Quasiparticle Decay Effects in the Superconducting Density of States: Evidence for d-Wave Pairing in the Cuprates

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Recent tunneling and photoemission data on the cuprate oxide superconductors may provide important information in choosing between proposed models for the superconducting order parameter in these materials. We show that corrections to the weak coupling mean-field approximation for a superconductor lead to different frequency thresholds for the spontaneous decay of the Bogoliubov quasiparticles for different order parameter symmetries and that these effects may be seen in the superconductor-insulator-superconductor tunneling conductance. Comparison with the recent data indicates that a $d_{x^2-y^2}$, rather than an s-wave, order parameter is a likely candidate for describing the cuprates.

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One of the unresolved questions in the study of the cuprate oxide superconductors concerns the nature of the superconducting order parameter. However, recent experimental tunneling data [1–3] on a wide variety of the cuprates, combined with angle resolved photoemission (ARPES) measurements on $Bi_2Sr_2CaCu_2O_8$ [4,5], may provide key evidence in resolving this issue. The type of superconducting order parameter present in the cuprates has important implications, not only for the description of the superconducting state, but also for theoretical descriptions of the origin of the unusual normal-state properties of these materials. Two recent approaches in particular illustrate this point. The phenomenological marginal Fermi liquid (MFL) hypothesis [6] leads to an s-wave pairing state. The almost antiferromagnetic Fermi liquid (AFL) model of Pines and co-workers [7,8] and the spin bag model of Schrieffer and co-workers [9,10] predict a d-wave order parameter. Other contributions to this debate include an analysis of NMR measurements favoring a d-wave state [11–13], of Raman spectra [14], and of the magnetic field dependence of the supercurrent for a $d_{x^2-y^2}$ order parameter [15].

The recent analysis [3] of experimentally measured superconductor-insulator-superconductor (S-I-S) tunneling conductance, $g_{SIS}=dI/dV$, reveals a dip in the g_{SIS} curves at a voltage corresponding to 3 times the measured peak position in the tunneling conductance for a number of the cuprate superconductors with a wide range of critical temperatures. This is also the case with numerically generated g_{SIS} using measured tunneling conductances on superconducting–insulator–normal-metal (S-I-N) junctions, g_{SIN}. The analysis of Zasadzinski *et al.* [3] is the first to identify the feature in g_{SIS} with a superconductor energy scale. This result is visible in S-I-S tunnel junctions based on 2:2:0:1 BSCCO ($Bi_2Sr_2Cu_1O_6$) ($T_c=5.5$ K), $Nd_{2-x}Ce_xCuO_{4-y}$ ($T_c=23$ K), 2:2:1:2 BSCCO ($Bi_2Sr_2CaCu_2O_8$) ($T_c=86$ K), and $Tl_2Ba_2CaCuO_8$ ($T_c=1000$ K). The same feature has also been measured by other groups [1,2] and is reminiscent of a dip seen on the high-energy side of the usual superconducting spectral weight peak in ARPES [4,5]. In the latter experiments, whose counterpart in conventional tunneling experiments is g_{SIN}, a precise determination of the "gap" is limited by resolution problems. The important point to note, however, is that the dip is seen at approximately twice the peak position. A dip, or any feature, at a voltage corresponding to twice the peak in g_{SIN} will show up as a dip or feature at 3 times this peak voltage in the corresponding g_{SIS} curve. The exact position and magnitude of this dip may help to decide whether an s-wave or a d-wave order parameter is appropriate for describing superconductivity in the cuprates. Furthermore, the momentum dependence of such a feature, probed in an ARPES experiment, for example, could provide important clues to the nature of the scattering mechanisms in the cuprates, the physics of their normal state and their transition to superconductivity.

In our calculation the dip in g_{SIS} is a consequence of deviations from weak coupling mean-field behavior of the superconductivity in these materials. Deviations from the mean-field treatment of superconductivity are expected to be more important in two dimensions (2D) than in three dimensions. The cuprate superconductors are a good place to look for these effects given that the CuO planes are an important feature of these compounds. Here we argue that the dip seen in g_{SIS} is a consequence of these effects and that the value of the biasing across the junction at which it occurs points to the conclusion that the superconducting order parameter in the cuprates is a d wave.

One consequence of deviations from a weak coupling mean-field treatment of superconductivity is that the single-particle states are associated with deformations of the condensate [16–18]. We show how these deviations from mean field also lead to changes in the density of states for superconductors, as seen in $g_{SIS}(eV)$, arising from quasiparticle decay processes. These decay processes are characterized solely by the gap function $\Delta(\mathbf{k})$, and the quasiparticle excitation spectrum. Consequently they are a probe of the nature of the order parameter. These decay processes have previously been considered by Pethick and co-workers [19,20] in their calculations of the transport properties of the B phase of superfluid ^{3}He close to T_c.

The starting point of the present analysis is a Hamiltonian, Eq. (1), describing a system of fermions interacting via a potential U(q):

$$H=\sum_{\mathbf{k},\sigma}\xi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\sum_{\mathbf{k}',\mathbf{k},\mathbf{q}}U(\mathbf{q})c^{\dagger}_{\mathbf{k}-\mathbf{q},\uparrow}c^{\dagger}_{-\mathbf{k}'+\mathbf{q},\downarrow}c_{-\mathbf{k}',\downarrow}c_{\mathbf{k},\uparrow}\,, \quad (1)$$

where $\xi_{\mathbf{k}}=-2t[\cos(k_xa)+\cos(k_ya)]-\mu$, a is the lattice spacing, μ is the chemical potential, and t is the hopping matrix element. One assumes that the ground state of the system at low temperatures is superconducting, the nature of which depends on $U(\mathbf{q})$. $\Delta(\mathbf{k})$ and the quasiparticle operators, $\gamma^{\dagger}_{\mathbf{k}\sigma}$ and $\gamma_{\mathbf{k}\sigma}$, are determined by the weak coupling approximation for the gap equation and the Hamiltonian is written in terms of these operators. The Hamiltonian becomes

$$H=\sum_{\mathbf{k}\sigma}E_{\mathbf{k}}\gamma^{\dagger}_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}+\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\alpha,\beta}U(\mathbf{q})[H_A(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\alpha,\beta)\gamma^{\dagger}_{\mathbf{k}_1\alpha}\gamma^{\dagger}_{\mathbf{k}_2\beta}\gamma^{\dagger}_{-\mathbf{k}_3\beta}\gamma_{\mathbf{k}_4\alpha}+H_B(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\alpha,\beta)\gamma^{\dagger}_{\mathbf{k}_1\alpha}\gamma^{\dagger}_{\mathbf{k}_2\beta}\gamma^{\dagger}_{\mathbf{k}_3\beta}\gamma^{\dagger}_{\mathbf{k}_4\alpha}$$
$$+H_C(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\alpha,\beta)\gamma^{\dagger}_{\mathbf{k}_1\alpha}\gamma^{\dagger}_{\mathbf{k}_2\beta}\gamma_{\mathbf{k}_3\beta}\gamma_{\mathbf{k}_4\alpha}+\text{H.c.}]\,, \quad (2)$$

where $\mathbf{k}_1=\mathbf{k}-\mathbf{q}$, $\mathbf{k}_2=-\mathbf{k}'+\mathbf{q}$, $\mathbf{k}_3=-\mathbf{k}'$, and $\mathbf{k}_4=\mathbf{k}$. The form of the vertices H_A, H_B, and H_C are given in Ref. [18] and depend on the usual coherence factors, $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. The deviations from this mean-field approximation are calculated to second order in the interactions. The contributions to the self-energy, $\Sigma(\mathbf{k},\omega)$, of the $\gamma^{\dagger}_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}$ propagator are shown in Fig. 1.

In Ref. [18] $U(\mathbf{q})$ was taken to be an attractive contact interaction and the corresponding superconductor to be s wave. Here we compare this case with a repulsive $U(\mathbf{q})$ which is strongly peaked at $\mathbf{q}=(\pm\pi/a,\pm\pi/a)$. This leads to a d-wave superconductor in the weak coupling approximation. Our model for $U(\mathbf{q})$ is motivated by the suggestion that the short-ranged antiferromagnetic order in the doped cuprates is responsible for the high value of T_c in the cuprates [7–10]. Experimental studies of spin fluctuations in the doped cuprates, which become superconductors at low temperatures, show a peak in $\chi(q,\omega)$ at $\mathbf{Q}=(\pi/a,\pi/a)$ which is smeared out over a range of the order of the inverse of the magnetic correlation length ξ [21]. The latter is typically of the order of several lattice spacings. We have taken a simple model for $U(\mathbf{q})$,

$$U(\mathbf{q})=\frac{U_0}{1+\xi^2|\mathbf{q}-(\pm\pi/a,\pm\pi/a)|^2}\,. \quad (3)$$

For both s- and d-wave cases the largest contributions to $\Sigma(\mathbf{k},\omega)$ come from $\Sigma_A(\mathbf{k},\omega)$ and $\Sigma_B(\mathbf{k},\omega)$ in Fig. 1. In the s-wave case $\Sigma_A(\mathbf{k},\omega)$ and $\Sigma_B(\mathbf{k},-\omega)$ are real until $|\omega|\geq 3\Delta_0$ where spontaneous decay is possible. For the $d_{x^2-y^2}$ case, $\Delta(\mathbf{k})=\frac{1}{2}\Delta_0[\cos(k_x)-\cos(k_y)]$ has nodes and this results in a lower threshold for quasiparticle decay. Δ_0 is determined by solving the weak coupling gap equation using $U(\mathbf{q})$. In Fig. 2 we show the $\text{Im}\Sigma_A(\mathbf{k},\omega)$ for the s-wave case with a contact interaction, $U=-1.22$, and the d-wave case with $U_0=14.707$ and $\xi=1$ in Eq. (3), giving $\Delta_0=0.1$ when $\mu=0$ for both H_A and H_B vertices in Eq. (2). Both $\text{Im}\Sigma_A(\mathbf{k},\omega)$ and $\text{Im}\Sigma_B(\mathbf{k},-\omega)$ increase rapidly for $\omega\geq 2\Delta_0$ and go over to a linear dependence on ω. In a more complete treatment of the antiferromagnetic spin fluctuations, which are responsible for the d-wave superconductivity, this linear

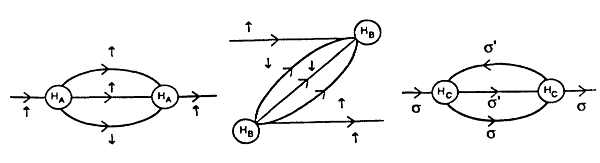

FIG. 1. Second-order contribution to the self-energy of the $\gamma^{\dagger}_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}$ propagator.

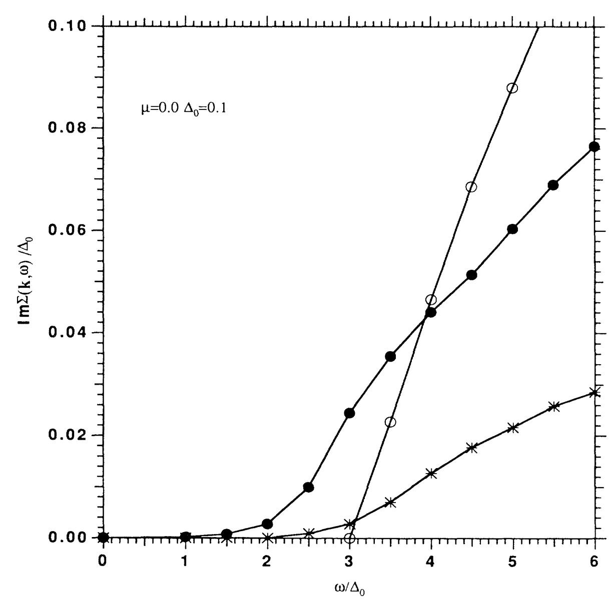

FIG. 2. $\text{Im}\Sigma_A(\mathbf{k},\omega)$ for the s wave at $\mathbf{k}=(k/\sqrt{2},k/\sqrt{2})$ (open circles) and for the d wave at $\mathbf{k}=(k/\sqrt{2},k/\sqrt{2})$ (solid circles) and at $\mathbf{k}=(k,0)$ (stars). $\mu=0$ and $\Delta_0=0.1$. In the s-wave case a contact interaction $\simeq -1.22$ was used and for the d-wave case $U(\mathbf{q})$ in Eq. (3) was used with $U_0\simeq 14.707$ and $\xi=1$.

dependence on ω is suppressed and $\text{Im}\Sigma_A(\mathbf{k},\omega)$ eventually falls as ω increases [8]. The magnitudes of $\text{Im}\Sigma_A(\mathbf{k},\omega)$ and $\text{Im}\Sigma_B(\mathbf{k},-\omega)$ with these parameters are $\sim 0.03\Delta_0$ at $\omega = 3\Delta_0$. This anisotropic dependence on $\mathbf{k}$ may also be reflected in ARPES [22]. The magnitude of $\text{Im}\Sigma(\mathbf{k},\omega)$ increases with increasing Δ_0. It also depends on μ and ξ. The more sharply peaked $U(\mathbf{q})$ is, the more $\text{Im}\Sigma(\mathbf{k},\omega)$ increases as $\mu \to 0$. For the value of ξ used here $\text{Im}\Sigma(\mathbf{k},\omega)$ has a sharper turn-on at $\omega \sim 2\Delta_0$ but the magnitude is practically unchanged as μ goes from 0 to -0.1. Comparing the results for the s-wave and d-wave cases, the microscopic calculations clearly show that spontaneous quasiparticle decay becomes appreciable at ω's smaller by $\sim\Delta_0$ in the d-wave case than in the s-wave case. $\Sigma_C(\mathbf{k},\omega)$ is negligible at low temperatures for both the s- and d-wave cases since it relies on the presence of thermal quasiparticles. Results for the extended s-wave order parameter $\Delta(\mathbf{k}) = \frac{1}{2}\Delta_0[\cos(k_x)+\cos(k_y)]$ show behavior that is very similar to the conventional isotropic s-wave case. We now show that the switching on of this decay channel may be seen in the tunneling conductance.

The current across an insulating barrier is given by [23]

$$I(eV) \propto \int_{-eV}^{0} d\omega\, N^R(\omega) N^L(\omega+eV)\,. \qquad (4)$$

$N^{(R,L)}(\omega)$ are the densities of states of the charge carriers on the left- and right-hand sides of the insulating barrier, which are determined by the imaginary part of the propagator $G(\mathbf{k},\omega) = \int dt\, e^{i\omega t}\langle 0|T[c^\dagger_{\mathbf{k}\sigma}(t), c_{\mathbf{k}\sigma}(0)]|0\rangle$. $c^\dagger_{\mathbf{k}\sigma}$ creates an electron in a plane wave state and $|0\rangle$ is the ground state on either side of the barrier. Rewriting $G(\mathbf{k},\omega)$ in terms of the $\gamma_{\mathbf{k}\sigma}$ propagators $N^L(\omega)$ contains the effect of the quasiparticle decay processes discussed above. For $\omega > 0$,

$$N^L(\omega) = \frac{1}{\pi}\sum_{\mathbf{k}} |\text{Im}G^L(\mathbf{k},\omega)| \simeq \frac{1}{2\pi}\sum_{\mathbf{k}} \frac{|\text{Im}\Sigma_A(\mathbf{k},\omega)|}{[\omega - E_{\mathbf{k}} - \text{Re}\Sigma_A(\mathbf{k},\omega)]^2 + [\text{Im}\Sigma_A(\mathbf{k},\omega)]^2}\,. \qquad (5)$$

The effects of spontaneous quasiparticle decay are more easily seen in $g_{\text{SIS}}(eV)$ curves than in $g_{\text{SIN}}(eV)$ curves. This is because two superconductor densities of states are convoluted with each other in $g_{\text{SIS}}(eV)$, whereas a superconducting and normal density of states are convoluted with each other in $g_{\text{SIN}}(eV)$. Examining Eq. (4) one sees that there is a big contribution to the current across the junction when $\omega = -\Delta_0$ and $\omega + eV = \Delta_0$, i.e., when the bias across the junction is $eV \simeq 2\Delta_0$. In the same way the effect of the decay processes can be seen in a d-wave superconductor when $\omega = -\Delta_0$ and $\omega + eV = 2\Delta_0$, the frequency at which the quasiparticle decay process starts to become appreciable in a d-wave superconductor. The calculated current is a monotonic function of eV with changes in slope at $eV = 2\Delta_0$ and at $eV = 3\Delta_0$ for a d-wave superconductor. Calculating $g_{\text{SIS}}(eV)$ picks out these values of eV at which the slope changes and it is the rapid increase in $\Sigma_A(\mathbf{k},\omega)$ at $\omega = 2\Delta_0$ which is responsible for the features at $eV = 3\Delta_0$. The corresponding value of eV for an s-wave superconductor is $\geq 4\Delta_0$.

In order to generate the g_{SIN} and g_{SIS} curves for a d-wave superconductor we introduce a phenomenological model in which $\text{Im}G(\mathbf{k},\omega)$ is replaced by a Lorentzian of the form

$$\text{Im}G(\mathbf{k},\omega) = \frac{1}{2\pi}\frac{\Gamma(\mathbf{k},\omega)}{(\omega - E_{\mathbf{k}})^2 + \Gamma(\mathbf{k},\omega)^2}\,, \qquad (6)$$

where $E_{\mathbf{k}}$ is a renormalized quasiparticle spectrum which has the same form as that given by the mean-field approximation but in which the parameters have been renormalized by the interactions. The qualitative features of the $\mathbf{k}$ and ω dependence of $\Gamma(\mathbf{k},\omega)$ are determined by our calculations of $\text{Im}\Sigma_A(\mathbf{k},\omega)$. Our model for $\Gamma(\mathbf{k},\omega)$, Eq. (7), has the rapid increase at $\omega \simeq 2\Delta_0$ and the anisotropy in $\mathbf{k}$ space seen in Fig. 2. These features are present for all parameters in the microscopic calculations and survive the effects of repeated scattering. We have

$$\Gamma(\mathbf{k},\omega) = \Gamma_0 + \frac{\Gamma_1}{2}\left[1 + \tanh\left(\frac{\omega - 2.5\Delta_0}{0.5\Delta_0}\right)\right] \times \left[1 - \frac{1}{2}\left(\frac{\Delta(\mathbf{k})}{\Delta_0}\right)^2\right]. \qquad (7)$$

Γ_0 and Γ_1 are taken to be free parameters. In Fig. 3 we compare $g_{\text{SIN}}(eV)$ and $g_{\text{SIS}}(eV)$ curves for the case where the frequency-dependent decay process is taken into account, $\Gamma_0 = 0.05\Delta_0$ and $\Gamma_1 = 0.5\Delta_0$ (full line), with the case where this frequency dependence is ignored, $\Gamma_0 = 0.05\Delta_0$ and $\Gamma_1 = 0$ (broken line). One sees that, as a consequence of the frequency-dependent damping due to the decay of Bogoliubov quasiparticles, there is a dip in $g_{\text{SIS}}(eV)$ for $3\Delta_0 \leq |eV| \leq 4\Delta_0$. This feature has been clearly identified in the experimental data by the work of Zasadzinski *et al.* [3]. This dip is completely missing from the $g_{\text{SIS}}(eV)$ where the frequency-dependent decay process is ignored (broken line). Looking at the $g_{\text{SIN}}(eV)$ curves (A) of Fig. 3, there is no strong feature and it would be difficult to identify the effect in experimental data. The assumption of an s-wave order parameter will always produce a dip in the g_{SIS} curves starting at $\geq 4\Delta_0$, which is not in agreement with the experimental data [3]. The size of Γ_1 in Fig. 3 is an order of magnitude larger than the size of $\text{Im}\Sigma(\mathbf{k},\omega)$ found in the microscopic calculations and so our microscopic calculations are used here only to motivate our phenomenological model for $\Gamma(\mathbf{k},\omega)$. The magnitude of $\text{Im}\Sigma(\mathbf{k},\omega)$ is enhanced by antiferromagnetic spin fluctuations which require going beyond second-order perturbation theory and allowing for repeated scattering through H_C [24].

In our calculation we have concentrated on spontane-

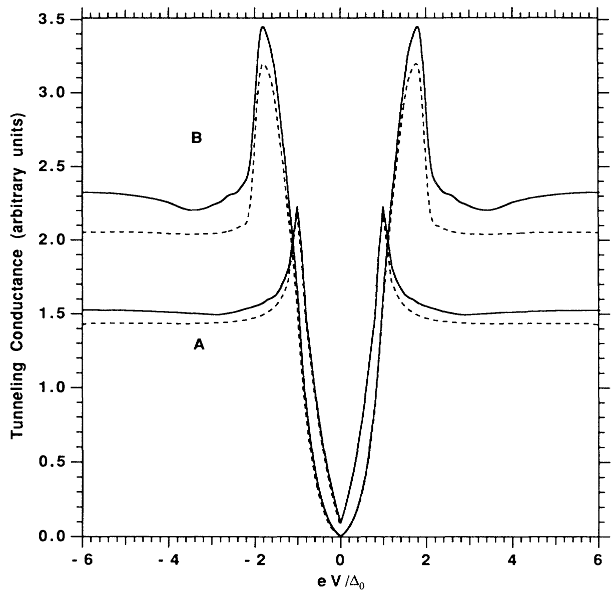

FIG. 3. Tunneling conductances, g_{SIN} (curves A) and g_{SIS} (curves B), as a function of the voltage across the junction, eV. The full line is the result with frequency-dependent damping given in Eq. (5), where $\Gamma_0=0.05\Delta_0$ and $\Gamma_1=0.5\Delta_0$. The broken line is the result for a frequency-independent damping, $\Gamma_1=0$. Here $\mu=-0.2$ and $\Delta_0=0.01$.

ous quasiparticle decay and have taken a simple model for the normal-state spectrum. In particular we have ignored the effects of interactions with this spectrum which have the effect of smoothing out sharp features associated with the tight-binding structure in the density of states. We consider a more realistic treatment of the normal-state spectrum and interaction effects in a forthcoming publication [24].

In conclusion we have postulated that features seen in the tunneling conductance of S-I-S junctions at bias voltages $eV \simeq 3\Delta_0$ [3] arise from quasiparticle decay. This quasiparticle decay is a correction to the weak coupling mean-field treatment of the quasiparticle states which can be significant in two-dimensional superconductors. The voltages at which these features are seen in $g_{\text{SIS}}(eV)$ have been identified with $3\Delta_0$ for a range of cuprate superconductors. This provides strong evidence for the $d_{x^2-y^2}$ order parameter in the cuprate superconductors.

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