Tunneling Density of States of High T_c Superconductors: d-Wave BCS Model versus SU(2) Slave-Boson Model

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Motivated by recent experimental measurements of the tunneling characteristics of high T_c materials using scanning tunneling spectroscopy, we have calculated the I-V and differential conductance curves in the superconducting state at zero temperature. Comparing BCS-like d-wave pairing and the SU(2) slave-boson approach, we find that the slave-boson model can explain the asymmetric background observed in experiments. The slave-boson model also predicts that the height of the conductance peak relative to the background is proportional to the hole doping concentration x, at least for underdoped samples. We also observe the absence of the van Hove singularity, and comment on possible implications.

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I. Introduction.—Tunneling spectroscopy has been one of the fundamental tools in studying the superconducting state of the high T_c materials. In recent years it has been possible to use the scanning tunneling microscope (STM) to perform reproducible experiments on single crystal $Bi_2Sr_2CaCu_2O_{8+\delta}$ cleaved in ultrahigh vacuum [1,2]. In contrast to photoemission experiments, which are local probes in wave-vector space, the STM is local in real space. Thus it does not provide any information that depends on momentum, however, it has much higher energy resolution. The density of states (DOS) obtained from the $\frac{dI}{dV}$ curve is a direct fingerprint of the single particle microscopic physics in the material and hence of some importance in constraining the possible theoretical models explaining the elusive high T_c physics.

The STM spectra for the superconducting phase exhibit unusual structure in the DOS when viewed in light of the Bardeen-Cooper-Schrieffer (BCS) theory even if effects such as energy dependence of the normal state density of states of sample and/or tip, existence of bandwidth cutoffs, unequal work functions of tip and sample, and energy-dependent transmission probabilities are included [3]. One notable feature in the tunneling spectra is the asymmetric background with an enhancement for hole tunneling into the sample. This feature is reproduced very well in our calculation based on the slave-boson theory. The slave-boson model also predicts that the strength of the background in the tunneling spectra does not scale with the doping x while the sharp conductance peak scales linearly with x. Thus, by measuring the relative strength of the background and the sharp conductance peak as a function of doping x, one can distinguish the BCS theory and the slave-boson theory experimentally.

We also observe the absence of the van Hove singularity, and comment on possible implications. One possible implication is particularly intriguing and consistent with photoemission results. That is the quasiparticles have a long lifetime, $\tau > 0.5$ meV, below the superconducting gap, and a very short lifetime, $\tau < 0.05$ meV (spin-charge separation) above the superconducting gap.

II. d-wave BCS.—The differential conductance $\frac{dI}{dV}$ displays, in the simplest case of constant DOS in the tip and energy-independent transition probability, the single electron DOS in the sample. This reflects the ability of the material to accommodate an extra electron or hole depending on the sample bias. Within the tunneling Hamiltonian formalism the tunneling current is given by [4]

$$j_T = 4\pi e\Gamma^2 \sum_{k,p} \int d\omega\, [A_{L-}(\omega,p)A_{R+}(\omega + V,k) - A_{L+}(\omega,p)A_{R-}(\omega + V,k)], \tag{1}$$

where the A_L's and A_R's are the spectral functions for the single electron Green's functions in the tip (L) and sample (R), respectively. V denotes the bias of the sample with respect to the tip and Γ is the tunneling matrix element assumed independent of energy. Notice that positive V corresponds to e^- tunneling into the sample.

For a free fermion system, which we suppose to represent the tip material, we have the standard form for the spectral function at zero temperature $A_{L+}(\omega,p) = \Theta(\omega)\delta(\omega - \xi_p)$ and $A_{L-}(\omega,p) = \Theta(-\omega)\delta(\omega - \xi_p)$, where $\xi_p = \epsilon_p - E_F$ denotes the particle spectrum in the tip with E_F the Fermi energy. $\Theta(\omega)$ is the Heaviside step function, where ω is measured with respect to the Fermi energy.

For the sample, we first consider the following single particle spectral distribution at zero temperature:

$$A_{R+}(\omega,p) = \Theta(\omega)u^2(p)\delta(\omega - E_p), \quad A_{R-}(\omega,p) = \Theta(-\omega)v^2(p)\delta(\omega + E_p), \tag{2}$$

where $u^2(p) = \frac{1}{2}(1 + \frac{\xi_p}{E_p})$ and $v^2(p) = \frac{1}{2}(1 - \frac{\xi_p}{E_p})$ are the BCS coherence factors, $E_p = \sqrt{\xi_p^2 + \Delta_p^2}$ is the

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dispersion relation of the quasiparticles in the superconducting state, and $\xi_p = \epsilon_p - E_F$ with ϵ_p the dispersion relation in the normal state. Here Δ_p denotes the gap function which is taken to have a d-wave symmetry in reciprocal space. Within the above approximation to the spectral functions, we obtain the following expressions for the single particle tunneling current:

$$j_T|_{V>0} = 4e\pi\Gamma^2 N(E_F) \sum_{k,E(k)\leq V} u^2(k),$$

$$j_T|_{V<0} = -4e\pi\Gamma^2 N(E_F) \sum_{k,E(k)\leq |V|} v^2(k).$$

Figure 1 plots the resulting differential conductance curve. With

$$\xi_k = t_0 + t_1(\cos k_x + \cos k_y) + t_2(\cos k_x \cos k_y) + t_3(\cos 2k_x + \cos 2k_y) + t_4(\cos 2k_x \cos k_y + \cos 2k_y \cos k_x) + t_5(\cos 2k_x \cos 2k_y) - E_F$$

as the dispersion relation for the quasiparticles in the ab plane of the sample and the matrix elements chosen as follows $[t_0, \ldots, t_5] = [0.1305, -0.2976, 0.1636, -0.026, -0.0559, 0.051]$ in eV, this is a tight binding fit to angle-resolved photoemission spectroscopy (ARPES) measurements performed by Norman *et al.* [5]. E_F has been adjusted to yield 10% hole doping, and $\Delta_k = \Delta_0(\cos k_x - \cos k_y)$ (with $\Delta_0 = 22$ meV) has the d-wave k-space symmetry mentioned previously.

With the hole doping at 10%, the van Hove singularity, present in the band structure, ends up on the hole side of the DOS very close to the Fermi energy. The fact that the van Hove singularity is close to the Fermi surface and hence should show up in the low energy single particle physics can be seen nicely in Fig. 1 in the form of the double peak structure. The coherence factors which mix particle and hole density of states lead to the van Hove singularity also showing up on the particle side of the $\frac{dI}{dV}$ curve, albeit with much smaller amplitude.

III. Slave bosons.—Next we consider the tunneling problem in light of the SU(2) slave-boson theory of Wen and Lee [6]. It is commonly believed that the simplest model that incorporates the strong correlation physics relevant for the high T_c cuprates is the t-J model. Because of the strong on-site Coulomb repulsion energy the doubly occupied states should not contribute to the low energy effective theory. Within the SU(2) approach this constraint is implemented via the introduction of a slave-boson doublet. The physical electron operator can then be written as an SU(2) singlet. Within this representation, the mean-field electron propagator is given by the product of the boson and the fermion propagators and was calculated in Ref. [7].

For our purpose we need only the $T = 0$ spectral functions which can be read off from the expression for the Green's function as

$$A_{R+}(\omega, k) = \Theta(\omega)\left\{\frac{x}{2} u_f^2(k)\delta[\omega - E^f(k)]\right\}$$

for the particle part and

$$A_{R-}(\omega, k) = \Theta(-\omega)\left\{\frac{x}{2} v_f^2(k)\delta[\omega + E^f(k)] + \frac{1}{2N}\sum_q [u_b(q-k)u_f(q) + v_b(q-k)v_f(q)]^2 \delta[\omega + E^f(q) + E^b_-(q-k)] + \frac{1}{2N}\sum_q [u_b(q-k)v_f(q) - v_b(q-k)u_f(q)]^2 \delta[\omega + E^f(q) + E^b_+(q-k)]\right\} \quad (3)$$

for the hole part of the spectrum. Here N denotes the number of sites and x is the hole doping concentration. The remaining variables are defined as follows: $u_{f,b}(k) = \frac{1}{2}\sqrt{1 + \frac{\epsilon(k)^{f,b}}{|E^{f,b}|}}$, $v_{f,b}(k) = \frac{1}{2}\frac{\Delta^{f,b}(k)}{|\Delta^{f,b}(k)|}\sqrt{1 - \frac{\epsilon(k)^{f,b}}{|E^{f,b}|}}$, $E^f(k) = \sqrt{[\epsilon^f(k)]^2 + [\Delta^f(k)]^2}$, and $E^b_\pm(k) = \pm\sqrt{[\epsilon^b(k)]^2 + [\Delta^b(k)]^2} - \mu_b$, where $\epsilon^f(k)$ and $\Delta^f(k)$ are the fermion dispersion and gap function, respectively, $\epsilon^b(k)$ and $\Delta^b(k)$ are the dispersions of the bosons, and μ_b is the boson chemical potential.

Notice that besides a coherent part for the spectral functions which resembles the form of the BCS spectral weight (2), albeit scaled by a factor of $\frac{x}{2}$, there is also an added incoherent contribution to the hole part of the spectral function (3).

To calculate the tunneling current we have used the fit to ARPES measurements as dispersion for the fermions (spinons) and a nearest neighbor tight binding dispersion

$$\epsilon^b = -2t^b(\cos k_x + \cos k_y)$$

for the bosonic degrees of freedom (holons) with t^b the hopping matrix element for the holons. It is important that we match the fermionic band structure with the ARPES measurements since the fermions have a bigger band mass and hence determine the dispersion relation seen in ARPES [6,8]. The electrons measured in those experiments are thought of (within spin-charge separating models) as bound states of the *heavy* spin degrees of freedom and the *light* charge degrees of freedom. Since we are interested in the low energy effective theory, the details of the broad dispersion for the holons (charge degrees of freedom) are not crucial and hence have been chosen to be as simple as possible. Furthermore, to arrive at Eq. (3) we assumed boson condensation of the holons.

With the above expressions for the spectral functions in the sample, we can calculate the tunneling current using Eq. (1) as

$$
\begin{aligned}
j_T|_{V>0} &= 4e\pi\Gamma^2 N(E_F) \sum_{k,E(k)\le V} \frac{x}{2}\, u_f^2(k) \\
j_T|_{V<0} &= -4e\pi\Gamma^2 N(E_F) \sum_{k,E(k)\le|V|} \frac{x}{2}\, v_f^2(k) + \frac{1}{2N} \sum_{k,q}^{-} [u_b(q-k)u_f(q) + v_b(q-k)v_f(q)]^2 \\
&\quad + \frac{1}{2N} \sum_{k,q}^{+} [u_b(q-k)v_f(q) - v_b(q-k)u_f(q)]^2,
\end{aligned} \tag{4}
$$

where $\sum_{k,q}^{\pm} = \sum_{k,q}\{\Theta[E^f(q) + E^b_{\pm}(q-k)] - \Theta[E^f(q) + E^b_{\pm}(q-k) - |V|]\}$.

When comparing the two $\frac{dI}{dV}$ curves in Figs. 1 and 2, one can see how the lowest energy physics is virtually identical. However, on energy scales bigger than $4\Delta_0$ a marked asymmetry in the background of the SU(2) model $\frac{dI}{dV}$ shows up with an increase in the hole tunneling spectral weight.

The inset of Fig. 2 depicts the incoherent contribution to the hole tunneling spectrum separately (scaling the height of Fig. 1 by $\frac{x}{2}$ and adding the incoherent hole contribution results in Fig. 2). The increase in the hole tunneling spectral weight arises due to the fact that removing an electron from the sample requires the recombination of the spin and charge degrees of freedom into a single entity. This yields a mixing in of the higher energy holon dispersion whose detailed form is not known within the effective low energy theory.

Another feature so far not discussed is the scaling with the hole doping of the conductance peak corresponding to electrons tunneling into the sample. By comparing Eqs. (3) and (4) we see that, within the SU(2) model, the peak height scales linearly with x, whereas there is no dependence of the peak height on doping within the d-wave approach. The doping dependence within SU(2) arises from the reduction of the overlap of the electron in the tip with the quasiparticle (as a bound state of holons and spinons) in the sample which, crudely speaking, means that an electron can only enter the sample on empty sites and then

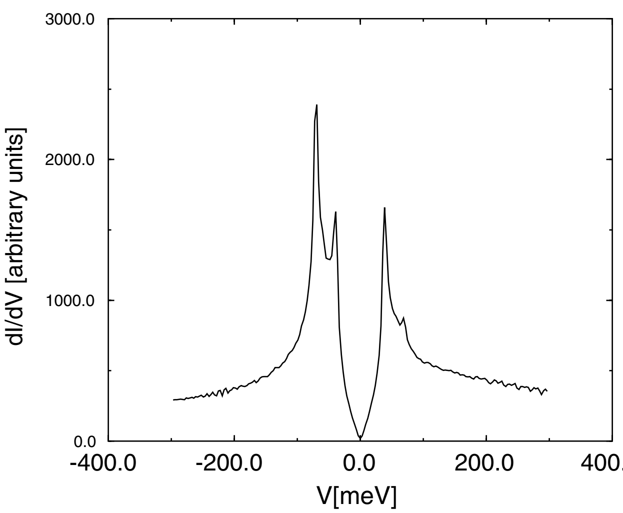

FIG. 1. The two peaks symmetrically located in height and energy with respect to zero bias are the usual peaks arising from the gap structure in the superconducting density of states. The two outer peaks are the remnants of the van Hove singularity. The wiggles in the background are due to the discreteness of k space when performing numerical calculation. The discreteness becomes amplified by the derivative taken in obtaining $\frac{dI}{dV}$ from the tunneling current (3). The resolution in voltage is 3 meV.

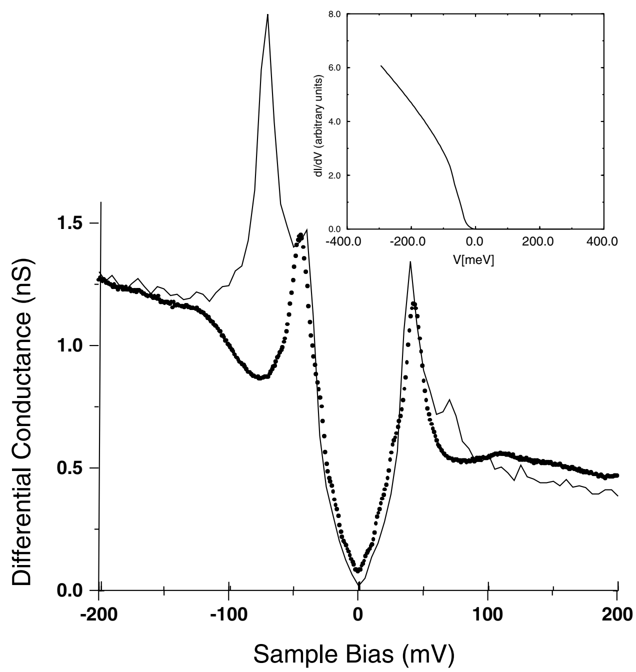

FIG. 2. Here we have set $t_1^f/2t^b = 1/2$. $\Delta^f = \Delta_0^f(\cos k_x - \cos k_y)$ and $\Delta^b = \Delta_0^b(\cos k_x - \cos k_y)$ with $\Delta_0^f/\Delta_0^b = 1/2$, where $t_1^f = -297.6$ meV from the ARPES fit and $\Delta_0^f = 22$ meV. Notice that the above ratios correspond to $J/t = 1/2$ within the t-J model. The solid curve is our slave-boson result. The wiggles in the background are more pronounced here, as compared with Fig. 1, due to smaller resolution in k space in calculating the convolution integrals (4). Here the resolution in V is 5 meV. The dots are the experimental result from Ref. [2]. The inset shows the incoherent part of the hole tunneling spectral weight. Notice that the exact shape of this curve should not be taken too literally; see discussion on boson band structure in the main text.

"decay" into its constituent parts. The only doping dependence within the d-wave approach arises due to the chemical potential which dictates the separation of the double peak structure but not its height. The linear scaling with x within the SU(2) slave-boson mean-field theory discussed here should be taken more as a qualitative than exact quantitative prediction, since it is a mean-field result. Recent photoemission experiments [9] by Ding *et al.* observed a linear x dependence of the quasiparticle peak, which fits the mean-field result of the SU(2) theory very well.

Thus, at the mean-field level we have found qualitatively different behaviors with regards to the x dependence of the hole tunneling background and the electron-tunneling peak within d-wave BCS and the SU(2) slave-boson theory. It is this difference in doping dependence, which should be experimentally testable and hence yield a feature distinguishable between the two models.

Furthermore, notice that the DOS contains singularities (for both BCS and the slave-boson model) at the electron-tunneling peak. The curvature of the measured dI/dV curve at these peaks should give us an upper bound on the quasiparticle decay rate at the energy scale of the superconducting gap. Based on new experimental data by Pan *et al.* [2], the quasiparticle decay rate can be as small as a few meV even for quasiparticles with energy as high as 40 meV. This is very different from the normal state, where the quasiparticle decay rate is of the same order of magnitude as the quasiparticle energy. We would also like to remark that, according to the photoemission and tunneling results for underdoped samples, the quasiparticle peak (with a width of order T) disappears completely above T_c while the gap remains at $(0, \pi)$. Based on the slave-boson theory, the sharp electron-tunneling peak arises due to the condensation of the holons (whose weight is proportional to x at $T = 0$). As T approaches T_c, the fraction of the condensed holons vanishes. If we assume that the holons are very incoherent above T_c, we can conclude that the sharp electron-tunneling peak should disappear above T_c. This picture from the slave-boson model is completely consistent with the observed results from photoemission experiments.

Another point to make here is about the van Hove singularity. Samples with small superconducting gaps ($\Delta \sim$ 25 meV) show a double peak structure in the tunneling dI/dV curve, and the double peak structure crosses over into a single peak for large superconducting gaps. At first sight, one might guess that the double peak structure is due to the van Hove singularity. However, after comparing the experimental line shape with the theoretical line shape, we conclude that the double peak cannot arise due to the van Hove singularity. This is because the experimental peaks at higher bias are quite symmetric, while the peaks from the van Hove singularity are very asymmetric (the peak at the hole side is much stronger than the peak on the electron side). Based on the dispersion obtained from the fitting of the ARPES measurements, the van Hove singularity should show up even for samples with larger gaps ($\Delta = 50$ meV). However, experimentally, one fails to see the van Hove singularity even when the gap is as small as 20 meV [2]. This seems to suggest that quasiparticles have a very short lifetime (spin-charge separation) above the superconducting gap, and hence the van Hove singularity cannot be observed. This leaves us with the question of where the double peak feature comes from if there are no well-defined quasiparticles above the superconducting gap. We hope that the double peak structure may give us some hints on how coherent quasiparticles emerge in the superconducting state from the incoherent normal state.

Finally, we would like to point out that the results of this paper are obtained from a mean-field calculation within the slave-boson theory. One naturally questions the reliability of the mean-field result and how much of our result remains valid after the gauge and other fluctuations are included. One of our main results is the explanation of the asymmetric tunneling background. It can be traced back to the strong on-site repulsion. It is much easier to remove an electron than to add an electron and create a doubly occupied site. We believe this result is robust and will survive the fluctuations around the mean-field state. The second main result is that the weight of the coherent quasiparticle tunneling peak is proportional to the doping x. After including the fluctuations, we believe that the weight of the coherent peak should have a similar doping dependence. This is because the coherent peak comes from the quasiparticle which is a bound state of a spinon and a holon. However, the detailed dependence may be of a more general form $x^{1+\alpha}$ (i.e., the fluctuations may correct the exponent) [10].

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