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The boundary effect in d-wave superconductors

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Abstract. We present a theory for the surface effect in d-wave superconductors. The quasiparticles in a superconductor occupying a half-space are described by the Bogoliubov–de Gennes equation. The asymptotic forms of the wave functions of the quasiparticles at large distances from the surface are discussed. This is the basic problem in solving the equation. We also review our recent results on the {100}- and {110}-surface effects in d-wave superconductors.

It is considered that the high-T_c superconductors are tight-binding systems [1]. The wave packet of each electron is confined to the space of a few atoms. Near the surface of such a superconductor, the wave functions of the electrons should be strongly deformed from that in the interior. In a junction between the high-T_c superconductors, the tunnelling probability of the particles depends on their wave functions near the surface. It is therefore reasonable that there should be remarkable interface effects in the phenomena of tunnelling in high-T_c superconductors.

Since the wave functions of electrons are confined to small regions, the short-range Coulomb repulsion between electrons should be very strong. Thereby, electron pairing on the same atom (corresponding to the s-wave component) should be substantially suppressed. It is acceptable that the predominant pairing component in high-T_c superconductors should have d-wave symmetry.

In high-T_c superconductors, the current carriers are considered to move in the copper–oxygen planes since the coupling between different layers is quite weak. For theoretical study, one usually uses a two-dimensional tight-binding model to describe the system [2]. The quasiparticles in an inhomogeneous superconductor are described by the Bogoliubov–de Gennes (BdG) equation [3]. A major task of theoretical study is to solve the BdG equation. We will discuss some basic problems encountered in solving the BdG equation. This is helpful for studying surface effects for more general cases. In addition, we will also review our recent results concerning the {100}- and {110}-surface effects [4, 5].

For simplicity, we consider here a semi-infinite square lattice with a straight boundary. Along the direction parallel to the boundary, the wave functions of the quasiparticles can be expanded in terms of plane waves. The unknown parts depend only on the coordinate in the normal direction. Therefore, the surface problems can be reduced to one-dimensional ones. In the present case, the BdG equation (defined for the one-dimensional chain) reads

$$\sum_j H_{ij}\psi(j) = E\psi(i) \tag{1}$$

where H_{ij} (a 2×2 matrix) is the Hamiltonian, $\psi(j)$ (a two-component spinor) is the wave function of the quasiparticles at coordinate j in the direction normal to the surface, and E is the corresponding eigen-energy.

To solve equation (1), one should know the asymptotic behaviours of the wave functions at large distances from the surface. Generally, there are two kinds of state: the bound states whose wave functions are confined to a region near the surface, and the free states in which the quasiparticles can move through the whole system. In the interior, since the system is homogeneous, the wave function of a free quasiparticle would approach to the plane wave. However, each energy level is degenerate. The energy of the free particles is a function of k_x and k_y, which are respectively the components of the momenta normal to and parallel to the boundary. As a simple example, one may consider the system with a {100} surface [4]. For given k_y, the plane waves of momenta k_x and $-k_x$ have the same energy $E(-k_x) = E(k_x)$. Even at lower energy levels, we have $E(q_x) = E(k_x)$, but $q_x \neq \pm k_x$. For the case of a tilted boundary, the degeneracy is more complicated. Therefore, at large distances, the wave function of any free quasiparticle should be a linear superposition of those degenerate plane waves. To analyse the superposition, we need to recognize the outgoing and incoming waves. They are distinguished by the sign of their group velocities, $v(k_x) = \mathrm{d}E(k_x)/\mathrm{d}k_x$. The outgoing and incoming waves have positive and negative group velocities, respectively. For the sake of description, we will use the subscripts $\alpha, \beta, \ldots$ to denote the incoming waves and $\mu, \nu, \ldots$ to denote the outgoing waves. An incoming wave after reflection by the surface can generate all of the components of the outgoing waves. Thus, an eigenfunction with an incoming wave of momentum k_α behaves as follows:

$$\psi_\alpha(j) \to \frac{\mathrm{i}}{\sqrt{2}}\left[\phi_\alpha(j) - \sum_\mu S_{\alpha\mu}\phi_\mu(j)\right] \qquad \text{as } j \to \infty \tag{2}$$

where $\mathrm{i}^2 = -1$, the ϕs (the wave functions of the plane waves) are the solutions to the homogeneous system, and the coefficient $S_{\alpha\mu}$ represents the amplitude of the outgoing wave of momentum k_μ. Note that, at an eigen-energy, the number of incoming waves is the same as that of the outgoing waves. Therefore, all of the $S_{\alpha\mu}$ compose a square matrix. It is unitary, as required by the particle-conservation law [6]. We put the factor $1/\sqrt{2}$ in equation (2) only for convenience—to ensure that the wave functions ψ_α and the ϕs satisfy the same normalization condition:

$$\sum_j \psi_\alpha^\dagger(j)\psi_\beta(j) = \delta_{\alpha\beta}\delta(E_\alpha - E_\beta). \tag{3}$$

In some special cases, the system is invariant under time reversal; the Hamiltonian H_{ij} is real. We can thereby obtain the symmetric matrix S by appropriately ordering the ϕ_α and ϕ_μ, and we can write it as

$$S = T'T \tag{4}$$

where T is a unitary matrix, and T' is the transverse of T. The eigenfunctions can be taken as $f(j) = T^*\psi(j)$ (with T^* the complex conjugate of T):

$$f(j) \to \frac{\mathrm{i}}{\sqrt{2}}[T^*\phi_{\mathrm{in}}(j) - T\phi_{\mathrm{out}}(j)] \qquad \text{as } j \to \infty \tag{5}$$

where $\phi_{\mathrm{in}}(j)$ and $\phi_{\mathrm{out}}(j)$ are incoming and outgoing wave functions, respectively, and we have denoted them in vector form: $\phi_{\mathrm{in}}^\dagger(j) = [\phi_\alpha^\dagger(j), \phi_\beta^\dagger(j), \ldots]$, etc. Fortunately, the validity of equation (4) corresponds to $\phi_{\mathrm{in}}^*(j) = \phi_{\mathrm{out}}(j)$. Thus we have a real function $f(j)$:

$$f(j) \to \sqrt{2}\,\mathrm{Im}[T\phi_{\mathrm{out}}(j)] \qquad \text{as } j \to \infty. \tag{6}$$

For the square lattice with a boundary corresponding to the surface {100} or {110}, the degeneracy is 2 or 4 depending on the energy. Thereby, T is a constant or a 2×2 unitary matrix. For the former case, the outgoing wave k_μ is degenerate with the incoming wave $k_\alpha = -k_\mu$; we have

$$T = \mathrm{e}^{\mathrm{i}\theta_\mu}$$

where θ_μ is the phase-shift [7]. For the latter case, two outgoing waves k_μ and k_ν with $k_\mu \neq k_\nu$ are degenerate with two incoming waves $k_\alpha = -k_\mu$ and $k_\beta = -k_\nu$; the matrix T is given by

$$T = \begin{pmatrix} a\mathrm{e}^{\mathrm{i}\theta_\mu} & -b\mathrm{e}^{\mathrm{i}\theta_\nu} \\ b^*\mathrm{e}^{\mathrm{i}\theta_\mu} & a\mathrm{e}^{\mathrm{i}\theta_\nu} \end{pmatrix}$$

where a is real, $b = |b|\mathrm{e}^{\mathrm{i}\theta}$ with $a^2 + |b|^2 = 1$. The phase θ reflects the effect of mixing of two outgoing waves; if $\theta = 0$, there exists a real matrix R such that RT is diagonal, so then the wave functions can be transformed to the same form as for the former case. Generally, under the influence of the surface effect, the mixing phase θ does not vanish. Note that all of the parameters a, b, and θ depend on the energy E. With the above analysis, one can get explicit expressions for the asymptotic wave functions as given in references [4] and [5].

Due to the surface effect, the density of states of the free quasiparticles is changed from that for the homogeneous system. In some cases, the total number of free states decreases. There must be bound surface states. Since all of the states compose a set that is a complete basis, their total number is the same as that of the homogeneous system. According to Levinson's theorem [6], the number N_b of bound surface states can be calculated from the S-matrix:

$$N_b = [\eta(E_{min}) - \eta(E_{max})]/\pi$$
$$\eta(E) = \frac{1}{2\mathrm{i}} \ln[\det(S)]$$

where $\eta(E)$ is the eigen-phase-shift.

Having the boundary conditions, one can then solve the BdG equation. Since the Hamiltonian H_{ij} contains the order parameters which are in turn determined from the solution to the BdG equation itself, we usually use the iteration method.

Recently, we have investigated the {100}- and {110}-surface effects in d-wave superconductors [4, 5]. The BdG equation has been solved self-consistently. For the {100} surface [4], two obvious features of the order parameters has been found.

(1) The pairing parameters of both x- and y-directions oscillate near the surface. This seems like the Friedel oscillation. The length scale of such an inhomogeneity is about ten lattice constants.

(2) Accompanying the oscillation, the d-wave symmetry is altered near the surface. At the surface, the y-direction pairing is suppressed to 60% of the bulk value, while the x-direction pairing is enhanced by 10%.

We have also studied the a-axis Josephson tunnelling between high-T_c superconductors [4]. With a model of tunnelling between the nearest-neighbour sites on the two interfaces, we calculated the temperature dependence of the Josephson critical current $J(T)$. The tunnelling current depends on the values of the wave functions at the surfaces. Since the functions are of standing waves, their magnitudes at the surface are substantially different from those of the plane waves. It is shown that our theoretical study is in very good agreement with the experiments [8–10]. Throughout the whole superconducting region, $0 < T/T_c < 1$, the experimental results for $J(T)/J(0)$ are well represented by the present theory. The present result is also indistinguishable from our earlier ones [11]. In the earlier calculation, we took the order parameters as constants even near the boundary. The BdG equation was then solved exactly; the wave functions are the analytic sine functions. At the boundary, as compared with those of the plane waves, the amplitudes of these standing waves are suppressed in the ranges $|k_x| < \pi/4$ and $3\pi/4 < |k_x| < \pi$, while they are enhanced for k_x in the rest of the range $(-\pi, \pi)$. The fact that two calculations give results that are almost the same implies that the main characteristic of the surface effect on the tunnelling in the weakly linked junctions can be captured by the simple sine functions. Even if it is based on the same tunnelling assumption, however, the prediction using plane-wave functions is explicitly different from the present one, but seems like the conventional BCS result. Obviously, the surface and thereby the interface effects are very much critical in the phenomena of tunnelling between high-T_c superconductors.

In the system with a {110} surface, Hu has predicted that there exist midgap states bound to the surface [12]. Since their density of states is sizable, these states contribute a peak to the tunnelling conductance at zero bias voltage between a normal conductor and a d-wave superconductor with the {110} interface. This prediction has been proved by experiments [13]. Besides the midgap states, we have also found from our theory that there can appear a number of surface states with non-zero energies [5]. The appearance of these states is related to the suppression of the order parameter near the surface [14]. The amplitudes of the order parameters for the a- and b-directions are the same, but are considerably suppressed in a region of length $\sim$70 lattice constants from the surface. In contrast to those of the midgap states, their energies disperse with the momentum parallel to the surface. So, these non-zero-energy bound surface states cannot result in peaks in the density of states as sharp as those for the midgap states. However, an enhancement in the tunnelling conductance at non-zero bias voltages (less than the pairing potential) can be expected in the junction with a {110} interface of the high-T_c superconductor.

Due to the anisotropic pairing, the surface properties of the high-T_c superconductors may depend sensitively on the surface orientation. It is therefore necessary to further investigate the general surface problems.

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