Pair Phase Fluctuations and the Pseudogap

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The single-particle density of states and the tunneling conductance are studied for a two-dimensional BCS-like Hamiltonian with a $d_{x^2-y^2}$-gap and phase fluctuations. The latter are treated by a classical Monte Carlo simulation of an XY model. Comparison of our results with recent scanning tunneling spectra of Bi-based high-T$_c$ cuprates supports the idea that the pseudogap behavior observed in these experiments can be understood as arising from phase fluctuations of a $d_{x^2-y^2}$ pairing gap whose amplitude forms on an energy scale set by $T_c^{MF}$ well above the actual superconducting transition.

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Intensive research has focused on the pseudogap regime, which is observed in the high-$T_c$ cuprates below a characteristic temperature that is higher than the transition temperature $T_c$. It occurs in a number of different experiments as a suppression of low-frequency spectral weight $\mathbf{1} \mathbf{2} \mathbf{3} \mathbf{4} \mathbf{5} \mathbf{6} \mathbf{7}$. This striking pseudogap behavior initiated a variety of proposals as to its origin $\mathbf{8} \mathbf{9} \mathbf{10} \mathbf{11} \mathbf{12} \mathbf{13} \mathbf{14} \mathbf{15}$. In this scenario, the key ideas of the cuprate phase fluctuation scenario: that is, we explore the notion that the pseudogap behavior initiated a variety of proposals as to its origin $\mathbf{8} \mathbf{9} \mathbf{10} \mathbf{11} \mathbf{12} \mathbf{13} \mathbf{14} \mathbf{15}$, since the analysis of the gap $\mathbf{6} \mathbf{7} \mathbf{12} \mathbf{13} \mathbf{14} \mathbf{15}$, because of the difficulty in determining the experimental consequences of the various theoretical proposals. In part, this reflects the possibility that there may be different pseudogap phenomena operating in different temperature and doping regimes. In part, this is because of the difficulty in determining the experimental consequences of the various theoretical proposals. In this paper, we focus on the pseudogap phenomena observed in scanning tunneling spectroscopy measurements $\mathbf{1} \mathbf{2}$ on Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) and Bi$_2$Sr$_2$CuO$_{6+\delta}$ (Bi2201). We provide a detailed numerical solution of a minimal model which, however, contains the key ideas of the cuprate phase fluctuation scenario: that is, we explore the notion that the pseudogap behavior observed in these experiments arises from phase fluctuations of the gap $\mathbf{8} \mathbf{9} \mathbf{10} \mathbf{11} \mathbf{12} \mathbf{13} \mathbf{14} \mathbf{15}$. In this scenario, below a mean field temperature scale $T_c^{MF}$, a $d_{x^2-y^2}$-wave gap amplitude is assumed to develop. However, the superconducting transition is suppressed to a considerably lower temperature $T_c$ by phase fluctuations $\mathbf{12}$. In the intermediate temperature regime between $T_c^{MF}$ and $T_c$, the phase fluctuations of the gap give rise to pseudogap phenomena.

We will study as a model for phase fluctuations a two-dimensional BCS Hamiltonian

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i \sigma} c_{j \sigma} + c^\dagger_{j \sigma} c_{i \sigma}) - \frac{1}{4} \sum_{\delta} \langle i | \delta \rangle (\Delta^\dagger_{i \delta} \langle \delta | i \rangle + \Delta^\dagger_{i \delta} \langle \delta | i \rangle),$$

(1)

where $c^\dagger_{i \sigma}$ creates an electron of spin $\sigma$ on the $i$th site and $t$ denotes an effective nearest-neighbor hopping. The $\langle i j \rangle$ sum is over nearest-neighbor sites of a 2D square lattice, and in the second term $\delta$ connects $i$ to its nearest-neighbor sites. In Eq. (1) one could, of course, add a next-nearest-neighbor hopping $t'$ and a chemical potential term. Here, for simplicity and to refrain from further approximations, we have set $t'$ and the chemical potential equal to zero $\mathbf{17}$. We will assume that below a mean field temperature $T_c^{MF}$, a $d_{x^2-y^2}$-gap amplitude forms with $\Delta \sim 2T_c^{MF}$. The detailed temperature dependence of $\Delta$ is not central, as we are not interested in the region around $T_c^{MF}$ where the pseudogap closes. The important point for our calculations is simply that a $d_{x^2-y^2}$-gap amplitude of order $2T_c^{MF}$ in magnitude forms as $T$ drops below $T_c^{MF}$ so that

$$\langle \Delta^\dagger_{i \delta} \rangle = \frac{1}{\sqrt{2}} (c^\dagger_{i \uparrow} c^\dagger_{i \downarrow} - c^\dagger_{i \downarrow} c^\dagger_{i \uparrow}) = \Delta e^{i \Phi_{\delta}},$$

(2)

with

$$\Phi_{\delta} = \begin{cases} (\phi_\uparrow + \phi_{i+\delta})/2 & \text{for } \delta \text{ in x-direction}, \\ (\phi_\downarrow + \phi_{i+\delta})/2 + \pi & \text{for } \delta \text{ in y-direction}. \end{cases}$$

(3)

We then determine the fluctuating phases from a Monte Carlo calculation using an effective 2D XY-free energy

$$F[\phi_i] = -E_1 \sum_{\langle ij \rangle} \cos (\phi_i - \phi_j),$$

(4)

with $E_1$ adjusted to set the Kosterlitz-Thouless $\mathbf{18}$ transition temperature $T_{KT}$ equal to some fraction of $T_c^{MF}$. Specifically, for the present calculation we will set $T_{KT} \simeq T_c^{MF}/5$. Here, we have the recent scanning tunneling results $\mathbf{10}$ for Bi$_2$Sr$_2$CuO$_{6+\delta}$ in mind, where $T_c \simeq 10K$ and the pseudogap regime extends to 50 or 60K, which we take as $T_c^{MF}$.

In principle, the XY action, which determines the fluctuations of the phases, arises from integrating out the shorter wavelength fermion degrees of freedom including those responsible for the local pair amplitude and the internal $d_{x^2-y^2}$ structure of the pairs. In general this leads
to a $\tau$-dependent quantum action as well as a coupling energy $E_1$, whose temperature dependence is determined by the many-body interactions of the microscopic system. There have been various discussions regarding the regime over which a classical action is appropriate for the cuprates \cite{21, 20, 19}. Here, however, we will proceed phenomenologically using the classical action, Eq. (4), and neglecting the temperature dependence of $E_1$. Furthermore, we will use the 2D form of Eq. (1). One knows that for the layered cuprates there is a crossover from 2D to 3D $XY$ behavior near $T_c$ \cite{22}. Our point of view is that away from this crossover regime, a 2D model is certainly suitable and on the finite size lattice that we will study, the system becomes effectively ordered as $T$ approaches $T_{KT}$ and the correlation length exceeds the lattice size. So $E_1$ will simply be used to set $T_{KT} \equiv T_c$. A crucial physical point that will be taken into account in our analysis is that the basic length scale of the $\varphi$-field is larger than the Cooper-pair size $\xi_0$. Thus, although this is a clearly simplified model, we believe that its solution provides useful insight into the experimental consequences of the phase fluctuation pseudogap scenario. It is the central aim of this paper to verify this by comparison with the STM experiments and reproduction of some of their characteristic and salient features.

The calculation of the density of states for an $L \times L$ periodic lattice now proceeds as follows \cite{27, 23, 24}. A set of phases $\{\varphi_i\}$ is generated by a Monte Carlo (MC) importance sampling procedure, in which the probability of a given configuration is proportional to exp$(-F[\varphi_i]/T)$ with $F$ given by Eq. (4). With $\{\varphi_i\}$ given, the Hamiltonian of Eq. (1) is diagonalized and the single particle density of states $N(\omega, T, \{\varphi_i\})$ is calculated. Further MC $\{\varphi_i\}$ configurations are generated and an average density of states $\langle N(\omega, T) \rangle = \langle N(\omega, T, \{\varphi_i\}) \rangle$ at a given temperature is determined.

As noted above, our point of view is that the $XY$ action, used in the MC simulations, in principle arises from integrating out the shorter wavelength fermion degrees of freedom up to the scale of the Cooper-pair size, so that only the center of mass pair phase fluctuations are important. Thus, the scale of the lattice spacing for $F[\varphi_i]$ is set by the pair size coherence length $\xi_0 \sim v_F/\pi\Delta_0$ and is of order 3 to 4 times the basic $Cu-Cu$ lattice spacing of the fermion Hamiltonian Eq. (1). Now the computationally intensive part of the calculation is the diagonalization of $H$ and in order to get meaningful results as $T$ approaches $T_{KT}$, we found it necessary to average over a large number of Monte Carlo $\{\varphi_i\}$ configurations. This requires that some compromise be made with respect to the lattice size. The results, we will present, are for a $32 \times 32$ Hamiltonian lattice. However, if we were to take $\xi_0 \sim 4$ lattice spacings, this would lead to only an $8 \times 8$ lattice for the $\varphi_i$ simulations. This would not allow a sufficient range for the Kosterlitz-Thouless phase coherence length to grow as $T$ approaches $T_{KT}$.

Thus, we have chosen to set $\Delta = 1.0t$ giving $\xi_0 \sim 1$ so that the $\varphi_i$ simulation can be carried out on the same $L \times L$ lattice that is used for the diagonalization of $H$. The important physical point is that this procedure effectively cuts off phase fluctuations on a scale less than the Cooper-pair size, $\xi_0$. Thus, the phase coherence length is always larger than the Cooper-pair size when $T$ is less than $T_{MF}$. Consequently, our results differ from earlier work \cite{23}, which found that the pseudogap regime due to fluctuating phases extended only about 20% above $T_c$, in contrast to the Bi tunneling experiments \cite{2, 3} and the recent Nernst-effect results \cite{8}. In the work of Ref. [25], parameters were used which set the basic scale of the phase correlation length to be much smaller than $\xi_0$ and, therefore, the phase correlation length exceeded $\xi_0$ only in a narrow temperature region set by a fraction of $T_{KT}$. We believe that this is not the correct phenomenology.

Results for $N(\omega, T)$ are shown in Fig. 1. For each temper-
For $T > T_c^{MF}$, the gap amplitude vanishes and the density of states exhibits the usual Van Hove peak at $\omega = 0$. For $T < T_c^{MF}$, the presence of a finite gap amplitude gives rise to a pseudogap whose size is set by $2\Delta$. Then, as $T$ approaches $T_{KT}$ and the $XY$ phase correlation length rapidly increases, coherence peaks evolve, the separation of which is determined by $2\Delta$. An important point is that the scale in temperature over which the evolution of the coherence peaks occurs, is set by some fraction of $T_{KT}$ which means that it appears suddenly on a scale set by $T_c^{MF}$.

An effective correlation length $\xi(T)$, extracted by fitting an exponential form to the correlation function

$$C(\ell) = \langle e^{-i\varphi + i\varphi'} \rangle$$

is plotted versus $T$ in Fig. 2 for our $32 \times 32$ lattice. The rapid onset of $\xi(T)$ as $T_{KT}$ is approached is clearly seen. It is this sudden increase of $\xi(T)$ that is responsible for the appearance of the coherence peaks as $T$ approaches $T_{KT}$. This effect is further enhanced by the 2D to 3D crossover that occurs in the actual materials.

In order to compare these results for $N(\omega, T)$ with scanning tunneling spectra $dI/dV$, we have calculated $dI(V, T)/dV$ using the standard quasi-particle expression for the tunneling current,

$$\frac{dI(V, T)}{dV} \propto \int N(\omega) \frac{\partial f(\omega - V)}{\partial V} \, d\omega.$$  

Here, $f(\omega) = (\exp(\omega/T) + 1)^{-1}$ is the usual Fermi factor. Results for $dI(V, T)/dV$ are displayed in Fig. 3. The effect of the Fermi factors is to provide a thermal smoothing of the quasi-particle density of states over a region of order $2T$. This becomes significant at the higher temperatures and the prominent pseudogap dependence of

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**FIG. 2:** The effective correlation length $\xi(T)$ versus $T/T_{KT}$ for the $32 \times 32$ lattice. Here $T_c^{MF}/T_{KT} \approx 5$ so that the pseudogap regime which extends from $T/T_{KT} \approx 1.5$ to $5$ is large compared to the superconducting region which extends from $0$ to $T/T_{KT} = 1$. The pronounced increase of $\xi(T)$ occurs over a narrow temperature region, on a scale set by $T_c^{MF}$, as $T_{KT}$ is approached.

**FIG. 3:** Tunneling conductance, $\frac{dI}{dV}$, normalized to its value at $T_c^{MF}$ and $V = 0$, for different temperatures. Solid curves are for $T = \{0.75, 1.25, 1.75, 3.00\} T_{KT}$, dashed curves for $T = \{1.00, 1.50, 2.00\} T_{KT}$ and $T_c^{MF} (\frac{dI}{dV}|_{V=0}$ is increasing with $T$).

$N(\omega, T)$ seen in Fig. 3 is smoothed out in $dI/dV$. In Fig. 3, $dI/dV$ results are shown as solid curves for $T = 0.75T_{KT}$ (Fig. 3a), $T = T_{KT}$ (Fig. 3b) and $T = 2T_{KT}$ (Fig. 3c). The dashed curve is for $T = T_c^{MF} \approx 5T_{KT}$. One sees that the size of the pseudogap scales with the spacing between the coherence peaks and evolves continuously out of the superconducting state. The pseudogap persists over a large temperature range measured in units of $T_{KT}$, becoming smoothed out by the thermal effects as $T$ approaches $T_c^{MF}$ and vanishing above $T_c^{MF}$.

Our numerical results for $dI(V, T)/dV$ are similar to recent scanning tunneling measurements of Bi2212 and Bi2201. Also in these experiments the superconducting gap for $T < T_{KT}$ evolves continuously into the pseudogap regime, which extends up to $T = T_c^{MF}$. The coherence peaks appear suddenly as $T_{KT}$ is approached. At higher temperatures, the pseudogap fills in rather than closing and the temperature range associated with the pseudogap regime can be large compared with the size of the superconducting regime.

Summarizing, in order to develop a more quantitative understanding for the role of phase fluctuations, we have provided a numerical solution of a simplified model which, nevertheless, contains the key ideas of the cuprate phase fluctuation pseudogap scenario. Here the center of mass pair-phase fluctuations of a BCS $d$-wave model were determined from a classical 2D $XY$ action by means of a Monte Carlo simulation. The resulting tunneling conductance ($dI/dV$) reproduces characteristic and salient features of recent STM studies of Bi2212 and Bi2201 suggesting that the pseudogap behavior observed in these experiments arises from phase fluctuations of the $d_{x^2-y^2}$-pairing gap.

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FIG. 4: Temperature dependence of $\frac{dI}{dV}$ normalized to its value at $T_{cMF}^{*}$ and $V = 0$. The solid curves are for $T = 0.75T_{KT}$ (a), $T = T_{KT}$ (b) and $T = 2T_{KT}$ (c). The dashed curve in all three figures is for $T = T_{cMF}^{*} \approx 5T_{KT}$.

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