the aid of (12), (13), and (37) we obtain

$$K_c(\xi, \xi') = \frac{\alpha}{\omega_e + |\xi| + |\xi'|} \left[\frac{\omega_e}{2} \ln \frac{1}{\alpha} + (|\xi| + |\xi'|) \ln \frac{4\varepsilon_F}{|\xi - \xi'|} \right] \quad (29)$$

with a logarithmic accuracy. Here $\alpha = e^2/\pi V_F$ is a Coulomb coupling constant.

The logarithmic singularity which appears in (29) is insignificant: it is due to an incomplete screening of the Coulomb interaction at $\omega = |\xi| + |\xi'| \neq 0$, and the nearer we are to the Fermi surface the smaller is the singularity. In particular, at the very Fermi surface K_c is finite:

$$K_c(0, 0) = (\alpha/2) \ln(1/\alpha) \equiv \mu \quad (30)$$

Note that the result (30) is of a general character and does not depend on a concrete approximation of ρ_c in the form (28). When $|\xi| > \varepsilon_F$ or $|\xi'| > \varepsilon_F$ we have

$$K_c(\xi, \xi') = (\alpha/r') \ln[(r + r')/|r - r'|] \quad (31)$$

where

$$r = \sqrt{1 + (\xi/\varepsilon_F)} \quad r' = \sqrt{1 + (\xi'/\varepsilon_F)}$$

It is seen from the expressions obtained that even at $\omega_e \ll \varepsilon_F$ the Coulomb part of $K_c(\xi, \xi')$ falls off at great distances $\sim \varepsilon_F$ from the Fermi surface. This fact is also due to the absence of screening of the Coulomb interaction at high frequencies.

Using (29) and (31) we can calculate now the effective frequency $\bar{\xi}$ given by (20):

$$\bar{\xi} \simeq \varepsilon_F \alpha^{1/3}$$

By (21) the total Coulomb contribution to the coupling constant g has the form

$$\chi_c(0) \equiv \mu^* = \mu/[1 + \mu \ln(\varepsilon_F \alpha^{1/3}/\theta)] \quad (32)$$

This is just the above-mentioned Coulomb pseudopotential.

Let us discuss now the phonon part of the interaction localized near the Fermi surface. We shall rewrite it in the form

$$K_{\text{ph}}(\xi, \xi') = -2 \int_0^\infty [dE v_{\text{ph}}(\xi, \xi', E)/(E + |\xi| + |\xi'|)] \quad (33)$$

where

$$v_{\text{ph}}(\xi, \xi', E) = \alpha \int_{|\xi - \xi'|/V_F}^{2p_F} (dq/q) \rho_{\text{ph}}(q, E) \quad (34)$$

Note that from (27) we get the following relation for the coupling constant with the phonons λ :

$$K_{\text{ph}}(0, 0) \equiv -\lambda = \alpha \int_0^{2p_F} (dq/q) \{ [1/\varepsilon(q, 0)] - [1/\varepsilon_c(q, 0)] \} \quad (35)$$

The quantity ρ_{ph} is nonzero only if $E < \xi_0$, where $\xi_0 \ll \omega_e$ is the characteristic phonon frequency. In this region, however, as is seen from (28), $\rho_c(q, E) = 0$. One can, therefore, set

$$\rho_{\text{ph}}(q, E) = \begin{cases} -1/\pi \operatorname{Im} [1/\varepsilon(q, E)] & E < \xi_0 \\ 0 & E > \xi_0 \end{cases}$$

$$\theta < \xi_0 \ll \omega_e, \varepsilon_F$$

Thus ρ_{ph} can be expressed in terms of the total spectral density ρ . Consider the two regions of integration in (34) and (35): $qV_F \lesssim \xi_0$ and $qV_F \gg \xi_0$. The contribution of the first is negligibly small due to a complete screening of the interaction at $q \rightarrow 0$, while in the second region ρ_{ph} can be written in the form

$$\rho_{\text{ph}}(q, E) = -(1/\pi) \operatorname{Im} \{ 1/[\varepsilon_{\text{ph}}(q, E) + (\kappa^2/q^2)] \} \quad \varepsilon(q, 0) = \varepsilon_{\text{ph}}(q, 0) + (\kappa^2/q^2)$$

Hence it is seen that the main contribution to the integral over q is given by the region $\kappa < q < 2p_F$. When estimating with a logarithmic accuracy, one can take the quantities $\rho(q, E)$ and $1/\varepsilon(q, 0)$ at $q \simeq 2p_F$.

Hence we have

$$v_{\text{ph}}(\xi, \xi', E) = \mu \rho(2p_F, E)$$

$$K_{\text{ph}}(\xi, \xi') = -2\mu \int_0^{\xi_0} [dE \rho(2p_F, E)/(E + |\xi| + |\xi'|)] \quad (36)$$

The quantity $K_{\text{ph}}(0, 0)$ determining, according to (23), the phonon contribution to T_c is given by the simple formula [see (35)]

$$\lambda = -K_{\text{ph}}(0, 0) = \mu \{ 1 - [1/\varepsilon(2p_F, 0)] \} \quad (37)$$

It is seen from (37) that the condition $1/\varepsilon(q, 0) \geq 0$ requires that the quantity λ be always smaller than μ (the phonon attraction is smaller than the Coulomb

repulsion) and reach the maximum value equal to μ at $\varepsilon(2p_F, 0) \rightarrow \infty$. It is, therefore, clear that the very existence of superconductivity in the case considered is connected with the suppression of the Coulomb repulsion in the Coulomb pseudopotential (32).

Using expressions (22) and (36) we see that the mean phonon frequency which determines the preexponent in T_c (23) is given by the expression

$$\ln \theta = \int_0^{\xi_0} (dE/E)\rho(2p_F, E) \ln E / \int_0^{\xi_0} (dE/E)\rho(2p_F, E) \quad (38)$$

It is thus seen that the preexponent in T_c is determined by the logarithmic average of the phonon frequencies over the phonon spectrum. In particular, this mean frequency does not necessarily coincide with the Debye frequency since the contribution of different phonons in θ depends on their coupling with the electrons.

Note that it is just this quantity (38) that determines the thermodynamical properties of a "hot" lattice. In particular, we have the relation $d\theta/dP = \alpha(P)/c(P)$, where α is the thermal expansion coefficient, c is the heat capacity, and P is the pressure.

The final expression for T_c , taking into account (23), (32), and (37), takes the form

$$T_c = \theta \exp \left\{ - \frac{1}{\mu \left[1 - \frac{1}{\varepsilon(2p_F, 0)} \right] - \frac{\mu}{1 + \mu \ln(\varepsilon_F \alpha^{1/3}/\theta)}} \right\} \quad (39)$$

and θ is given by (38).

5. DISCUSSION

As an example of the use of the results obtained we shall consider a practically important case, when the phonon frequency spectrum consists of a number of discrete branches.

Neglecting the phonon damping we may write*

$$\varepsilon_{\text{ph}}(2p_F, \omega) = 1 + \sum_{\nu} [f_{\nu}/(\omega_{0\nu}^2 - \omega^2 - i\delta)]$$

where f_{ν} are the coefficients that can be connected with the oscillator strengths, and $\omega_{0\nu}$ are "bare" phonon frequencies. At $q = 2p_F$ the polarizability $\alpha_c \simeq \kappa^2/4p_F^2 \ll 1$ and $\varepsilon_{\text{ph}} \simeq \varepsilon$. Hence the equation $\varepsilon_{\text{ph}}(2p_F, \omega) = 0$ determines the eigenvalues of the system. If the phonon damping is small, the spectral

*It can be shown that the damping does not change significantly the results obtained below.

density ρ can be written in the following form:

$$\rho = \delta \left\{ 1 - \sum_{\nu} [f_{\nu} / (\omega_{0\nu}^2 - \omega^2)] \right\}$$

Introducing dimensionless constants of the phonon coupling

$$a_{\nu} = [\omega^2 (\partial \varepsilon_{\text{ph}} / \partial \omega^2)]_{\omega = \omega_{\nu}}$$

we obtain from (36) and (37)

$$\lambda = \mu \sum_{\nu} a_{\nu} = \mu \left\{ \sum_{\nu} (f_{\nu} / \omega_{0\nu}^2) / [1 + \sum_{\nu} (f_{\nu} / \omega_{0\nu}^2)] \right\} \quad (40)$$

It follows from (38) that the mean logarithmic frequency is

$$\ln \theta = \sum_{\nu} \alpha_{\nu} \ln \omega_{\nu} / \sum_{\nu} a_{\nu}$$

Using these expressions we get from (39)

$$T_c = \prod_{\nu} \omega_{\nu}^{a_{\nu} / \sum_{\nu} a_{\nu}} \exp \left\{ - \frac{1}{\lambda - \frac{\mu}{1 + \mu \ln (\varepsilon_F \alpha^{1/3} / \theta)}} \right\} \quad (41)$$

It is seen from (41) that, generally speaking, the existence of high frequencies ω_{ν} in the system can lead to the increase of T_c , but only if the coupling of the electrons with these oscillations is rather strong.

This is just the situation with the so-called generalized "jellium" model,¹¹ illustrating the possibility of increasing T_c when some additional polarization modes with a high oscillator strength are introduced in the system (see Refs. 10 and 15).

It should be noted, however, that even if the phonon frequencies and the coupling constants λ and μ are considered as independent parameters, the increase of θ does not always cause the growth of T_c .

In fact, it is seen from (39) and (32) that with the increase of θ , μ^* also increases, and, therefore, the exponent decreases. Sooner or later this effect will exceed the increase of the preexponential factor. To estimate the limiting value of θ^{max} at which T_c has its maximum value T_c^{max} , note that from the stability condition $1/\varepsilon(q, 0) \geq 0$ we get that $\lambda \leq \mu$ [see (37)]. Then considering the most favorable case $\lambda = \mu$ and optimizing expression (41) with respect to θ we have[†]

$$\begin{aligned} \theta^{\text{max}} &= \varepsilon_F e^{-2/\lambda} \\ T_c^{\text{max}} &= \varepsilon_F e^{-3/\lambda} \end{aligned} \quad (42)$$

[†]The authors are grateful to L. N. Bulaevskii who has pointed out to us the possibility of obtaining an upper limit on T_c , from expression (39).

Expression (42) for the maximum critical temperature is obtained in the weak-coupling approximation, and therefore the numerical estimates on the basis of (42) are not reliable enough. If we still try to estimate T_c^{\max} by this formula taking $\lambda \simeq 1/2$ and $\varepsilon_F \simeq 10$ eV, we obtain $T_c^{\max} \simeq 300$ K, which is rather an optimistic result.

In a similar way the estimates of T_c for the case of strong coupling were obtained in Ref. 13. These estimates give the values of T_c^{\max} smaller by an order of magnitude. It should be mentioned, however, that the numerical results are rather sensitive to many details of the description of the system due to the exponential dependence of T_c on the parameters; in the case of strong coupling it is rather difficult to estimate the accuracy of the formulas for T_c used in Ref. 13, particularly with respect to a description of the Coulomb effects (for more details see Ref. 14). Therefore the question of the maximum value of T_c^{\max} seems to be open.

ACKNOWLEDGMENTS

The authors are grateful to Prof. V. L. Ginzburg and the participants of his seminar for fruitful discussions and also to Z. Radovich who has pointed out the way to simplify the calculations.

REFERENCES

1. J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).
2. D. Pines and P. Nosieres, *The Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. 1.
3. N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *New Method in the Theory of Superconductivity* (Consultants Bureau, New York, 1959).
4. G. M. Eliashberg, *Soviet Phys.—JETP* **38**, 966 (1960); **39**, 1437 (1960).
5. P. Morel and P. W. Anderson, *Phys. Rev.* **125**, 1263 (1962).
6. J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964).
7. W. A. McMillan, *Phys. Rev.* **167**, 331 (1967).
8. E. G. Batyjev, *Soviet Phys.—Solid State* **6**, 3554 (1964).
9. G. Gusman and R. Brout, *J. Phys. Chem. Solids* **26**, 223 (1965).
10. D. A. Kirzhnits, E. G. Maksimov, and D. I. Khomskii, Preprint N 108, Lebedev Physical Inst., 1970.
11. J. P. Hurault, *J. Phys. Chem. Solids* **29**, 1765 (1968).
12. L. Hedin and S. Lundqvist, *Solid State Physics*, F. Seitz, ed. (Academic Press, New York, 1969), Vol. 23, p. 2.
13. M. L. Cohen and P. W. Anderson, Preprint SST/50/1971, Cavendish Lab., 1971.
14. V. L. Ginzburg and D. A. Kirzhnits, Preprint N 17, Lebedev Physical Inst., 1972.
15. V. L. Ginzburg, *Usp. Fiz. Nauk* **101**, 185 (1970) [English transl., *Soviet Phys.—Usp.* **13**, 335 (1970)].