Tunneling-Hamiltonian method in the theory of the Josephson effect

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The temperature dependence of the critical Josephson current at an atomically sharp tunnel junction between two superconductors is quite different from that in the ordinary theory of a 3D tunneling Hamiltonian. The cases which come closest to that described in this letter are high T_c superconductors with a quasi-2D structure and a short coherence length. © *1995 American Institute of Physics.*

The tunneling-Hamiltonian method developed in Refs. 1 and 2 is used to calculate the tunneling current between two weakly coupled superconductors. In this method, an interface between the two superconductors is not explicitly introduced. The states in the "left" and "right" superconductors are assumed to be classified in the same way as in unbounded bulk systems. In this letter we wish to demonstrate that incorporating the interface explicitly in the case of an atomically sharp tunnel junction can lead to a substantial change in the temperature dependence of the critical current for a superconductor with a short coherence length. The atomically sharp interface cannot be taken into account by a semiclassical method. A convenient approach starts from the tight-binding method and is widely used in calculations of the tunneling properties of surfaces in scanning tunneling microscopy.

The tunneling coupling in the method of Refs. 1 and 2 is described by the Hamiltonian

$$H_T=\sum_{\mathbf{p},\mathbf{q},\sigma}[T_{\mathbf{p},\mathbf{q}}c^+_{L\mathbf{p}\sigma}c_{R\mathbf{q}\sigma}+\text{H.a.}], \tag{1}$$

where $T_{\mathbf{p},\mathbf{q}}$ is the tunneling matrix element, and $c^+_{L,R\mathbf{p},\mathbf{q}\sigma}$ are creation operators in the left (L) and right (R) superconductors.

In second-order perturbation theory in $T_{\mathbf{p},\mathbf{q}}$, the expression for the tunneling current reduces to[1–3]

$$I_c=4\pi eT\sum_{\omega_n,\mathbf{p},\mathbf{q},\sigma}|T_{\mathbf{p},\mathbf{q}}|^2\,\text{Im}\{F^+_L(\omega_n,\mathbf{p})F_R(\omega_n,\mathbf{q})\}, \tag{2}$$

where $F_{L,R}(\omega_n,\mathbf{p},\mathbf{q})$ are the Gor'kov Green's functions, and $\omega_n=\pi(2n+1)$ is the Matsubara frequency. Furthermore, if $T_{\mathbf{p},\mathbf{q}}$ depends only weakly on $\mathbf{p}$ and $\mathbf{q}$ (tunneling occurs from all states $L\mathbf{p}$ to all $R\mathbf{q}$, with identical amplitudes), the integration of $\mathbf{p}$ and $\mathbf{q}$ can be carried out independently. The result is the known expression[3]

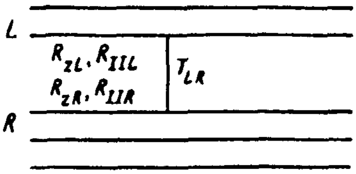

FIG. 1.

$$I_c=\frac{\pi}{eR_N}\sum_{\omega_n}\frac{\Delta_L\Delta_R}{\sqrt{\omega_n^2+\Delta_L^2}\sqrt{\omega_n^2+\Delta_R^2}}.$$

Under the condition $\Delta_R=\Delta_R=\Delta$ this expression reduces to

$$I_c=\frac{\pi\Delta}{2eR_N}\tanh\left(\frac{\Delta}{2T}\right), \tag{3}$$

where R_N is the resistance of the normal junction. We assume for definiteness that the superconducting order parameter is the same in the L and R systems.

We consider a planar, atomically sharp interface between two superconductors (Fig. 1). In calculating the tunneling current, it is convenient to start with a Hamiltonian in the coordinate representation:

$$H_T=\sum_{\mathbf{R}_L,\mathbf{R}_{R,\sigma}}[T_{\mathbf{R}_L\mathbf{R}_R}c^+_{\mathbf{R}_{L\sigma}}c_{\mathbf{R}_{R\sigma}}+\text{ H.a.}], \tag{4}$$

where $T_{\mathbf{R}_L\mathbf{R}_R}$ is the amplitude for a transition from a site $\mathbf{R}_L$ in the left system to site $\mathbf{R}_R$ in the right system (Fig. 1). From this point on, the method for calculating the tunneling current is essentially the same as for ballistic perpendicular transport in semiconductor superlattices. In second order, the expression for the tunneling current is

$$I_c=4\pi eT\sum_{\omega_n,\mathbf{R}_L,\mathbf{R}_R,\mathbf{R}'_L,\mathbf{R}'_{R,\sigma}}\text{Im}\{T_{\mathbf{R}_R\mathbf{R}_L}F^+_{\mathbf{R}_L\mathbf{R}'_L}(\omega_n)T_{\mathbf{R}'_L\mathbf{R}'_R}F_{\mathbf{R}'_R\mathbf{R}_R}(\omega_n)\}, \tag{5}$$

where $F_{\mathbf{R}_L\mathbf{R}'_L}(\omega_n)$ and $F_{\mathbf{R}'_R\mathbf{R}_R}(\omega_n)$ are Gor'kov Green's functions for the L and R half-spaces, calculated for the case in which there is no interaction between these half-spaces. Expression (5) requires knowledge of $F_{\mathbf{R}_L\mathbf{R}'_L}(\omega_n)$ for a half-space; we accordingly need to be specific about the geometry of the surface and the band structure. We can make some further simplifications by assuming that tunneling occurs only from the outermost plane in the L system to the outermost plane in the R system. In this case, expression (5) can be put in the form

$$I_c=4\pi eT\sum_{\omega_n,\mathbf{k}_\parallel}|T_{LR}(\mathbf{k}_\parallel)|^2\text{Im}\{F^+_L(\omega_n,\mathbf{k}_\parallel)F_R(\omega_n,\mathbf{k}_\parallel)\}, \tag{6}$$

where

$$F_L^+(\omega_n,\mathbf{k}_\parallel)=\sum_{\mathbf{R}_{L\parallel},\mathbf{R}'_{L\parallel}} F(\omega_n,\mathbf{R}_{zL},\mathbf{R}_{L\parallel};\mathbf{R}_{zL'},\mathbf{R}'_{L\parallel})\exp\{i(\mathbf{R}_{L\parallel}-\mathbf{R}'_{L\parallel})\},$$

where $R_{zL,zR}$ are the z coordinates of the outermost L and R planes, respectively. We then find

$$T_{LR}(\mathbf{k}_\parallel)=\sum_{\mathbf{R}_{L\parallel}\mathbf{R}_{R\parallel}} T_{\mathbf{R}_L\mathbf{R}_R}\exp\{i(\mathbf{R}_{R\parallel}-\mathbf{R}_{L\parallel})\}.$$

By virtue of translational invariance we can always take Fourier transformations in a plane. The physical meaning here is that the parallel component of the quasimomentum along the surface is conserved in tunneling across the boundary. If the tunneling does not occur exclusively from the outermost layer, in contrast, then the transition amplitudes $F(\omega_n,\mathbf{R}_{zL},\mathbf{R}_{L\parallel};R'_{zL},\mathbf{R}'_{L\parallel})$ which couple different points R_{zL} and R'_{zL}, with $\mathbf{k}_\parallel$ conserved, will appear in Eq. (6). If the coherence length is short, nondiagonal transition amplitudes of this sort should also be small.

The function $T_{LR}(\mathbf{k}_\parallel)$ depends weakly on $\mathbf{k}_\parallel$. The reason is that $T_{\mathbf{R}_L\mathbf{R}_R}$ is a sharp function of $\mathbf{R}_L-\mathbf{R}_R$. The tunneling matrix element falls off at least exponentially as the points $\mathbf{R}_L$ and $\mathbf{R}_R$ undergo a relative shift (with fixed R_{zL} and R_{zR}). It is the sharp decrease in the tunneling matrix element which makes it possible to observe the atomic relief on atomically clean surfaces in scanning tunneling microscopy.

As a limiting case we assume $T_{\mathbf{R}_L\mathbf{R}_R}=T_{LR}\delta(\mathbf{R}_L-\mathbf{R}_R)$. In this case, the tunneling occurs between points in the outmost planes, which are beside each other. In this limit $T_{\mathbf{R}_L\mathbf{R}_R}$ is independent of $\mathbf{k}_\parallel$, and the expression for the current becomes

$$I_c=4\pi eT|T_{LR}|^2\sum_{\mathbf{k}_\parallel,\omega_n}\mathrm{Im}\{F_L^+(\omega_n,\mathbf{k}_\parallel)F_R(\omega_n,\mathbf{k}_\parallel)\}. \qquad (7)$$

The difference between expressions (7) and (2) is that the momentum $\mathbf{k}_\parallel$ is common to the Green's functions of the L and R systems, in which the momenta $\mathbf{p}$ and $\mathbf{q}$ are "decoupled," and a tunneling occurs from all $\mathbf{p}$ states to all $\mathbf{q}$ states. In the case at hand, the parallel component of the quasimomentum is conserved in the tunneling. The effect should be to reduce the phase volume and the critical current.

To calculate the temperature dependence $I_c(T)$ and the superconducting Green's function $F(\omega_n,\mathbf{k}_\parallel)$, we use the approximation of a cylindrical Fermi surface. This approximation is not a supplement to the preceding one; it is a consequence of the circumstance that the tunneling occurs from only the outermost planes. For s-wave superconducting pairing we have

$$F_{L,R}(\omega_n,\mathbf{k}_\parallel)=\frac{\Delta_{L,R}}{\omega_n^2+\xi_{\mathbf{k}_\parallel}^2+\Delta_{L,R}^2}, \qquad (8)$$

where $\xi_{\mathbf{k}_\parallel}$ is the energy of the electrons with respect to the Fermi level. For the current we have

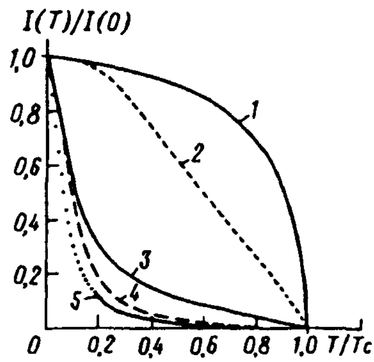

FIG. 2.

$$I_c=4\pi e N_{\parallel}^2|T_{LR}|^2 T\sum_{\omega_n}\frac{\Delta_L\Delta_R}{\sqrt{\omega_n^2+\Delta_L^2}\sqrt{\omega_n^2+\Delta_R^2}(\sqrt{\omega_n^2+\Delta_L^2}+\sqrt{\omega_n^2+\Delta_R^2})}.$$

With $\Delta_L=\Delta_R=\Delta$ we find

$$I_c=2\pi e N_{\parallel}^2|T_{LR}|^2\Delta^2 T\sum_{\omega_n}\frac{1}{(\omega_n^2+\Delta^2)^{3/2}},\tag{9}$$

where $N_{\parallel}$ is the partial density of states at the outermost layer at the Fermi level. For simplicity we have assumed $\Delta_L=\Delta_R=\Delta$. For $d_{x^2-y^2}$ pairing, we use the Green's function in the form

$$F_{L,R}(\omega_n,\mathbf{k}_{\parallel})=\frac{\Delta_{L,R}(\hat{\mathbf{k}}_x^2-\hat{\mathbf{k}}_y^2)}{\omega_n^2+\xi_{\mathbf{k}_{\parallel}}^2+\Delta_{L,R}^2(\hat{\mathbf{k}}_x^2-\hat{\mathbf{k}}_y^2)^2},\tag{10}$$

where $\hat{\mathbf{k}}_x$ and $\hat{\mathbf{k}}_y$ are unit vectors.

Figure 2 shows the temperature dependence of the critical current. Curve 1 shows the dependence $\Delta(T)$, for which we used the standard approximation $\Delta(T)=\Delta_0\tanh(1.74\sqrt{T_c/T-1})$; this approximation gives a good description of the temperature dependence of the exact BCS solution. Curves 2 and 3 show the behavior of the critical current for s- and d-wave pairing, respectively, for standard tunneling theory. Curves 4 and 5 show the corresponding behavior for s- and d-wave pairing in our own case. It follows from a comparison of these curves that the temperature dependence of the critical Josephson current in the 2D case is considerably sharper. This sharp decay is actually due to the decrease in the phase volume during tunneling.

In reality, tunneling occurs from several closest planes. The actual experimental situation is something between the two cases described above. The cases which are closest to the situation described above are apparently high-T_c superconductors, which have a layered (quasi-2D) structure and a short coherence length.

In a recent paper,[4] the discrepancy between the temperature dependence of the critical Josephson current seen experimentally[5] and the standard theory was interpreted on the basis of a mixed $s+id$ pairing. The circumstance described above may be one more (and no less important) cause of the sharp decay of the critical current with the temperature that is observed.

In summary, for an atomically sharp tunneling interface and for a well-expressed layered (quasi-2D) structure, the temperature dependence of the critical current is considerably sharper. The standard 3D theory of tunneling works well for superconductors with an isotropic band structure, a large coherence length, and a smooth boundary.

The dependence of the Josephson tunneling current on the atomic structure of the tunneling junction described here is not surprising. A dependence of this sort, for the normal tunneling current, has been known in the physics of surfaces and in scanning tunneling microscopy (indeed, the very method is based on this dependence), where it is possible to produce controllable, atomically sharp interfaces in ultrahigh vacuum by molecular beam epitaxy.

In the case of an atomically sharp boundary, the change in the superconducting order parameter itself at the interface may be important. This question requires a separate study.

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