Superconductivity in systems with strong electron-phonon interaction

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The superconducting state is studied in systems with strong electron-phonon interaction. The Éliashberg integral equations are reduced to a form which makes their analysis and numerical solution simpler. It is shown that in the limit of large coupling constants, $\lambda \gg 1$, and for $T = 0$ the energy gap Δ_0 has an asymptotic form $\propto \sqrt{\lambda}\,\bar{\omega}$. It is also shown that for finite temperatures the density of electronic states is nonzero for all ω and the superconducting spectrum has excitations with energies "inside the gap," which, in the case of strong coupling, results in a substantial redistribution of the number of normal and superconducting electrons, the properties of such superconductors being markedly different from those given by the BCS model.

1. INTRODUCTION

The Éliashberg equations[1,2] have been studied for a long time. As is known, in the Éliashberg theory a superconductor is fully characterized by the spectral function of the electron-phonon coupling $\alpha^2(\omega)F(\omega)$ (see, e.g., Refs. 3 and 4) and the mean interaction value by a dimensionless coupling constant $\lambda = 2\int_0^\infty d\omega[\alpha^2(\omega)F(\omega)/\omega]$. Éliashberg[1,2] and other authors (see the review in Ref. 3) have shown that for small coupling constants these equations lead to practically the same results for excitation spectra and thermodynamic and kinetic characteristics of superconductors as the Bardeen–Cooper–Schrieffer (BCS) theory.

Important distinctions arise only for fairly large values of the coupling constant λ. The effect of strong coupling, $\lambda \gg 1$, has been studied at length for the superconducting transition critical temperature T_c. In particular, Allen and Dynes[5] have shown that in the limit $\lambda \gg 1$ T_c obeys a power law

$$T_c \propto \lambda^{1/2}.$$

Thermodynamic properties of superconductors with large coupling constants λ have also been studied in detail. In these studies it was possible to solve the Éliashberg equations only at discrete points of the imaginary axis (the Matsubara frequencies), using a simple and convenient technique.[6]

Less attention has been paid to the excitation spectra and dynamic properties of the superconductors with strong coupling, since in this case it is necessary to find the solutions of the Éliashberg equations on the real axis of the variable ω. These problems are studied in the present paper.

2. GENERAL ANALYSIS OF THE ELIASHBERG EQUATIONS FOR SYSTEMS WITH STRONG ELECTRON-PHONON COUPLING

Analytic continuations of the Éliashberg temperature equations from the upper half-plane of the variable ω to the real axis have the form[3,4]

$$\hat{\Sigma}_{\mathbf{p}}(\omega) = -\int \frac{d\mathbf{p}'}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{dz}{2\pi} \alpha^2(\mathbf{p},\mathbf{p}')F(\mathbf{p}-\mathbf{p}',z)$$

$$\int_{-\infty}^{\infty} d\omega' \hat{\tau}_3 \,\mathrm{Im}\, \hat{G}_{\mathbf{p}}^R(\omega')\hat{\tau}_3 \frac{\mathrm{th}(\omega'/2T)+\mathrm{cth}(z/2T)}{\omega-z-\omega'+i\delta}, \qquad (1)$$

where $\hat{G}_p^R(\omega)$ and $\hat{\Sigma}_p(\omega)$ are respectively the matrix retarded electronic Green's function and self-energy, $\alpha^2(\mathbf{p},\mathbf{p}')$ is the squared modulus of the electron-phonon scattering matrix element, $F(\mathbf{p}-\mathbf{p}',z)$ is the spectral density of the phonon Green's function, and $\hat{\tau}_i$ are Pauli matrices. The integral Éliashberg equations (1) are highly complicated for analysis and numerical solution, owing to the singular energy dependence of the electron-phonon coupling. Therefore they are used relatively rarely.

Let us represent the electron-phonon coupling in (1) as the sum of a regular and a singular part. To do this, we add and subtract $\tanh(\omega - z)/2T$ in the numerator in (1) and integrate the singular part of the electron-phonon coupling over $d\omega'$, using the dispersion relation for the retarded electron Green's function:

$$\hat{G}_{\mathbf{p}}^R(\omega) = -\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{d\omega'}{\omega-\omega'+i\delta}\,\mathrm{Im}\,\hat{G}_{\mathbf{p}}^R(\omega').$$

As a result, Eqs. (1) will have the form

$$\hat{\Sigma}_{\mathbf{p}}(\omega) = -\int \frac{d\mathbf{p}'}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega' \hat{\tau}_3 \,\mathrm{Im}\, \hat{G}_{\mathbf{p}}^R(\omega')\hat{\tau}_3 \int_{-\infty}^{\infty} \frac{dz}{2\pi} \alpha^2(\mathbf{p},\mathbf{p}')$$

$$\times F(\mathbf{p}-\mathbf{p}',z) \frac{\mathrm{th}(\omega'/2T)-\mathrm{th}[(\omega-z)/2T]}{\omega-z-\omega'}$$

$$-\int \frac{d\mathbf{p}'}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{dz}{2\pi} \alpha^2(\mathbf{p},\mathbf{p}')$$

$$\times F(\mathbf{p}-\mathbf{p}',z) \left[\mathrm{cth}\frac{z}{2T} + \mathrm{th}\frac{\omega-z}{2T}\right] \hat{\tau}_3 \hat{G}_{\mathbf{p}}^R(\omega-z)\hat{\tau}_3. \qquad (2)$$

We expand next the self-energy $\hat{\Sigma}_p(\omega)$ in terms of Pauli matrices:

$$\hat{\Sigma}_{\mathbf{p}}(\omega) = [1 - Z_{\mathbf{p}}(\omega)]\,\omega\hat{\tau}_0 + \Sigma_{\mathbf{p}}(\omega)\hat{\tau}_1$$

(Σ denotes the anomalous self-energy part). Using the explicit form of the electronic Green's function

$$\hat{G}_{\mathbf{p}}^R(\omega) = \frac{\omega Z_{\mathbf{p}}(\omega)\hat{\tau}_0 + \Sigma_{\mathbf{p}}(\omega)\hat{\tau}_1 + \varepsilon_{\mathbf{p}}\hat{\tau}_3}{\omega^2 Z_{\mathbf{p}}^2(\omega) - \Sigma_{\mathbf{p}}^2(\omega) - \varepsilon_{\mathbf{p}}^2},$$

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we average (2) over the momenta in the usual manner (see Refs. 3 and 4). As a result we get

$$\hat{\Sigma}(\omega)=\frac{1}{2}\int_{-\infty}^{\infty} d\omega'\hat{\tau}_3 \operatorname{Im} \hat{g}^R(\omega')\hat{\tau}_3 \int_{-\infty}^{\infty} dz\alpha^2(z)F(z)$$

$$\times\frac{\operatorname{th}(\omega'/2T)-\operatorname{th}[(\omega-z)/2T]}{\omega-z-\omega'}-\frac{\pi}{2}\int_{-\infty}^{\infty} dz\alpha^2(z)F(z)$$

$$\times\left[\operatorname{cth}\frac{z}{2T}+\operatorname{th}\frac{\omega-z}{2T}\right]\hat{\tau}_3\hat{g}^R(\omega-z)\hat{\tau}_3, \qquad (3)$$

where we have introduced the spectral function $\alpha^2(\omega)F(\omega)$ of the electron-phonon coupling, the averaged electronic Green's function

$$\hat{g}^R(\omega)=i\frac{\omega\hat{\tau}_0+\Delta(\omega)\hat{\tau}_1}{[\omega^2-\Delta^2(\omega)]^{1/2}}\operatorname{sign}\omega$$

and the superconducting gap $\Delta(\omega)=\Sigma(\omega)/Z(\omega)$. Using the symmetry properties $\Delta(-\omega)=\Delta^*(\omega)$, $Z(-\omega)=Z^*(\omega)$, and $\alpha^2(-\omega)F(-\omega)=-\alpha^2(\omega)F(\omega)$, we rewrite the equations in the form

$$\Sigma(\omega)\equiv Z(\omega)\Delta(\omega)=\int_0^{\infty} d\omega' \operatorname{Re}\frac{\Delta(\omega')}{[\omega'^2-\Delta^2(\omega')]^{1/2}}K_s(\omega,\omega')$$

$$+i\pi\int_0^{\infty} d\omega'\alpha^2(\omega')F(\omega')\left\{\frac{\Delta(\omega+\omega')}{[(\omega+\omega')^2-\Delta^2(\omega+\omega')]^{1/2}}\right.$$

$$\times[n(\omega')+f(\omega+\omega')]$$

$$+\operatorname{sign}(\omega-\omega')\frac{\Delta(\omega-\omega')}{[(\omega-\omega')^2-\Delta^2(\omega-\omega')]^{1/2}}$$

$$\left.\times[n(\omega')+f(\omega'-\omega)]\right\}, \qquad (4)$$

$$Z(\omega)=1+\int_0^{\infty} d\omega' \operatorname{Re}\frac{\omega'}{[\omega'^2-\Delta^2(\omega')]^{1/2}}K_n(\omega,\omega')$$

$$+\frac{i\pi}{\omega}\int_0^{\infty} d\omega'\alpha^2(\omega')F(\omega')\left\{\frac{\omega+\omega'}{[(\omega+\omega')^2-\Delta^2(\omega+\omega')]^{1/2}}\right.$$

$$\times[n(\omega')+f(\omega+\omega')]+\operatorname{sign}(\omega-\omega')\frac{\omega-\omega'}{[(\omega-\omega')^2-\Delta^2(\omega-\omega')]^{1/2}}$$

$$\left.\times[n(\omega')+f(\omega'-\omega)]\right\}, \qquad (5)$$

$$K_s(\omega,\omega')=\frac{1}{2}\int_0^{\infty} dz\alpha^2(z)F(z)\,[k(\omega',\omega,z)$$

$$-k(\omega',-\omega,-z)+k(\omega',-\omega,z)-k(\omega',\omega,-z)],$$

$$K_n(\omega,\omega')=-\frac{1}{2\omega}\int_0^{\infty} dz\alpha^2(z)F(z)\,[k(\omega',\omega,z)$$

$$+k(\omega',-\omega,-z)-k(\omega',-\omega,z)-k(\omega',\omega,-z)],$$

$$k(\omega',\omega,z)=\frac{\operatorname{th}(\omega'/2T)+\operatorname{th}[(\omega+z)/2T]}{\omega'+\omega+z},$$

where $f(\omega)$ and $n(\omega)$ are the Fermi and Bose distributions respectively. The kernels $K_s(\omega,\omega')$ and $K_n(\omega,\omega')$ in Eqs. (4) and (5) are regular short-range Fredholm functions. In fact, writing $k(\omega',\omega,z)$ in the form

$$k(\omega',\omega,z)=\frac{1}{\operatorname{ch}(\omega'/2T)}\,\frac{1}{\operatorname{ch}[(\omega+z)/2T]}\,\frac{\operatorname{sh}[(\omega'+\omega+z)/2T]}{\omega'+\omega+z}$$

we make sure that this function has no singularities for real variables. In the complex plane of the variable ω' the function $k(\omega',\omega,z)$ has poles at the points $\omega_n'=2i\pi T(n+1/2)$. Therefore the terms in Eqs. (3)–(5) determined by the regular part K may be written in a somewhat different way. Passing to the contour integration in the complex ω' plane in the regular terms in (3) and taking into account the Green's function analytic properties, we find for Eq. (4):

$$\Sigma(\omega)=\pi T\sum_{n=-\infty}^{n=\infty}K_s(\omega-i\omega_n)\frac{\Delta(i\omega_n)}{[\omega_n^2+\Delta(i\omega_n)]^{1/2}}$$

$$+i\pi\int_0^{\infty} dz\alpha^2(z)F(z)\left\{\frac{\Delta(\omega+z)}{[(\omega+z)^2-\Delta^2(\omega+z)]^{1/2}}[n(z)+f(\omega+z)]\right.$$

$$\left.+\operatorname{sign}(\omega-z)\frac{\Delta(\omega-z)}{[(\omega-z)^2-\Delta^2(\omega-z)]^{1/2}}[n(z)+f(z-\omega)]\right\}, \qquad (4a)$$

where

$$K_s(\omega-i\omega_n)=\int_0^{\infty} dz\alpha^2(z)F(z)\frac{2z}{z^2-(\omega-i\omega_n)^2}.$$

Equation (5) may be rewritten in a similar manner. Equations of this very type have been found by Marsiglio *et al.*,[7] who have suggested to use them for the analytic continuation of the functions $\Delta(i\omega_n)$ and $Z(i\omega_n)$ obtained as a result of the solution of the Éliashberg equations at the Matsubara frequencies $i\omega_n$. The analytic continuation is achieved in Ref. 7 by solving twice the Éliashberg equations. First, they are solved on the imaginary axis, then the found solutions are used to calculate the regular terms (inhomogeneities) in (4a), which, in their turn, are used to find the analytic continuation in question. According to the authors of Ref. 7, this method of analytic continuation is especially convenient for the determination of the energy gap, as $T\to 0$, in the very-strong-coupling case. In the case of Eqs. (4) and (5) obtained above it is not necessary to solve the equations on the imaginary axis, since the regular terms with the Fredholm kernels K do not lead to additional complications in the solution of these equations. To make sure of this, we consider the case $T=0$, when Eqs. (4) and (5) can be written as

$$\Delta(\omega)=\frac{\int_{\Delta_0}^{\infty} d\omega' \operatorname{Re}\frac{\Delta(\omega')}{[\omega'^2-\Delta^2(\omega')]^{1/2}}K_s(\omega',\omega)}{1+\int_{\Delta_0}^{\infty} d\omega' \operatorname{Re}\frac{\omega'}{[\omega'^2-\Delta^2(\omega')]^{1/2}}K_n(\omega',\omega)}$$

$$+\frac{i\pi\int_0^{\omega} d\omega'\alpha^2(\omega-\omega')F(\omega-\omega')\frac{\Delta(\omega')-\Delta(\omega)(\omega'/\omega)}{[\omega'^2-\Delta^2(\omega')]^{1/2}}}{1+\int_{\Delta_0}^{\infty} d\omega' \operatorname{Re}\frac{\omega'}{[\omega'^2-\Delta^2(\omega')]^{1/2}}K_n(\omega',\omega)},$$

$$K_s(\omega'\omega) = \int_\omega^\infty dz\alpha^2(z)F(z)\left(\frac{1}{\omega'+z+\omega} + \frac{1}{\omega'+z-\omega}\right)$$
$$+ \int_0^\omega dz\alpha^2(z)F(z)\left(\frac{1}{\omega'+z+\omega} - \frac{1}{\omega'-z+\omega}\right),$$

$$K_n(\omega',\omega) = -\frac{1}{\omega}\int_\omega^\infty dz\alpha^2(z)F(z)\left(\frac{1}{\omega'+z+\omega} - \frac{1}{\omega'+z-\omega}\right)$$
$$-\frac{1}{\omega}\int_0^\omega dz\alpha^2(z)F(z)\left(\frac{1}{\omega'+z+\omega} - \frac{1}{\omega'-z+\omega}\right). \qquad (6)$$

It is seen that the regular parts of the interaction, K_s and K_n, are localized in the phonon energy range where the interaction K_s corresponds to attraction and is of order $K_s(0,0) = \lambda$. Outside the phonon spectrum the K_s and K_n moduli decrease rapidly, and K_s corresponds to repulsion. Thus, the attraction range of the interaction K_s is bounded by a characteristic phonon frequency $\overline{\omega}$.

The second term in (6), of the resonant type, connected with the singular part of the electron-phonon coupling, is completely different. This term, in contrast to the regular one, strongly depends on the specific form of the spectral function. The resonant contribution is small in the low energy range $\omega \ll \overline{\omega}$, owing to the smallness of the spectral function $\alpha^2(\omega)F(\omega)$, and reaches a maximum only at ω of order $\overline{\omega} + \Delta_0$, where Δ_0 is the energy gap defined for $T = 0$ as $\Delta_0 = \Delta(\Delta_0)$.

In the weak-coupling case, when the energy gap is much smaller than $\overline{\omega}$, it is the regular term that gives the main contribution to Δ_0. In this case we arrive at the usual exponential dependence of the gap on the BCS coupling constant λ: $\Delta_0 \propto \exp(-\lambda/1+\lambda)$. Evidently, if we consider only this interaction, which reverses its sign near the phonon spectrum boundary, we find that the energy gap is smaller than $\overline{\omega}$ for arbitrarily large coupling constants λ. On the contrary, if we allow for the singular part of the interaction, the attraction range becomes dependent on the coupling constant and increases to $\sim\overline{\omega} + \Delta_0$, which corresponds to the usual notions about the attraction potential in a superconductor, with quasiparticle dispersion law taken into account. In the strong-coupling case, it is most difficult to study the second term in (6) analytically. Therefore we will use the results of numerical analysis with the model spectral function $\alpha_m^2(\omega)F_m(\omega)$ of the electron-phonon coupling shown in Fig. 1.[1)] The solution $\Delta(\omega)$ of Eq. (6) for $\lambda = 20$ is plotted in Fig. 2. The regular-term contribution [the first term in (6)] is shown in the same figure. As seen from Fig. 2, the regular contribution [the inhomogeneity in (4a)] is localized in an energy range of order $\overline{\omega}(\sim 1)$ and is small, in comparison with the resonant contribution, outside this range, particularly at $\omega \sim \Delta_0$.

Let us consider briefly the problem, highly popular in the literature, of superconducting properties in the limit $\lambda \gg 1$. The limiting behavior of the superconducting transition critical temperature was first studied by Allen and Dynes,[5] who showed that $T_c \propto \sqrt{\lambda}$. As far as the energy gap behavior in the limit $\lambda \gg 1$ is concerned, there are substantial differences. Some authors[8,9] argue that $\Delta_0 \sim \sqrt{\lambda}$, others[10,11] that $\Delta_0 \propto \lambda$. In the limit $\lambda \gg 1$ the energy gap is mainly determined by the resonant term in (6), while the regular-term contribution is, at least numerically, small. Using the simplest model for the function $\alpha^2(\omega)F(\omega)$ in the form of one Einstein maximum centered at $\omega = \overline{\omega}$, i.e., $\alpha^2(\omega)F(\omega) = (\lambda\overline{\omega}/2)\,\delta(\omega - \overline{\omega})$, we can rewrite the equation for $\Delta(\omega)$ in the form

$$\Delta(\omega) = \frac{\pi\lambda\overline{\omega}}{2}\frac{\Delta(\omega-\overline{\omega}) - (\omega-\overline{\omega})\Delta(\omega)/\omega}{[\Delta^2(\omega-\overline{\omega}) - (\omega-\overline{\omega})^2]^{1/2}}.$$

Further, we introduce the function $\varphi(\omega) = \Delta(\omega)/\omega$ and change over to the variable $y = \omega - \overline{\omega}$. Expanding the function $\varphi(y+\overline{\omega})$ in terms of $\overline{\omega}/\Delta_0$ and using only the lowest term, we get

$$\varphi(y) = \frac{\pi\lambda\overline{\omega}^2\varphi'(y)}{2y[\varphi^2(y)-1]^{1/2}}.$$

The solution of this differential equation has the form

$$\varphi(y) = \left[\sin\frac{y^2}{\pi\lambda\overline{\omega}^2}\right]^{-1}. \qquad (7)$$

Setting $\varphi(\Delta_0) = 1$, we find that $\Delta_0 = \pi\overline{\omega}\sqrt{\lambda}/\sqrt{2}$.

Thus, for large λ the energy gap has the same asymptote as T_c. The specific value of the constant in this asymptote should, certainly, be obtained from the exact solution of Eq. (6). It can be shown that the asymptote $\Delta_0 \propto \sqrt{\lambda}$ is reached under when the condition $d\Delta(\omega)/d\omega|_{\omega=\Delta_0} = 1$, which is

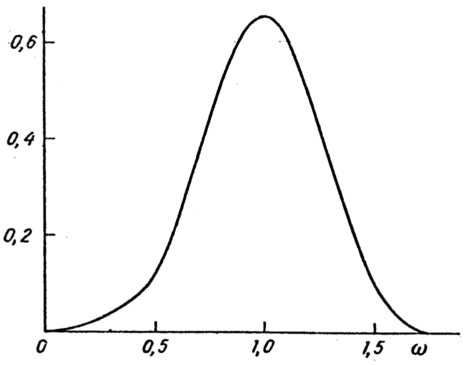

FIG. 1. The model spectral function $\alpha_m^2(\omega)F_m(\omega)$.

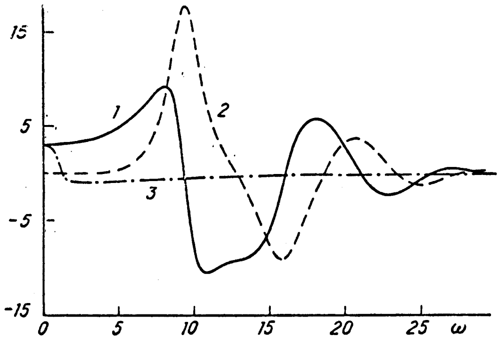

FIG. 2. Re$\Delta(\omega)$ (*1*), Im$\Delta(\omega)$ (*2*) and regular part of $\Delta(\omega)$ (*3*) for $\lambda = 20$ and $T = 0$.

satisfied by the solution (7). As seen from the numerical analysis carried out by Marsiglio and Carbotte,[9] this condition does not hold even for $\lambda = 200$, therefore Δ_0 for smaller values of λ (as in Refs. 10 and 11, where $\lambda < 40$) can be approximated to equal accuracy by a power law: $\Delta_0 \approx \lambda^p \bar{\omega}$, where $\frac{1}{2} \lesssim p \lesssim 1$.

Consider now the properties of the equations and their solutions obtained above at finite temperatures. As already noted, the regular kernels $K_s(\omega,\omega')$ and $K_n(\omega,\omega')$ are localized near the energy $\bar{\omega}$. At finite temperatures K_s and K_n are smeared. In particular, for small ω' $K_s(\omega,\omega')$ vanishes as $\tanh\omega'/2T$. The function $K_s(\omega,\omega')$ at $T = 0.1$ is shown in Fig. 3. Both for $T = 0$ and finite temperatures it is quite close to $\lambda \tanh(\omega'/2T)\theta(\bar{\omega} - \omega')\theta(\bar{\omega} - \omega)$, i.e., to the BCS model interaction. As seen from (3), at $T \ll \bar{\omega}$ the resonant contributions to $\Sigma(\omega)$ are important only for $\omega \sim \bar{\omega}$. In the weak-coupling case, the absolute values of $\Sigma(\omega)$ in the range of characteristic phonon frequencies are small in comparison with ω, therefore, the resonant terms have a small effect on the thermodynamic properties as well. In particular, the ratio $2\Delta_0/T_c$ has its BCS value 3.52. Thus, the power dependences on the coupling constant and considerable deviations from the BCS value of the ratio $2\Delta_0/T_c$, taking place in the strong-electron-phonon-coupling case, are connected with the resonant terms and characterize their relative magnitude.

For finite temperatures the allowance for the resonant interaction is, in principle, important also for small ω, since it leads to an $\mathrm{Im}Z(\omega)$ divergence and to gapless superconductivity.[2,12] We are going to study this problem at length in the next section.

3. ENERGY GAP AND DENSITY OF ELECTRONIC STATES IN SUPERCONDUCTORS WITH STRONG ELECTRON-PHONON COUPLING

In the BCS theory the density of electronic states in superconductors has the form

$$N(\omega) = \mathrm{Re}\frac{\omega}{[\omega^2 - \Delta^2(T)]^{1/2}}, \tag{8}$$

where $\Delta(T)$ is the temperature-dependent energy gap. As seen from Eq. (8), $N(\omega) \equiv 0$ for energies lower than the gap. Consider now what happens in systems with electron-phonon coupling. To this end, we write the renormalized function $Z(\omega)$ and the superconducting gap $\Delta(\omega)$ in the form

$$Z(\omega,T) = \mathrm{Re}\,Z(\omega,T) + i\frac{\Gamma(\omega,T)}{\omega}$$

$$\Delta(\omega,T) = \frac{\Sigma(\omega,T)}{\mathrm{Re}\,Z(\omega,T) + i\Gamma(\omega,T)/\omega} = \omega\frac{\tilde{\Sigma}(\omega,T)}{\omega + i\tilde{\Gamma}(\omega,T)}.$$

Here

$$\tilde{\Sigma}(\omega,T) = \frac{\Sigma(\omega,T)}{\mathrm{Re}\,Z(\omega,T)},$$

$$\tilde{\Gamma}(\omega,T) = \frac{\pi}{\mathrm{Re}\,Z(\omega,T)}\int_0^\infty d\omega'\alpha^2(\omega')F(\omega')$$

$$\times\left\{\frac{\omega+\omega'}{[(\omega+\omega')^2 - \Delta^2(\omega+\omega')]^{1/2}}[n(\omega') + f(\omega+\omega')]\right.$$

$$\left.+\mathrm{sign}(\omega-\omega')\frac{\omega-\omega'}{[(\omega-\omega')^2 + \Delta^2(\omega-\omega')]^{1/2}}[n(\omega') + f(\omega'-\omega)]\right\}. \tag{9}$$

The function $\tilde{\Gamma}(\omega,T)$ is the renormalized inverse electron relaxation time. The density $N(\omega)$ of the electronic states could also be rewritten with the help of the introduced functions $\tilde{\Sigma}(\omega,T)$ and $\tilde{\Gamma}(\omega,T)$:

$$N(\omega) = \mathrm{Re}\frac{\omega + i\tilde{\Gamma}(\omega,T)}{\{[\omega + i\tilde{\Gamma}(\omega,T)]^2 - \tilde{\Sigma}^2(\omega,T)\}^{1/2}}. \tag{10}$$

Equation similar to Eq. (10),

$$N(\omega) = \mathrm{Re}\frac{\omega + i\tilde{\Gamma}(T)}{\{[\omega + i\tilde{\Gamma}(T)]^2 - \tilde{\Sigma}^2(T)\}^{1/2}} \tag{10a}$$

is used in fitting experimental data to describe the density of states in superconductors with allowance for pair breaking. The function $\tilde{\Gamma}(T)$ is regarded as a parameter indicative of pair-breaking processes, and $\tilde{\Sigma}(T)$ has the meaning of the order parameter. The processes leading to pair breaking are scattering by magnetic impurities, proximity to the normal metal, and some others. As seen from (10), similar pair-breaking processes exist also in systems with electron-phonon coupling. At $T = 0$, as follows from the solution of the Éliashberg equations, the function $\tilde{\Gamma}(\omega,T)$ vanishes for $\omega < \Delta_0$, where Δ_0 is the energy gap defined by the equation $\mathrm{Re}\Delta(\Delta_0) = \Delta_0$ or by the similar equation $\mathrm{Re}\tilde{\Sigma}(\Delta_0,0) = \Delta_0$. At finite temperatures the function $\tilde{\Gamma}(\omega,T)$ is nonzero for any ω, including $\omega = 0$. This means, as already noted in Refs. 2 and 12, that in the superconductor excitation spectrum the energy gap is absent at $T \neq 0$ and,

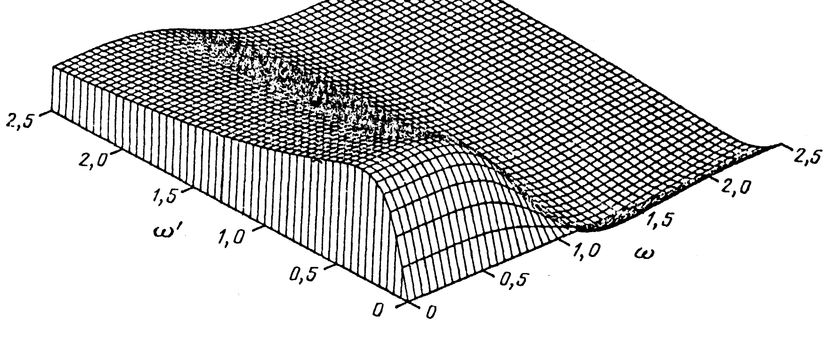

FIG. 3. The regular part of the electron-phonon coupling $K_s(\omega,\omega')$ for the temperature $T/\bar{\omega} = 0.1$.

consequently, there are normal quasiparticles of infinitesimal energy, since even as $\omega \to 0$ the density of states $N(\omega) = \Gamma/\sqrt{\Gamma^2 + \Sigma^2}$ is nonzero. The question is whether this fact is important quantitatively.

The possible behavior of the density of states is given already by the simplest formula (10a). It is easy to make sure that the maximum of the density of states (10a) is shifted with respect to the order parameter $\tilde{\Sigma}(T)$ by a value of order $\sim \tilde{\Gamma}(T)$, therefore two types of temperature dependence of the maximum position are possible. In the case when the damping $\tilde{\Gamma}(T)$ grows slowly with temperature in comparison with the decrease of the order parameter $\tilde{\Sigma}(T)$, the maximum of the density of states follows the function $\tilde{\Sigma}(T)$. Such a dependence corresponds to the gap behavior in the BCS theory. If, however, $\tilde{\Gamma}(T)$ grows more quickly than $\tilde{\Sigma}(T)$ decreases, the maximum is shifted towards higher energies with temperature, and its smearing becomes the main effect. In the immediate vicinity of T_c the position of the maximum of the density of states is not connected with the order parameter. Near the critical temperature the expression for the density of states can be expanded in the small parameter Σ/Γ and represented in the form

$$N(\omega)=1+\frac{1}{2}\,\mathrm{Re}\left[\frac{\Sigma(T)}{\omega+i\Gamma(T_c)}\right]^2 .$$

In this case the position of the density-of-states maximum does not depend on $\tilde{\Sigma}$ (and temperature) and it tends to $\sqrt{3}\,\tilde{\Gamma}(T_c)$ as $T \to T_c$.

In the weak-coupling case, in the most important frequency range $\omega \ll \overline{\omega}$ the functions $\tilde{\Sigma}(\omega,T)$ and $\tilde{\Gamma}(\omega,T)$ can be replaced by their amplitudes at the point $\omega = 0$. As seen from (9), in this case the inverse electron relaxation time $\tilde{\Gamma}(0,T)$ is small $[\Gamma \sim \lambda T(T/\overline{\omega})^2$ at low temperatures $T \ll \overline{\omega}$ even in the normal state$]$, therefore the density of states (10) differs little from the BCS density of states (8), and thermal excitations "across the gap" dominate in the spectrum. Their energies lie in the region of the $N(\omega)$ maximum, whose position is governed by the order parameter $\tilde{\Sigma}(0,T)$. Thus, a superconductor with a weak electron-phonon coupling deviates from the BCS theory only in a narrow T_c vicinity. Therefore, for such superconductors the energy gap, to good accuracy, could be understood to be the position of the density-of-states maximum, and the temperature dependence of the latter could be regarded as the energy-gap temperature dependence. In fact, this is usually done in the tunnel experiments, for example.

Let us try now, with the help of a numerical solution of the Éliashberg equations with a model function $\alpha^2(\omega)F(\omega)$, to find how the BCS model differs from the systems with a strong electron-phonon coupling. Figure 4 shows the density of states for different temperatures $(t = T/T_c > 0.35)$ and coupling constants. As seen from Fig. 4, at finite temperatures the density of states is a continuous function with a maximum and with distinct regions of low $[N(\omega) < 1$ "inside the gap"$]$ and high ("the gap region") densities of states. The quasiparticle state occupation versus the energy ω is shown in Fig. 5 together with the ratio of quasiparticles with energies smaller than ω to the total number of quasiparticles

$$n_n(\omega)=\int_0^{\omega} d\omega' f(\omega')N(\omega') \Big/ \int_0^{\infty} d\omega' f(\omega')N(\omega').$$

The dashed line shows the region "inside the gap." The form of $N(\omega,T)$ and the quasiparticle state occupation for the coupling constant $\lambda = 2$ are shown in Figs. 4a and 5a. Figure 6 shows the temperature dependences $\tilde{\Sigma}(0,T)$ and $\tilde{\Gamma}(0,T)$ approximately representing the amplitudes of the functions $\tilde{\Sigma}(\omega,T)$ and $\tilde{\Gamma}(\omega,T)$, together with the position of the density-of-states maximum as a function of temperature, $\Delta_0(T)$. As seen from Figs. 4–6, in spite of a strong smearing of the peak, there is an energy range ("the gap region") which contains a large number of thermal excitations and whose position in the whole temperature range (excluding the T_c vicinity) correlates with the behavior of $\tilde{\Sigma}(0,T)$. In this sense, the average amplitude of the function $\tilde{\Sigma}(\omega,T)$ could be roughly considered as an order parameter. This corresponds on the whole to the superconducting-gap notions, as is also confirmed by the presence of a residual co-

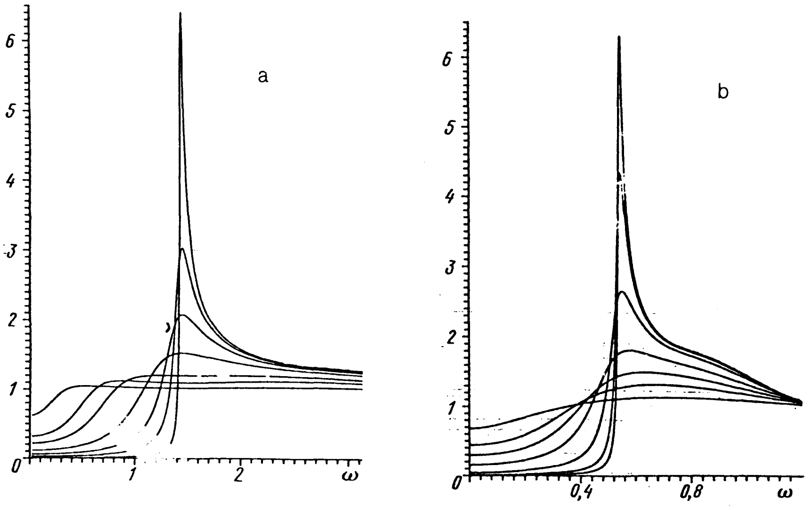

FIG. 4. The density of electronic states for $T/T_c > 0.35$ and coupling constants $\lambda = 2$ (a) and $\lambda = 5$ (b).

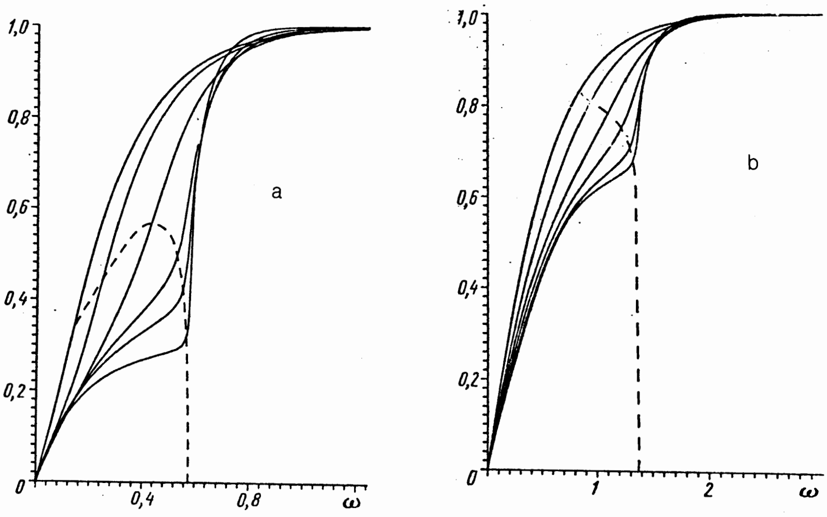

FIG. 5. The relative number of quasiparticles with energies smaller than ω at temperatures $T/T_c > 0.35$ for the coupling constants $\lambda = 2$ (a) and $\lambda = 5$ (b).

herent maximum in the temperature dependence of the nuclear-spin relaxation rate (see Fig. 7).

As the coupling constant increases, the smearing of the peak and the occupation of the low-frequency states also increase. Thus, the function $N(\omega,T)$ in Fig. 4b ($\lambda = 5$) refers to another behavior of the density of states, characterized by strong damping. In this case the structure of the density of states does not correlate with the amplitude of the function $\tilde{\Sigma}(\omega,T)$. In spite of the fact that the $N(\omega,T)$ maximum has a large amplitude for some temperatures, the relative number of quasiparticles in "the gap region," as shown in Fig. 5b, is small and the region itself is unimportant for the quasiparticle thermodynamics. A large number of quasiparticles is "inside the gap," where the density of states has a weak energy dependence. Such states could be regarded as gapless and treated in the framework of the two-liquid model. As a parameter characterizing the gapless state, it is natural to use a quantity proportional to the mean density of states "inside the gap" (a similar situation takes place also for $\lambda = 3.5$).

The existence of a mechanism of quasiparticle state occupation other than the BCS one leads to a change in the ratio of the numbers of normal, (n_n), and superconducting, ($n_s = 1 - n_n$), electrons, which can be estimated from the temperature dependence of the London penetration depth

$$\frac{1}{\lambda_L^2(T)} = \frac{2\pi ne^2}{m}\int_0^\infty d\omega \,\mathrm{th}\frac{\omega}{2T}\,\mathrm{Re}\frac{\Delta^2(\omega)}{[\omega^2-\Delta^2(\omega)]^{1/2}Z(\omega)}$$
$$= \frac{2\pi ne^2}{m^*}n_s,$$

shown in Fig. 7. As is seen, the number of normal electrons at a given temperature t grows with the coupling constant. The temperature dependence of the nuclear spin relaxation rate,

$$K(T) = \frac{1}{T}\int_0^\infty d\omega \frac{1}{\mathrm{ch}^2(\omega/2T)}\left\{\left[\mathrm{Re}\frac{\omega}{[\omega^2-\Delta^2(\omega)]^{1/2}}\right]^2 + \left[\mathrm{Re}\frac{\Delta(\omega)}{[\omega^2-\Delta^2(\omega)]^{1/2}}\right]^2\right\}$$

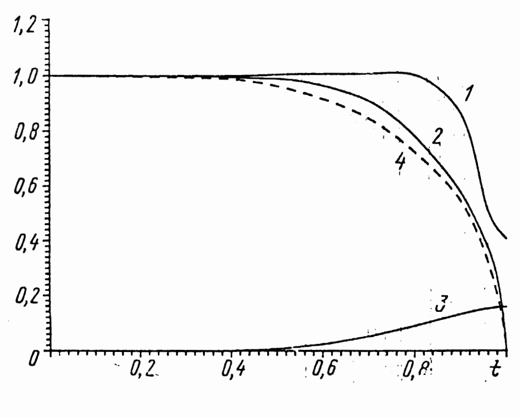

FIG. 6. Relative-temperature dependences of the normalized functions $\Delta_0(t)$ (1), $\tilde{\Sigma}(0,t)$ (2), and $\tilde{\Gamma}(0,t)$ (3) for $\lambda = 2$; the BCS $\Delta(t)$ (4) is also shown.

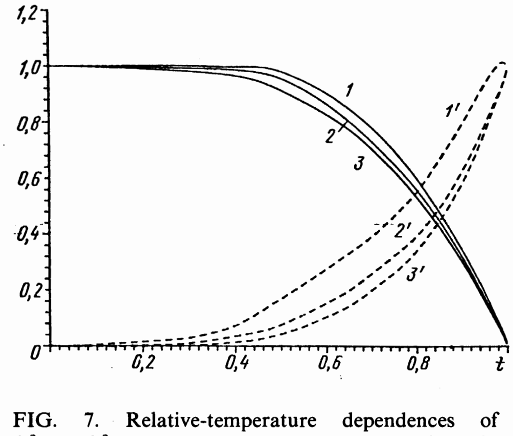

FIG. 7. Relative-temperature dependences of the functions $\lambda_L^2(0)/\lambda_L^2(t)$ (solid lines) and $K(t)$ (dashed lines) for the coupling constants 2 (1,1'), 3.5 (2,2') and 5 (3,3') (from the top to the bottom respectively).

shown in Fig. 7 does not have a coherent maximum in the gapless state and can be approximated by a power function with an exponent increasing with the coupling constant.

The strong coupling effects considered above are encountered in real high-T_c superconductors.[13,14] In particular, the state of BiSrCaCuO at $t>0.7$ can be regarded as gapless,[15] and its conductivity described by the two-liquid model with the parameter $n_s = 1 - t^4$ (Refs. 16 and 17), which formally coincides with n_s in the Gorter–Casimir model. The temperature functions $n_s(t)$ and $K(t)$ for BiSrCaCuO, whose coupling constant is 2.04, but whose spectral function $\alpha^2(\omega)F(\omega)$ is more smeared than in our case (and, consequently, the damping is stronger), occupy intermediate position in Fig. 7 between the curves corresponding to $\lambda = 2$ and $\lambda = 3.5$. As follows from Fig. 7, the equality of $n_n(t)$ and $K(t) \approx t^4$ dependences observed in BiSrCaCuO and other high-T_c superconductors[17-19] is, probably, characteristic of BiSrCaCuO and other superconductors with close parameters, but is not universal in the strong-coupling limit.

4. CONCLUSION

Let us list briefly the results of our studies. The electron-phonon coupling in the integral Éliashberg equations is represented as the sum of a singular and a regular part close to the model BCS coupling. Such a representation is convenient for the analysis and numerical solution on the real axis of the variable energy ω. The analytic study of the singular-part contribution, dominant in the large-coupling-constant limit, yields for the energy gap at $T=0$ the asymptote $\Delta_0 \sim \sqrt{\lambda}\,\overline{\omega}$.

A consistent analysis of the density of electronic states for superconductors with strong electron-phonon coupling has been carried out. It is shown that at finite temperatures the density of states is nonzero for all ω, giving rise to excitations with "inside-the-gap" energies in the superconductor spectrum. Such a mechanism of quasiparticle state occupation causes the number of normal electrons at a given temperature $t = T/T_c$ to increase with the constant λ of electron-phonon coupling. In the case of a sufficiently strong coupling ($\lambda > 2$) a gapless state sets in near T_c in a temperature range, growing with λ. A number of experimental studies indicate such a possibility.

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[1)] The function $\alpha_m^2(\omega)F_m(\omega)$ is normalized by the condition $2\int_0^\infty d\omega[\alpha_m^2(\omega)F_m(\omega)/\omega] = 1$, so that the spectral function of a superconductor with a coupling constant λ has the form $\lambda\alpha_m^2(\omega)F_m(\omega)$. In what follows we use the energy units normalized to the characteristic phonon frequency $\overline{\omega}$.

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