Determination of the energy gap parameter and of the electron-phonon interaction in superconductors from the tunnel data

A. A. Galkin, A. I. D'yachenko, and V. M. Svistunov

Donets Physico-technical Institute, Ukrainian Academy of Sciences
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It is shown that the complex energy-gap parameter of an isotropic strongly coupled superconductor can be directly determined from the tunnel density of states. A linear second-order integral equation is obtained for the electron-phonon interaction function without resorting to a Coulomb pseudopotential or to a cutoff parameter. The equation is solved for a number of pure metals and alloys.

1. The electron tunneling method makes it possible to obtain most complete information on superconducting properties of materials. There are also prospects of using the tunnel effect to determine a number of parameters that characterize a substance in the normal state. Tunneling has in fact become a most precise tool for the study of details of the interaction of electrons with a lattice, which is the principal interaction responsible for the superconductivity[1,2]. It appears that the electron-tunneling method is useful also in searches for other superconductivity mechanisms[3]. At the same time, it is probable that not all the possibilities of the tunnel effect have been realized as yet. One cannot exclude the possibility that further development of the quantitative theory of single-particle tunneling in solids and an improvement in the methods of extracting physical information from tunnel data will lead to qualitatively new results.

The calculation of the tunnel density of states

$$N_\tau(\omega)=\mathrm{Re}\frac{\omega}{[\omega^2-\Delta^2(\omega)]^{1/2}}$$

is based on the Migdal-Éliashberg theory[4], according to which the connection between the electron-phonon interaction parameters and the energy-gap parameter $\Delta(\omega)$ of a superconductor is described by the system of equations[5]

$$\Delta(\omega)=\frac{1}{Z(\omega)}\int_{\Delta_0}^{\omega_c}d\nu\,\mathrm{Re}\left(\frac{\Delta(\nu)}{[\nu^2-\Delta^2(\nu)]^{1/2}}\right)[K^+(\omega,\nu)-\mu^*],\qquad(1)$$

$$[1-Z(\omega)]\omega=\int_{\Delta_0}^{\infty}d\nu\,\mathrm{Re}\left(\frac{\nu}{[\nu^2-\Delta^2(\nu)]^{1/2}}\right)K^-(\omega,\nu),$$

where

$$K^\pm(\omega,\nu)=\int d\omega_q g(\omega_q)\left(\frac{1}{\omega_q+\nu+\omega+i0^+}\pm\frac{1}{\omega_q+\nu-\omega-i0^+}\right)$$

$Z(\omega)$ is a renormalization function, Δ_0 is the energy gap in the excitation spectrum of the superconductor, μ^* and ω_c are respectively the Coulomb pseudopotential and the cutoff parameter introduced in[6], and $g(\omega)$ is the effective electron-phonon interaction averaged over the Fermi surface. The function $g(\omega)$ and its derivative $dg(\omega)/d\omega$ describe fully the structure of the phonon density of states.

MacMillan and Rowell[7] have proposed a method of reconstructing $g(\omega)$ and μ^* from the tunnel characteristics by inverting Eqs. (1) with a computer. A comparison of the neutron-diffraction data on the phonon spectra with the tunnel data shows the latter to be reliable[8]. The determination of the function $g(\omega)$, which describes the electron-phonon interaction in metals, from the tunnel experiments is therefore bound to attract attention at present.

At the same time, the cumbersome calculations, which call for high-productivity computers, make the use of the method of MacMillan and Rowell[7] in the analysis of the tunnel result quite complicated, for it is necessary to have six to eight solutions of the system (1) for $\Delta(\omega)$ in order to find a function $\mathrm{Re}[\omega/(\omega^2-\Delta^2(\omega))^{1/2}]$, that differs from the experimental $N_T(\omega)$ with accuracy to 10^{-3}. During each iteration stage, μ^* must be chosen such that the calculated Δ_0 coincides with the experimental value of Δ_0. In these operations, μ^* is in fact a fit parameter that is quite sensitive to the experimental value[1)] of Δ_0 and to the cutoff limit ω_c, and influences the calculated function $g(\omega)$. It is not surprising that the values of μ^* given in various papers for the same metals are quite different.

In this paper we develop a qualitatively different approach to the interpretation of the tunnel data. It is based on the fact that if the energy-gap parameter $\Delta(\omega)$ is known, then Eqs. (1) become linear and can be easily solved with respect to $g(\omega)$. As the initial data for the determination of $\Delta(\omega)$ we use directly the experimental tunnel density of states. In this operation, when $g(\omega)$ is reconstructed it is not necessary to calculate the parameter μ^*, the determination of which is not always justified.

2. We consider an isotropic semiconductor with a single observable gap Δ_0. In this case (see the Appendix) the function

$$\Phi(z)=i/[z^2-\Delta^2(z)]^{1/2}$$

is analytic in the region D that includes the entire Z plane, with the exception of cuts $(-\infty,-\Delta_0)$ and $(\Delta_0,+\infty)$ on the real axis.

Using the contour L (Fig. 1) (L ∈ D) and Eqs. (A.7) and (A.8), we obtain a dispersion relation for $\Phi(z)$:

$$\mathrm{Im}\frac{1}{[\omega^2-\Delta^2(\omega)]^{1/2}}=\frac{2}{\pi}\int_{\Delta_0}^{\infty}\mathrm{Re}\frac{\nu}{[\nu^2-\Delta^2(\nu)]^{1/2}}\frac{d\nu}{\omega^2-\nu^2},\qquad(2)$$

which connects directly the measured tunnel density of states $n_T(\omega)$ with $\mathrm{Im}[\omega^2-\Delta^2(\omega)]^{-1/2}$. Expression (2) it makes it possible to calculate the function

$$\frac{\omega}{[\omega^2-\Delta^2(\omega)]^{1/2}}=N_\tau(\omega)+i\,\mathrm{Im}\frac{\omega}{[\omega^2-\Delta^2(\omega)]^{1/2}}\qquad(3)$$

at $\Delta_0<\omega<\omega_T$.[2)] With the aid of (3), after simple algebraic transformations, we obtain a function $\Delta(\omega)$ that corresponds exactly to $N_T(\omega)$.

Since $\Delta(\omega)$ has been determined, we obtain from

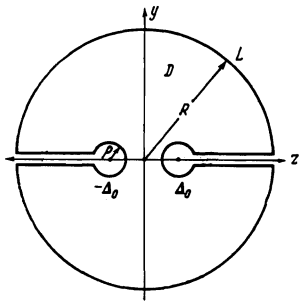

FIG. 1. Integration contour for the determination of the dispersion relation (2).

Im $(\Delta(\omega)Z(\omega))$ and from (1) for the determination of $g(\omega)$ the following linear integral equation of the first kind:

$$\int_0^{\omega-\Delta_0} g(\nu)\,\mathrm{Re}\left[\Delta(\omega-\nu)-\frac{\mathrm{Re}\,\Delta(\omega)}{\omega}(\omega-\nu)\right] \times[(\omega-\nu)^2-\Delta^2(\omega-\nu)]^{-1/2}\,d\nu=\mathrm{Im}\,\Delta(\omega) -\frac{\mathrm{Im}\,\Delta(\omega)}{\omega}\int_{\Delta_0}^{\infty} d\nu\,\mathrm{Re}\frac{\nu}{[\nu^2-\Delta^2(\nu)]^{1/2}} \times\int d\omega_q\,g(\omega_q)\left(\frac{1}{\nu+\omega_q+\omega}-\frac{1}{\nu+\omega_q-\omega}\right),$$

or in operator form

$$\hat{A}g=\hat{B}+\hat{C}g. \tag{4}$$

If we use piecewise-linear interpolation for $g(\omega)$ then the integral operator $\hat{A}$ is represented by a lower triangular matrix with a leading diagonal, for which the triangular inverse matrix $\hat{A}^{-1}$ can be calculated rapidly and very accurately. Multiplying (4) by $\hat{A}^{-1}$, we obtain a linear integral equation of the second kind:

$$g=\hat{A}^{-1}\hat{B}+\hat{A}^{-1}\hat{C}g. \tag{5}$$

Using the identity

$$\int_{\Delta_0}^{\infty}\frac{\nu\,d\nu}{(\nu^2-\Delta_0^2)^{1/2}(\nu^2-\omega^2)}\equiv 0 \text{ for } \omega\neq\Delta_0,$$

we rewrite (2) in the form

$$\mathrm{Im}\frac{1}{[\omega^2-\Delta^2(\omega)]^{1/2}}=\frac{2}{\pi}\int_{\Delta_0}^{\infty}\frac{N_\tau(\nu)-N_{\mathrm{BCS}}(\nu)}{\omega^2-\nu^2}\,d\nu, \tag{6}$$

where $N_{\mathrm{BCS}}(\nu)=\nu/(\nu^2-\Delta_0^2)^{1/2}$ is the density of the electronic BCS states. It is seen from (6) that an important role in the determination of $\Delta(\omega)$ is played not by $N_T(\omega)$ but by the deviation of $N_T(\omega)$ from $N_{\mathrm{BCS}}(\omega)$.

Thus, the problem of reconstructing $g(\omega)$ from $N_T(\omega)$ reduces to a calculation of the integral (6) and to the solution of the linear integral equation (5), and a unique solution is obtained, something not obvious when the procedure proposed in[7] is used.

A program for the determination of $g(\omega)$ can be easily written for a medium-class computer (Minsk-22, Minsk-32, M-220), and is easy to reach a calculation accuracy not worse than obtained in experiment. The calculation of $g(\omega)$ for Pb and $Pb_{90}Bi_{10}$, using the tabulated data for $N_T(\omega)$ from[10], have shown good agreement with the results of[10]–see Fig. 2. Figure 3 shows $g(\omega)$ for the Bi-Tl alloy investigated in our laboratory[11][3)].

3. 1) An integral equation for $g(\omega)$ was obtained from the imaginary part of $\varphi(\omega)=\Delta(\omega)Z(\omega)$. It does not include the cutoff potential $\omega_c(\omega_c\sim 5\omega_p)$ or the Coulomb pseudopotential μ^*. When $g(\omega)$ is reconstructed from $N_T(\omega)$, the Coulomb interaction is therefore taken into account not in the static approximation as in (1), but

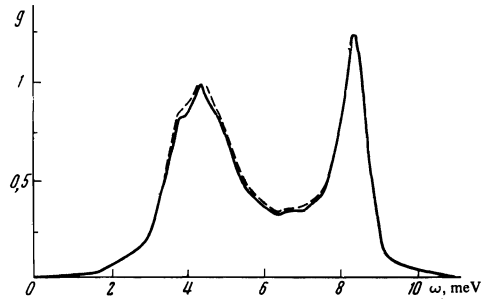

FIG. 2. Comparison of $g(\omega)$ of lead, reconstructed by the method of [7] (dashed line), with that obtained form Eq. (5) (solid line).

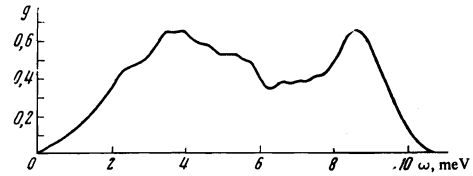

FIG. 3. The function $g(\omega)$ for the alloy $Bi_{65}Tl_{35}$.

in the long-wave approximation, when the slight contribution of the imaginary part of the Coulomb interaction to $\mathrm{Im}\varphi(\omega)$ can be neglected at frequencies much lower than the plasma frequency. The value of μ^* needed for applications, if $g(\omega)$ is known and ω_c is specified, is determined from the equation

$$\Delta_0 Z(\Delta_0)=\mathrm{Re}\,\varphi(\Delta_0).$$

2) From the value of $g(\omega)$ we can determine, with high accuracy, the most important parameters of a metal in the superconducting state, such as the critical temperature T_c, the temperature dependence of the energy gap, the critical magnetic field, the temperature dependence of the Josephson current, the energy of the low-temperature interaction, etc.[1]. The renormalization coefficient

$$Z_n=1+2\int_0^{\infty}\frac{g(\omega)}{\omega}d\omega$$

for metals in the normal state determines the change of the effective mass of the density of states and of the electron velocity near the Fermi surface[2].

3) Using $g(\omega)$, and especially its derivative, we can not only find the positions of some of the Van Hove singularities, but also determine their type, something difficult to do if only the dependence of d^2I/dE^2 on U is known[12].

When the position and type of several of the critical points of $g(\omega)$ are known, then it is possible in principle to reconstruct the phonon spectrum $\omega=\omega(k)$ of the investigated material, but this question is beyond the scope of the present article.

4) The dispersion relation (2) is generalized to the case when it is important to take into account the temperature T:

$$\mathrm{Im}\frac{1}{[\omega^2-\Delta^2(\omega,T)]^{1/2}}=\frac{2}{\pi}\int_0^{\infty}N_\tau(\nu,T)\frac{d\nu}{\omega^2-\nu^2}. \tag{7}$$

If the tunnel density of states at a finite temperature $N_T(\nu, T)$ is determined, then from (7) and from the equation

$$\mathrm{Re}\,\Delta(\Delta_0(T),T)=\Delta_0(T)$$

we obtain the value of $\Delta_0(T)$, which should coincide within reasonable limits with the experimentally observed gap. We thus obtain a criterion with which to check whe-

ther the tunnel characteristics have been correctly plotted.

5) In the derivation of Eq. (2) we used rather general analytic properties of $\Delta(\omega)$ and $g(\omega)$, properties possessed not only by the electron-phonon interaction. Generally speaking, the tunnel density of states $N_T(\omega)$, and consequently also $\Delta(\omega)$ and $g(\omega)$, contain contributions of all the interactions of the electron, both in the investigated metal and inside the tunnel barrier. This imposes "stringent" requirements on the tunnel experiment and on the interpretation of the results.

The effect exerted on $N_T(\omega)$ by the passage of the electron in the interior of the barrier can be neglected if magnetic impurities that lead to the so called "zero-point" anomalies[1] are not present in the "tunnel." The action of the magnetic impurities and of a number of other factors, which perhaps are still unknown to us, can be excluded by a careful renormalization of the tunnel conductivity $\sigma(U) = (dI/dU)_S/(dI/dU)_n$[1]. The quantitative tunnel information concerning $\Delta(\omega)$ and $g(\omega)$ can be trusted only when $\sigma(0) \sim 10^{-3}$ [1]. For junctions of the S_1-I-S_2 type, there should be distinctly observed a region of negative resistance at

$$\Delta_0^{(1)}-\Delta_0^{(2)}<U<\Delta_0^{(1)}+\Delta_0^{(2)}.$$

If the tunnel junction, the measurement, and the reduction of the tunnel characteristics are all in accord with these requirements, then a quantitative analysis carried out on the basis of the obtained value of $g(\omega)$ yields indeed information on the electron-phonon interaction, or points to the existence of other interaction mechanisms. This question calls for special theoretical and experimental investigations. One can hope that objective and detailed data on the experimental situation and on the details of the calculation of the tunnel curves will contribute to further progress in research on the superconducting and normal states of solids.

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APPENDIX

From among all the continuous bounded functions $g(\omega)$, we are interested only in the function for which the solution of the system (1) is continuous and bounded, with the equation

$$\omega=\Delta(\omega)$$

having at $\omega > 0$ a single root $\omega = \Delta_0$. In this case we have

$$g(0)=0 \qquad (A.1)$$

and it follows from the system (1)[4] that an analytic continuation of the function $\Delta(\omega)$ into the complex z plane yields a function $\Delta(z)$ that is analytic in the domain D (Fig. 1) with cuts $(-\infty, -\Delta_0)$ and $(\Delta_0, +\infty)$, with

$$\Delta(z^*)=\Delta^*(z), \quad \Delta(-z)=\Delta(z). \qquad (A.2)$$

We shall show that the function

$$\eta(z)=z^2-\Delta^2(z) \qquad (A.3)$$

has no roots in the domain D.

According to the statements made above, $\eta(\omega)$ has only two roots on the real axis, at the points $\omega = \pm\Delta_0$ which do not belong to the contour L. Using (8.1) and Eq. (1), we can show that on circles with sufficiently small radius ρ, we have the function $\eta(\rho e^{i\varphi})$ has no roots. On semicircles with radius R, at $R \gg \omega_c$,

$$|\Delta(z)| \ll R, \qquad (A.4)$$

i.e., $\eta(z)$ has no roots. We can thus always choose ρ and R such that the function $\eta(z)$ has no roots on the contour L. According to the well known Cauchy theorem the number of roots of $\eta(z)$ inside the contour L is equal to the change of the argument of $\eta(z)$ after tracing the contour L, divided by 2π. Let us examine the change of the argument of $\eta(z)$ on going along the contour L as $R \to \infty$ and $\rho \to 0$:

$$\Delta \arg \eta(z)\big|_{\substack{R\to\infty\\ \rho\to 0}} = \Delta \arg \eta(\operatorname{Im} z=0) + \Delta \arg \eta(Re^{i\varphi}) + \Delta \arg \eta(z=\Delta_0+\rho e^{i\varphi}) + \Delta \arg \eta(z=\rho e^{i\varphi}-\Delta_0) = 0+4\pi-2\pi-2\pi=0. \qquad (A.5)$$

Thus, $\eta(z)$ has no roots inside the contour L as $\rho \to 0$ and $R \to \infty$, meaning that $\eta(z)$ has no roots in the entire domain D.

The continuous function $\eta(\omega)$ has a single root Δ_0 at $\omega > 0$ and $\lim[|\Delta(\omega)|/\omega] = 0$ at $\omega \to \infty$, from which it follows that $\operatorname{Re} \Delta(\omega) \equiv \Delta(\omega) < \omega$ for $|\omega| < \Delta_0$, i.e., the function

$$\Phi(\omega)=\frac{i}{\eta^{1/2}(\omega)}=\frac{i}{[\omega^2-\Delta^2(\omega)]^{1/2}} \qquad (A.6)$$

is real on the real axis at $|\omega| < \Delta_0$.

We continue $\Phi(\omega)$ analytically into the complex z plane through the segment $(-\Delta_0, \Delta_0)$ on the real axis. We obtain a function $\phi(z)$ that is analytic in the domain D, with

$$\Phi(z)=\Phi(-z), \quad \lim|\Phi(z)|=0 \text{ as } |z|\to\infty \qquad (A.7)$$

and from the Schwartz symmetry principle it follows that

$$\Phi(z^*)=\Phi^*(z). \qquad (A.8)$$

[1)] At the real accuracy ~1 % with which Δ_0 is determined, the changes in μ^* can reach ~40% [9].

[2)] Usually $\omega_T \sim 5\omega_D$ and is so chosen that the conductivities in the normal and superconducting states are practically the same following a displacement on a barrier equal to ω_T.

[3)] At the first All-Union Conference on High-Pressure Physics and Technology [11], results were also reported on the effect of pressure on the function $g(\omega)$ obtained for the alloys Bi-Tl, Pb-In, and Pb-Bi by the method proposed here.

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