TUNNELING BETWEEN SUPERCONDUCTORS*

Vinay Ambegaokar and Alexis Baratoff†
Department of Physics and Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York
(Received 22 April 1963)

In a recent note, Josephson[1] has predicted some new effects in the tunneling characteristics of a system of two superconductors separated by an oxide layer. The effects are an oscillating supercurrent of frequency $2eV/h$ (where V is the applied voltage), and a possible dc supercurrent at zero voltage.[2] In this Letter we reproduce and somewhat generalize Josephson's calculation by another method, the method of the thermodynamic Green's functions, which brings out the assumptions that are made and is sufficiently general to apply to superconductors with strong electron-phonon coupling. In addition, we show that in the model of Bardeen, Cooper, and Schrieffer a simple prediction for the temperature dependence of the dc supercurrent follows from the theory. This prediction should, of course, be experimentally tested.

From our point of view, Josephson's effects occur because the amplitudes for condensed pair formation and disruption (Gor'kov's F functions), which are nonlocally dependent on the energy gap, may overlap in the oxide layer even though the gap is essentially zero there. A key assumption in Josephson's calculation is that the F functions in the representation of the single-particle states of the semi-infinite metals on either side have the same form as those for the bulk superconductor in the representation of plane waves. A similar assumption is customarily made for quasi-particle tunneling and is experimentally verified. The approximation for the F functions seems reasonable to us, provided that the barrier is considerably thinner than the superconducting coherence length.

Our starting point is the Hamiltonian[3-5]

$$H = H_l + H_r + V, \tag{1}$$

where H_l and H_r are the many-body Hamiltonians for the superconductors on the left and right and V is the term that couples them, namely,

$$V = \sum_{k,q,\alpha} (T_{kq} c_{k\alpha}{}^{+} d_{q\alpha} + T_{kq}{}^{*} d_{q\alpha}{}^{+} c_{k\alpha}). \tag{2}$$

Here $c_{k\alpha}$ and $d_{q\alpha}$ are annihilation operators for single-particle states on the left and right, α is the spin index, and the explicit form of the matrix elements T_{kq} between states of approximately equal energy is[3]

$$T_{kq} = \hbar \int \{(\hbar/2mi)[\varphi_k{}^{*}(\vec{x}) \partial \chi_q(\vec{x})/\partial z - \chi_q(\vec{x}) \partial \varphi_k{}^{*}(\vec{x})/\partial z] - (e/mc) A_z \varphi_k{}^{*} \chi_q\}_{z=z_0} dx dy. \tag{3}$$

Above $\varphi_k(\vec{x})$ and $\chi_q(\vec{x})$ are the wave functions for the states with quantum numbers k and q, the z axis is normal to the barrier, z_0 lies in the barrier, and A is the self-consistent vector potential. The use of the Hamiltonian (1) in first-order perturbation-theory calculations has been recently justified by Prange.[5]

The number operator for electrons on the left is given by

$$N_l = \sum_{k\alpha} c_{k\alpha}{}^{+} c_{k\alpha}. \tag{4}$$

As in the treatment of reference 4, we use the equation of motion for this operator to compute the rate of change of its expectation value:

$$i\langle \dot{N}_l \rangle = \langle [N_l, H] \rangle = 2i \operatorname{Im} \sum_{kq\alpha} T_{kq} \langle c_{k\alpha}{}^{+} d_{q\alpha} \rangle. \tag{5}$$

The expectation value in (5) is in the grand ensemble describing the two superconductors with, however, different chemical potentials on the two sides. In the first order of perturbation theory, one has

$$\langle c_{k\alpha}{}^{+} d_{q\alpha} \rangle = -i \int_{-\infty}^{t} d\bar{t} \langle [c_{k\alpha}{}^{+}(t) d_{q\alpha}(t), V(\bar{t})] \rangle, \tag{6}$$

where the operators on the right are in the interaction representation. The usual tunneling current is obtained by making a Hartree-Fock factorization of the contribution to (6) of the second term of (2). Josephson's effects come from the first term of (2) and reflect the macroscopic occupation of ground-pair states in both superconductors. For this term one has to calculate the expectation value of the operator $c_k{}^{+} d_q c_{k'}{}^{+} d_{q'}$. This operator has no diagonal matrix element between states with definite numbers of particles on the left and right. However, in the limit of zero voltage there is a highly degenerate set of states with the same total number of electrons N but differing numbers of ground-state pairs on the left and right, and a

diagonal matrix element exists between phase-coherent superpositions of these states.[1,6] For finite voltages, Josephson apparently assumes that the same coherent superposition of states can be achieved during the tunneling process, but questions of stability appear to us to remain open in this case. The coherent superpositions of states may be chosen to have the property[6]

$$P_l P_r^{+} |N, \alpha\rangle = e^{-i\alpha} |N, \alpha\rangle, \tag{7}$$

where P_l and P_r^{+} annihilate and create ground-state pairs. The tunneling rate may now be written in terms of the single-particle Green's function G and the Gor'kov amplitudes F and $\bar{F}$. Anticipating that the magnetic field will be confined to the barrier region, we may assume these quantities to be diagonal in the representation of Eq. (3). They are defined according to

$$G_{\alpha\beta}(k;t,t') = -iT\langle c_{k\alpha}(t) c_{k\beta}^{+}(t')\rangle,$$

$$F_{\alpha\beta}(k;t,t') = T\langle P_r^{+} c_{k\alpha}(t) c_{k\alpha}(t')\rangle,$$

$$\bar{F}_{\alpha\beta}(k;t,t') = T\langle P_r c_{-k\alpha}(t) c_{k\beta}(t')\rangle, \tag{8}$$

where T is Wick's time-ordering operator. On substituting (2) in (5), making the appropriate factorizations, and doing the spin sums as in Gor'kov's first paper,[7] one finds

$$\langle \dot{N}_l \rangle = -2\,\mathrm{Re} \sum_{kq\alpha} \int_{-\infty}^{t} d\bar{t} \{ e^{i\alpha} T_{kq} T_{-k-q} [\bar{F}^{>}(k;t,\bar{t}) F^{<}(q;\bar{t},t) - \bar{F}^{<}(k;t,\bar{t}) F^{>}(q;\bar{t},t)]$$

$$+ T_{kq} T_{kq}^{*} [G^{<}(k;\bar{t}-t) G^{>}(q;t-\bar{t}) - G^{>}(k;\bar{t}-t) G^{<}(q;t-\bar{t})] \}. \tag{9}$$

The factors that occur in (9) are not time-ordered products; the superscripts indicate the order of the field operators. To exhibit the structure of (9), it is convenient to introduce the spectral functions[8] for G, F, and $\bar{F}$. For the single-particle Green's function, the spectral function A is given by the relation

$$G^{\gtrless}(q,\omega) = \mp i A(q,\omega) f^{\pm}(\omega), \tag{10}$$

where

$$f^{\pm}(\omega) = \{\exp[\mp\beta(\omega-\mu)] + 1\}^{-1}, \tag{11}$$

β being $(kT)^{-1}$ and μ the chemical potential. For F and $\bar{F}$, we may write

$$F(q;t,t') = e^{-2i\mu t'} \Phi(q;t-t'), \tag{12}$$

with

$$\Phi^{\gtrless}(q,\omega) = \mp i B(q,\omega) f^{\pm}(\omega) \tag{13}$$

and

$$\bar{F}(q;t,t') = e^{2i\mu t} \bar{\Phi}(q;t-t'), \tag{14}$$

with

$$\bar{\Phi}^{\gtrless}(q,\omega) = \mp i \bar{B}(q,\omega) f^{\pm}(\omega). \tag{15}$$

Introducing these spectral forms, one obtains

$$\langle \dot{N}_l \rangle = 2\,\mathrm{Im} \sum_{kq\alpha} \int_{-\infty}^{\infty} \frac{d\omega d\omega'}{(2\pi)^2} [f_l^{-}(\omega) - f_r^{-}(\omega')]$$

$$\times \left\{ |T_{kq}|^2 \frac{A(k,\omega) A(q,\omega')}{\omega - \omega' + i\eta} + e^{i\alpha} T_{kq} T_{-k-q} \exp[2i(\mu_l - \mu_r)t] \frac{\bar{B}(k,\omega) B(q,\omega')}{\omega - \omega' - i\eta} \right\}. \tag{16}$$

If the metals on both sides are in the normal state or if only one is superconducting, the second term in the square bracket is not present. In Eq. (16) no assumption about the strength of the electron-phonon interaction has been made. In particular, for strongly coupled superconductors the spectral functions will not be sharply peaked. The usual quasi-particle tunneling current[3,4] is obtained by using for the normal metal the bulk form

$$A(k,\omega) = 2\pi\delta(\omega - \epsilon_k - \mu), \tag{17}$$

and for the superconductor the form corresponding to the Bardeen-Cooper-Schrieffer theory

$$A(k,\omega) = \pi[(1 + \epsilon_k/E_k)\delta(\omega - E_k - \mu) + (1 - \epsilon_k/E_k)\delta(\omega + E_k - \mu)], \tag{18}$$

where $E_k = (\epsilon_k^2 + \Delta^2)^{1/2}$, and Δ is the gap.

Making the same bulk approximation for the anomalous terms, one has

$$B(q,\omega) = -(\pi i \Delta/E_q)[\delta(\omega - \mu - E_q) - \delta(\omega - \mu + E_q)], \tag{19}$$

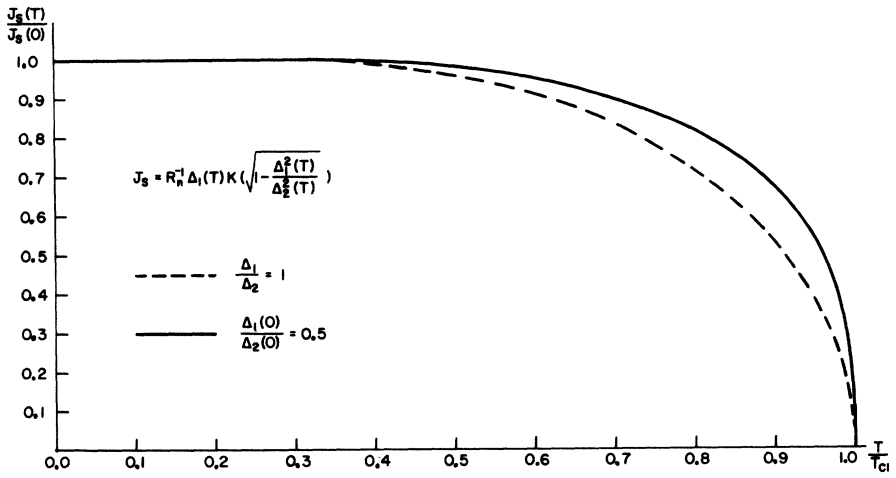

FIG. 1. Reduced dc Josephson current versus reduced temperature. T_{c1} is the smaller of the two critical temperatures. The dashed line applies to the case of equal energy gaps; the temperature dependence reduces to that of the gap alone. The solid line corresponds to $\Delta_1(0)/\Delta_2(0) = 0.5$, and applies approximately to a Sn-Pb sandwich. The BCS temperature dependence of the gap is assumed in both cases. Barring other complications from the strong electron-phonon coupling in lead, such an approximation is good for Al-Pb or Sn-Pb sandwiches since the gap of lead varies little over the interesting temperature range.

and

$$\overline{B}(q,\omega) = (\Delta^*/\Delta)B(q,\omega). \tag{20}$$

With these substitutions, (15) reduces to the form given by Josephson and shows his effects. In particular, the zero-voltage current is seen to be

$$e\langle\dot{N}_l\rangle = \sin(\alpha+\alpha')\Bigg\{4e\sum_{kq\alpha}|T_{kq}T_{-k-q}\Delta_l^*\Delta_r|/4E_qE_k \times P\left[\frac{f^-(E_q)-f^-(E_k)}{E_q-E_k}+\frac{f^+(E_q)-f^-(E_k)}{E_q+E_k}\right]\Bigg\},$$

$$\equiv J_S\sin(\alpha+\alpha'). \tag{21}$$

Above, α' is the argument of the quantities whose absolute value is indicated. Note that (21) is explicitly gauge invariant. The relative phase $(\alpha+\alpha')$ is strongly dependent on the transverse dimensions of the junction[6] and on the external magnetic field.[1,2]

Assuming specular transmission, integrating over k_x, k_y, q_x, q_y, and neglecting the energy dependence of T_{kq} (as is experimentally justified), one finds

$$J_S = \frac{e\overline{T}\Delta_1\Delta_2}{\pi^2\hbar}P\int_0^\infty\frac{d\epsilon_1}{E_1}\int_0^\infty\frac{d\epsilon_2}{E_2}\left[\frac{1}{E_1+E_2}+\frac{2E_1f^-(E_2)}{E_2^2-E_1^2}+\frac{2E_2f^-(E_1)}{E_1^2-E_2^2}\right]. \tag{22}$$

The last two terms give no contribution to the principal value integral and the first may be evaluated in terms of the complete elliptic integral of the first kind. Then, noting that the normal state resistance R_n is given by $2\pi h/e^2\overline{T}$, one finds the simple formula

$$J_S = R_n^{-1}\Delta_1(T)K([1-\Delta_1^2(T)/\Delta_2^2(T)]^{1/2}), \tag{23}$$

where Δ_1 (in eV) is the smaller of the two energy gaps. Since $K(0) = \frac{1}{2}\pi$, one has the result that when Δ is the same on both sides, J_S is the current that flows in the normal state at an applied voltage of $\frac{1}{2}\pi\Delta$.[9] The equivalent voltage for differing superconductors may be easily calculated from (23). J_S is an upper limit for the maximum supercurrent. Equation (23) is plotted in reduced form in Fig. 1, using the BCS temperature dependence of the gap.[10] The solid line applies approximately to a tin-lead sandwich.

Finally, it may be worth mentioning that the electronic contribution to the free energy from the overlap of pair functions may be easily calculated from the well-known formula

$$\Delta F = \int_0^1(d\lambda/\lambda)\langle\lambda V\rangle, \tag{24}$$

where λ is an explicit coupling constant. In the first order of perturbation theory, one obtains

$$\Delta F = -(\hbar/2e)J_S\cos(\alpha+\alpha'). \tag{25}$$

This is the generalization to finite temperatures of the binding energy.[2,6]

It is a pleasure to thank Dr. P. W. Anderson and Professor J. R. Schrieffer for discussions. We are also grateful to Professor J. Bardeen and Mr. B. D. Josephson for an educational correspondence, and to Professor R. A. Ferrell and Professor R. E. Prange for copies of their work in advance of publication.

*Work supported in part by the U. S. Office of Naval Research and by the Advanced Research Projects Agency.

†National Science Foundation Predoctoral Fellow.

[1]B. D. Josephson, Phys. Letters 1, 251 (1962).

[2]The probable observation of the dc effect has been recently reported by P. W. Anderson and J. M. Rowell, Phys. Rev. Letters 10, 230 (1963).

[3]J. Bardeen, Phys. Rev. Letters 6, 57 (1961); 9, 147 (1962).

[4]M. H. Cohen, L. M. Falicov, and J. C. Phillips, Phys. Rev. Letters 8, 316 (1962); Proceedings of the Eighth International Conference on Low-Temperature Physics, London, 1962 (Butterworths Scientific Publications, Ltd., London, 1962), p. 163.

[5]R. E. Prange (to be published).

[6]R. A. Ferrell and R. E. Prange (to be published).

[7]L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. 34, 735 (1958) [translation: Soviet Phys. - JETP 7, 505 (1958)].

[8]P. C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959).

[9]B. D. Josephson[1] gave the equivalent voltage as $2\pi\Delta$, but has independently arrived at the correct value quoted in the text (private communication).

[10]B. Muhlschlegel, Z. Physik 155, 313 (1959).

MAGNETIC SCATTERING OF NEUTRONS BY NONCOLLINEAR SPIN DENSITIES*

M. Blume
Physics Department, Brookhaven National Laboratory, Upton, New York
(Received 1 May 1963)

In the Heitler-London model of a ferromagnet, one associates with each magnetic ion a spin density which points in the direction of the over-all magnetization. This spin density points in the same direction in all parts of the ion. It is entirely possible, however, for a spin density in a ferromagnet to be such that the integral of the density over a unit cell points in the direction of the net magnetization, while the density in different regions of the cell is not collinear with the net magnetization. Such a density might occur in an anisotropic metallic ferromagnet, such as hexagonal cobalt, or in an antiferromagnetic or spiral spin structure. In addition, Overhauser's spin-density-wave[1] theory of metallic magnetism can lead to a density of this form.

It is the purpose of this Letter to point out that it is possible, using neutron scattering techniques, to distinguish noncollinear spin densities from the common variety, and to indicate the simple generalizations of the theory of neutron scattering which are necessary to account for these phenomena. For clarity, we will consider a ferromagnet with one atom per unit cell, but the expressions are easily generalized to more complicated spin structures. We will also consider magnetization densities which arise predominantly from electronic spins, so that orbital scattering can be neglected. To a first approximation the inclusion of orbital effects will not change our results, but taking full account of orbital moments and anisotropic orbital scattering would complicate the discussion unnecessarily.[2] Accordingly, we may fix our attention on ferromagnetic cobalt or, with a slight generalization, on antiferromagnetic chromium. The results of the theory may be summarized most easily by pointing out that all of the usual formulas for magnetic scattering[3] are still valid on introduction of a noncollinear density, provided that the unit vector which defines the direction of the magnetization is in the new expressions replaced by a unit vector whose direction varies as a function of the scattering vector $\vec{K}$.

To derive these results we consider first the cross section for elastic magnetic scattering of an unpolarized beam of slow neutrons[3]:

$$\frac{d\sigma}{d\Omega'}=\left(\frac{\gamma e^2}{mc^2}\right)^2 |\langle q|\sum_i \exp(i\vec{K}\cdot\vec{r}_i)\hat{K}\times(\vec{s}_i\times\hat{K})|q\rangle|^2. \quad (1)$$

Here $\gamma=-1.91$ is the gyromagnetic ratio of the neutron, and m, $\vec{r}_i$, and $\vec{s}_i$ are, respectively, the mass, position, and spin of the ith electron in the solid. The summation is over all electrons in the solid, and the matrix element is taken in the ground state $|q\rangle$ of the ferromagnet. $\vec{K}=\vec{k}-\vec{k}'$ is the difference between the initial and final wave vector of the neutron, and $\hat{K}$ is a unit vector in the direction of $\vec{K}$. Writing out the matrix element