Tunneling and Superconductivity of Strongly Repulsive Electrons

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We show that superconductive pairing is possible in the presence of an arbitrarily strong short-range repulsion between electrons if the gap is an odd function of $k-k_F$. We discuss how the behavior of $\Delta(k-k_F)$ close to the Fermi surface is related to (i) the low-energy tunneling density of states, and (ii) the attractive part of the potential. We show that some features of the tunneling data in high-T_c cuprates, including the fact that the maximum hardly moves when T approaches T_c, are natural consequences of this type of pairing.

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In the BCS theory of superconductivity [1], pairing is due to an attractive potential between electrons. Although the interaction does not have to be attractive for all wave vectors, it is often assumed that the effective interaction close to the Fermi surface has to be attractive at least in some region of the phase space in order to get pairing. According to this argument, the only way to get superconductivity for strongly repulsive electrons is to generate an attractive interaction that dominates the repulsion in some part of the phase space. A number of such scenarios have been put forward in the context of high-T_c cuprates.

In this paper, our first aim is to show that this argument is wrong, and that pairing is possible even if the repulsive part of the potential is arbitrarily strong. To avoid unnecessary complications, we concentrate on a weak-coupling theory, in which case the gap function $\Delta(\mathbf{k},\omega)$ depends only on $\mathbf{k}$, and we furthermore assume that $\Delta(\mathbf{k})$ is a function of $\epsilon_\mathbf{k}$ only, where $\epsilon_\mathbf{k}$ is the quasiparticle energy measured from the Fermi level. For free electrons, this means that the gap is isotropic.

At $T=0$, the gap function is found by solving the equation

$$\Delta(\epsilon)=-N(0)\int_{-\omega_c}^{\omega_c} d\epsilon' V(\epsilon,\epsilon')\frac{\Delta(\epsilon')}{2[\epsilon'^2+\Delta(\epsilon')^2]^{1/2}}, \qquad (1)$$

where, as usual, the density of states $N(\epsilon)$ is assumed not to vary significantly within ω_c of the Fermi level.

We start by studying a toy model where $V(\epsilon,\epsilon')=V_1(\epsilon,\epsilon')+V_2(\epsilon,\epsilon')$ is the sum of a repulsion and an attraction defined by

$$V_1(\epsilon,\epsilon')=\begin{cases}U>0 \text{ if } |\epsilon|,|\epsilon'|<\omega_1,\\ 0 \text{ otherwise,}\end{cases} \qquad (2)$$

$$V_2(\epsilon,\epsilon')=\begin{cases}-V<0 \text{ if } |\epsilon|,|\epsilon'|<\omega_2' \text{ and } |\epsilon-\epsilon'|<\omega_2,\\ 0 \text{ otherwise.}\end{cases} \qquad (3)$$

In what follows we take $\omega_2'=\omega_2$ for simplicity and we look for even and odd solutions for $\Delta(\epsilon)$. The BCS type of solution is even, and we start with this case. The gap equation can then be written ($\epsilon>0$)

$$\Delta_e(\epsilon)=-UN(0)\int_0^{\omega_1} d\epsilon'\frac{\Delta_e(\epsilon')}{[\epsilon'^2+\Delta_e(\epsilon')^2]^{1/2}}+VN(0)\int_0^{\omega_2} d\epsilon'[v_2(\epsilon,\epsilon')+v_2(\epsilon,-\epsilon')]\frac{\Delta_e(\epsilon')}{[\epsilon'^2+\Delta_e(\epsilon')^2]^{1/2}}, \qquad (4)$$

where $v_2(\epsilon,\epsilon')=-V_2(\epsilon,\epsilon')/V$ is positive and of order 1. A quick inspection of the signs tells us that the $V=0$ equation has only $\Delta_e(\epsilon)=0$ as a solution, while the $U=0$ equation has a nonvanishing solution. So, increasing U at fixed V, we expect to reduce the gap, until U reaches a critical value U_c where the only solution is $\Delta_e(\epsilon)=0$. This is effectively confirmed by a numerical analysis of Eq. (4). So, pairing of even symmetry is possible only if the repulsion is not too strong.

In the odd case, the situation is quite different. The repulsive part of the potential is even in ϵ' and drops from the equation. With the simple choice of V_2 of Eq. (3), the resulting equation can be solved analytically and has a nonvanishing solution when $VN(0)>2$:

$$\Delta_0(\epsilon)=\begin{cases}\epsilon\{[VN(0)/2]^2-1\}^{1/2} \text{ if } |\epsilon|<\omega_2,\\ 0 \text{ otherwise.}\end{cases} \qquad (5)$$

This solution is lower in energy than $\Delta=0$, with a condensation energy

$$W(\Delta_0)-W(\Delta=0)=-\omega_2^2\left(\frac{1}{VN(0)}+\frac{VN(0)}{4}-1\right). \qquad (6)$$

Let us emphasize that this result is independent of U, so that there is actually pairing for arbitrarily strong repulsion. In particular, for $\omega_1 \geq \omega_2$ and $U > V$, there is pairing although the interaction is everywhere repulsive. An odd gap does not care about the absolute value of the interaction, it is sensitive only to its variation. If particle-hole symmetry is present in the normal state, it is broken by an odd gap. However, the quasiparticle energy remains particle-hole symmetric; only Josephson tunneling can reveal the fact that the gap is odd around the Fermi surface. More generally, odd pairing can be expected to occur when (i) $V_1(\epsilon,\epsilon')$ is large, so that even pairing is impossible; (ii) $V_1(\epsilon,-\epsilon')\simeq V_1(\epsilon,\epsilon')$, so that the repulsion cannot reduce $\Delta_0(\epsilon)$ significantly; (iii) $V_2(\epsilon,-\epsilon')\neq V_2(\epsilon,\epsilon')$, so that the attraction is effective in building up $\Delta_0(\epsilon)$. The first two conditions are met by a strong local repulsion, as in the large-U Hubbard model, while the third one is not very restrictive. Attractions via exchange of bosons typically yield

$$V_2(\epsilon,\epsilon') \propto \frac{1}{(\epsilon-\epsilon')^2-\omega^2}\,, \tag{7}$$

which indeed fulfills the third condition. "Extended s-wave" pairing [2] on a square lattice with nearest-neighbor hopping is an example of odd pairing when there is one electron per site [3]. The type of odd gap we are considering is to be distinguished from the odd-in-frequency gap discussed by Berezinskii [4] and, more recently, by Allen [5].

High-T_c cuprates have been proposed as candidates for this new type of pairing, most recently by Anderson [6]. To go beyond the hypothesis, we start by looking at a physical property that is very sensitive to the details of the gap function, namely, the tunneling density of states $N_T(E)$. When Δ depends on ϵ, $N_T(E)$ is given by [7]

$$N_T(E)\equiv\frac{\rho(E)}{N(0)}=\frac{E}{\epsilon+\Delta(\epsilon)d\Delta(\epsilon)/d\epsilon}\,, \tag{8}$$

where $E=[\epsilon^2+\Delta(\epsilon)^2]^{1/2}$. From Eq. (8), it is clear that if $\Delta(\epsilon)\propto \operatorname{sgn}\epsilon|\epsilon|^\alpha$, then $N_T(E)\propto|E|^{-1+1/\alpha}$. Hence, a natural consequence of odd pairing is that there is no well-defined gap in tunneling [8]: If $\alpha=1$ (toy model), one has gapless superconductivity [$N_T(E)=2/VN(0)$ for $E<\omega_2VN(0)/2$, and 1 otherwise]; if $\alpha<1$, the density of states increases from $N_T(E)=0$ at $E=0$. Experimentally, there is evidence that the tunneling density of states of high-T_c cuprates vanishes only for $E=0$ (at $T=0$). While this part of the data is consistent with odd pairing, this fact alone does not provide strong evidence in its favor. It is well known that any gap function with zeros on the Fermi surface will have the same effect. Odd pairing is a special case where the gap function vanishes everywhere on the Fermi surface. An alternative explanation of the nonvanishing tunneling density of states has been proposed by Kirtley and Scalapino [9].

There is, however, another particular feature of the tunneling density of states in high-T_c cuprates, namely, the fact that the maximum hardly moves when the temperature approaches T_c. In regular BCS, the gap $\Delta(T)$ vanishes at T_c, and the maximum of the tunneling density of states, which occurs for $E_0=\Delta(T)$, moves to the Fermi level as $T\to T_c$. If $\Delta(\mathbf{k};T)$ vanishes on part of the Fermi surface, the peak occurs for $E_0=\max_{k=k_F}\Delta(\mathbf{k};T)$ and, as in the regular BCS case, moves to the Fermi level as $T\to T_c$. This is why we have not considered this type of gap function (e.g., d wave) for which the repulsion drops from the gap equation for symmetry reasons. To our knowledge, the only explanation so far has been proposed by Allen and Rainer within a conventional strong-coupling approach [10].

Let us see what kind of T dependence one gets with odd pairing. As the gap vanishes everywhere on the Fermi surface, the maximum in $N_T(E)$ can no longer occur for $E_0=\max_{k=k_F}\Delta(k)$ because this quantity vanishes. In fact, if the gap reaches its maximum value Δ_0 for an energy ϵ_0, it is easy to see that the maximum in $N_T(E)$ occurs for $E_0\simeq(\epsilon_0^2+\Delta_0^2)^{1/2}$. If the gap builds up very fast, i.e., if $\epsilon_0\ll\Delta_0$, then one recovers the BCS result $E_0=\Delta_0$. On the other hand, if the energy at which the gap is maximum is much bigger than the gap itself, $E_0\simeq\epsilon_0$. But as $T\to T_c$, $\Delta\to 0$, and this condition is always satisfied, so that $E_0\simeq\epsilon_0$ does not go to zero with the gap. In principle, ϵ_0 is itself a function of T. But as we shall see in an example, the main effect of temperature is to reduce the overall magnitude of the gap function, while its shape, and in particular the energy ϵ_0 where Δ is maximum, is essentially unaffected [11].

To illustrate this point, we need to solve the T-dependent gap equation,

$$\Delta(\epsilon)=-N(0)\int_{-\omega_c}^{\omega_c}d\epsilon'\,V_2(\epsilon,\epsilon')\frac{\Delta(\epsilon')}{2[\epsilon'^2+\Delta(\epsilon')^2]^{1/2}}\times\tanh\frac{[\epsilon'^2+\Delta(\epsilon')^2]^{1/2}}{2T}\,, \tag{9}$$

for a given potential $V_2(\epsilon,\epsilon')$. As we do not want to study the gapless case, we cannot use the potential of Eq. (3), but first have to find a form of the interaction that yields a power law $\Delta(\epsilon)\propto\operatorname{sgn}\epsilon|\epsilon|^\alpha$, $\alpha<1$. Since $V_2(\epsilon,\epsilon')$ is a function of two variables, there are infinitely many solutions, and further constraints are needed to determine the interaction completely. The ultimate goal is to find a microscopic model that produces such an interaction, but this difficult problem is beyond the scope of the present analysis. In fact, for our purpose, which is to illustrate the T dependence of $N_T(E)$, the precise form of $V_2(\epsilon,\epsilon')$ is unimportant. A model potential that is simple and not too singular would be sufficient [12]. Guided by the type of attraction that arises from exchange of bosons, we look for solutions $V_2(\epsilon,\epsilon')$ that depend only on $|\epsilon-\epsilon'|$. The equation to be solved is again Eq. (1), but $\Delta(\epsilon)$ is now a given function with a power-law singularity at $\epsilon=0$, and $V(\epsilon-\epsilon')$ is the unknown. By extending the integration limits to infinity [with $\Delta(\epsilon)=0$ for $|\epsilon|>\omega_c$], this equation can be formally solved by Fourier transform. This is, however, numerically complex and analytically obscure, so we try to find a model potential to use in Eq. (9) which gives the desired *low-energy* behavior of $\Delta(\epsilon)$. If $\alpha<1$, then, for small ϵ, $[\epsilon^2+\Delta(\epsilon)^2]^{1/2}\simeq|\Delta(\epsilon)|$, and Eq. (1) becomes

$$\Delta(\epsilon)=-N(0)\int_{-\omega_c}^{\omega_c}d\epsilon' V(\epsilon-\epsilon')\mathrm{sgn}\epsilon'/2 \tag{10}$$

and yields $V(\epsilon-\epsilon')=-(d\Delta/d\epsilon)(\epsilon-\epsilon')$ in the limit $\omega_c\to\infty$. This suggests that to get $\Delta(\epsilon)\propto\mathrm{sgn}\epsilon|\epsilon|^\alpha$, one could choose a potential $V(\epsilon-\epsilon')\propto-|\epsilon-\epsilon'|^{\alpha-1}$.

Now, we have to decide which power law we want to reproduce for $\Delta(\epsilon)$. This power law is reflected not only in the low-energy tunneling density of states, which, as we saw, is then given by $N_T(E)\propto|E|^{-1+1/\alpha}$, but also in the temperature dependence of the penetration depth, which can be shown [13] to follow the same power law $\lambda(T)\propto T^{-1+1/\alpha}$. In the case of high-$T_c$ cuprates, the experimental situation is not yet completely clear. For the tunneling data, some groups have reported a linear behavior [14], while others found a higher power law [15]. For the penetration depth, many groups have interpreted their data with an exponential behavior, although any power law $\lambda(T)\propto T^\beta$, $\beta\geq2$, cannot be excluded [16]. So we assume $\alpha=\frac{1}{3}$, which gives $N_T(E)\propto E^2$. Then we solve Eq. (9) with a model potential $V_2(\epsilon,\epsilon')$ defined by

$$V_2(\epsilon,\epsilon')=\begin{cases}-V(|\epsilon-\epsilon'|/\omega_c)^{-2/3} & \text{if } |\epsilon|,|\epsilon'|<\omega_c,\\ 0 & \text{otherwise.}\end{cases} \tag{11}$$

The solution of Eq. (9) was obtained by iteration in $\Delta(\epsilon)$. To enhance the precision for small ϵ, we discretized according to $\epsilon_n=\epsilon(n/N)^3$, where $N=500$ is the total number of points, and we checked that $\Delta(\epsilon)\propto\epsilon^{1/3}$ for small ϵ at $T=0$. The results for $\Delta(\epsilon)$ and $N_T(E)$ at various temperatures are plotted in Figs. 1 and 2 for $N(0)V=0.24$. The most remarkable feature is that, as we expected, the peak in the tunneling density of states hardly shifts when $T\to T_c$. In fact, for the model of Figs. 1 and 2, the peak does not move very much in the whole range of temperature, in agreement with tunneling data obtained on high-T_c cuprates. This is due to the fact that Δ_0 is already comparable to ϵ_0 at $T=0$.

Finally, another point that is worth discussing is the value of the ratio $2\Delta/kT_c$. The values quoted in many experimental papers are obtained by taking for Δ the position of the maximum in $N_T(E)$. The values obtained in this way are often much bigger than the weak-coupling BCS values ($2\Delta/kT_c\sim3.5$), and this is put forward as evidence that high-T_c cuprates are strong-coupling superconductors. In fact, within our weak-coupling model, the same procedure yields $2\Delta/kT_c\sim5$, a value typical of strong coupling. So, it is possible to get big values of this ratio even within weak coupling if the pairing is odd.

In summary, we have shown that within a weak-coupling approach superconductive pairing of odd symmetry can occur for arbitrarily strong short-range repulsions. We have shown that some of the features of the tunneling data in high-T_c cuprates can be accounted for within a weak-coupling approach using an odd gap func-

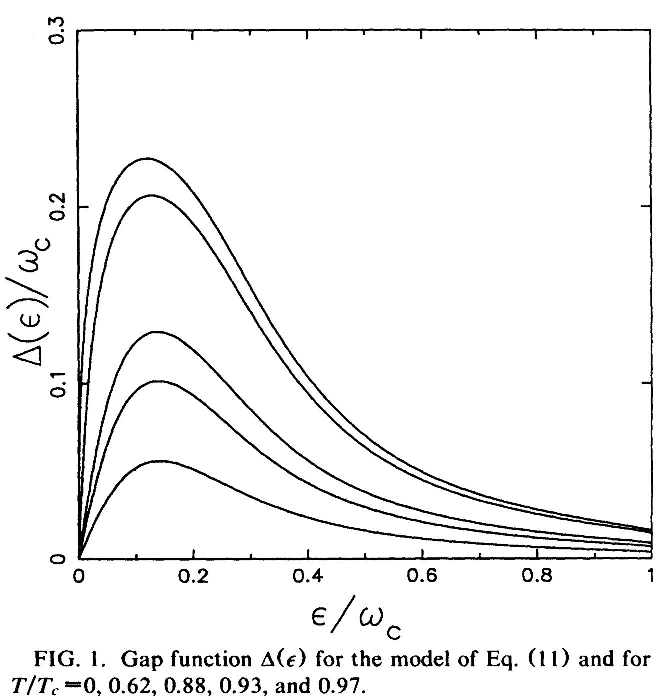

FIG. 1. Gap function $\Delta(\epsilon)$ for the model of Eq. (11) and for $T/T_c=0$, 0.62, 0.88, 0.93, and 0.97.

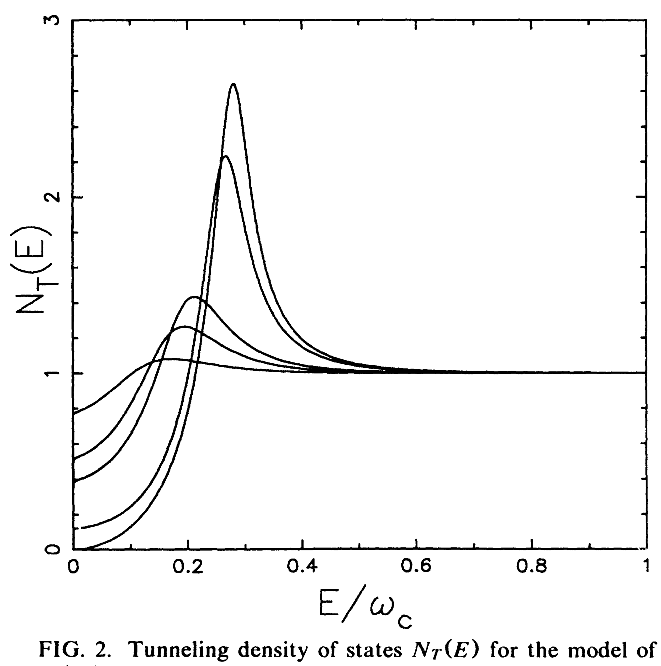

FIG. 2. Tunneling density of states $N_T(E)$ for the model of Eq. (11) and for $T/T_c=0$, 0.62, 0.88, 0.93, and 0.97. Note that for a direct comparison with experiments, a thermal broadening should be included.

tion $\Delta(k-k_F)$. More work is needed to propose realistic interactions leading to odd pairing and to analyze other properties within this context.

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