Pair Density Wave in the Pseudogap State of High Temperature Superconductors

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Recent scanning tunneling microscopy (STM) experiments of Bi2Sr2CaCu2O8+δ have shown evidence of real-space organization of electronic states at low energies in the pseudogap state. We argue based on symmetry considerations as well as model calculations that the experimentally observed modulations are due to a density wave of d-wave Cooper-pairs without global phase coherence. We show that STM measurements can distinguish a pair-densit-wave from more typical electronic modulations such as those due to charge density wave ordering or scattering from an onsite periodic potential.

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One of the major challenges in condensed matter physics today is to understand the electronic phase diagram of high temperature cuprate superconductors. At the center of the debate is the nature of electronic states in lightly hole-doped cuprates, which has attracted a great deal of attention because of the observation of a pseudogap in the density of states (DOS) in these compounds. To understand this phenomenon, some have focused on the smooth evolution of the pseudogap energy scale. The origin of DOS modulation in the superconducting state has been for the most part attributed to quantum interference of quasi-particles, although potential relevance of electronic ordering has also been considered.

In this Letter, we focus on the STM resolved modulations of the DOS in the pseudogap state and propose that these are a consequence of a novel density wave associated with d-wave Cooper pairs, first proposed in the context of the charge ordering in the vicinity of vortices. This state, illustrated in Fig. (1) of Ref. 24, has a rotationally symmetric charge periodicity of $4a \times 4a$ near doping level $x = 1/8$. This state also arises naturally in the plaquette boson approach of Altman and Auerbach or in the large $N$ approximation of the $t - J$ model. It differs from the stripe state in terms of the rotation symmetry, and differs from the Wigner crystal state of the holes, which would have a charge periodicity of $\sqrt{3}a \times \sqrt{3}a$ at the same doping level.

Recently, mapping of the electronic states with the scanning tunneling microscope (STM) has demonstrated a link between the observation of real space electronic patterns and the pseudogap in DOS of underdoped Bi2Sr2CaCu2O8+δ samples. In this experiment, STM was used to detect a dispersionless modulation of the low energy electronic states, showing an unusual enhancement of the intensity of modulated patterns within the pseudogap energy scale. The pseudogap modulations bears similarity to those observed near the vortex cores, but seems to be distinct from the STM features in the superconducting state, which exhibit energy dispersion. The origin of DOS modulation in the superconducting state has been for the most part attributed to quantum interference of quasi-particles, although potential relevance of electronic ordering has also been considered.

In Refs. 21, 24, 25, 26, 27, 28, it was argued that the energy dependence of the tunneling intensity can be used to identify the type of ordering in the superconducting state.
range pairing correlations.

To model the experimental findings, we study quasiparticle spectrum based on solutions of the Bogoliubov-de Gennes (BdG) equations for a d-wave superconductor, while taking into account classical phase fluctuations to model the pseudogap state

\[
\left( \begin{array}{cc} \hat{\mathcal{H}}_0 & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{\mathcal{H}}_0 \end{array} \right) \left( \begin{array}{c} u_n(r) \\ v_n(r) \end{array} \right) = E_n \left( \begin{array}{c} u_n(r) \\ v_n(r) \end{array} \right) \tag{1}
\]

with \( \hat{\mathcal{H}}_0\psi_n(r) = -t\sum_\delta \psi_n(r + \delta) - \mu(r)\psi_n(r) \) and \( \hat{\Delta}\psi_n(r) = \sum_\delta \Delta(r, \delta)\psi_n(r + \delta) \) subjected to the self-consistent condition

\[
\Delta(r, \delta) = \frac{V(r, r')}{2} \sum_n [u_n(r)v_n^*(r') + u_n(r')v_n^*(r)] 
\times \tanh\left( \frac{\beta E_n}{2} \right), \tag{2}
\]

where \( r' = r + \delta \) and \( \delta \) denote a nearest-neighbor vector, \( \psi_n(r) \) can be \( u_n(r) \) or \( v_n(r) \). \( \beta = 1/k_B T \) is the inverse of temperature \( T \). We assume \( V(r, r') = (V(r) + V(r'))/2 \) and focus on the periodic pairing and chemical potentials, namely, \( V(r) = V_0 - \sum_Q \Delta V(Q) \cos Q \cdot r \) and \( \mu(r) = \mu_0 - \sum_Q \Delta \mu(Q) \cos Q \cdot r \).

To describe the pseudogap state above \( T_c \), we consider only classical phase fluctuations i.e. the phase field \( \phi(r) \) is independent of time. The pairing operator takes the form

\[
\hat{\Delta} = \frac{1}{2} e^{i\phi(r)/2} [\Delta(r)d(p) + d(p)\Delta(r)] e^{-i\phi(r)/2} \tag{3}
\]

where the differential operators \( d(p) = 2[\cos(p_xa) - \cos(p_ya)] \). In the superconducting state, the phase field \( \phi(r) \) is rigid while in the pseudogap its fluctuations destroy long range phase coherence. Note that in the superconducting state, even in the presence of pairing modulations, the spectrum remains gapless at four points on the Fermi surface.

The local DOS (LDOS) is a functional of the phase configuration, \( \phi(x) \), given by

\[
\rho(r, E, \{\phi(x)\}) = -\sum_n \left[ |u_n(r)|^2 f'(E_n - E) \\
+ |v_n(r)|^2 f'(E_n + E) \right], \tag{4}
\]

where the \((u_n(r), v_n(r))\) and \( E_n \) are respectively eigenfunctions and eigenenergies of \( \hat{H} \) for the phase configuration \( \phi(x) \). \( f'(E) = -\beta/4 \cos^2(\beta E) \) is the derivative of the Fermi distribution function. The Fourier transform of \( \rho(r, E, \{\phi(x)\}) \) is

\[
\rho(q, E, \{\phi(x)\}) = \frac{1}{L^2} \sum_r \cos(q \cdot r)\rho(r, E, \{\phi(x)\}) \tag{5}
\]

with \( L^2 \) the number of the sites.

Before presenting the numerical results, we analyze the symmetry of \( \rho(q, E, \{\phi(x)\}) \) when the average of chemical potential \( \mu(r) \) is zero. First, we consider the effect of a CDW described by a periodic chemical potential \( \mu(r) \) oscillating around zero average with periodicity \( L_\mu \). The Hamiltonian has the following symmetry: if \((u_n(r), v_n(r))\) is an eigenstate with energy \( E_n \) and phase configuration \( \phi(x) \), then \((-1)^{x+y}(-v_n^*(r + L_\mu/2), u_n^*(r + L_\mu/2))\) is an eigenstate with the same energy \( E_n \) for the phase configuration \( \phi(x) = \phi(x + L_\mu/2) \). We used the fact that the factor \((-1)^{x+y}\) introduces a minus sign to both the hopping and the pairing terms leaving the chemical potential term untouched, while the shift by \( L_\mu/2 \) changes the sign of the chemical potential term. In addition the standard Bogoliubov-de Gennes symmetry has been used. For the superconducting state where \( \phi(x) \) is \( x \)-independent one can easily show \( \rho(Q_\mu, E, \{\phi(x)\}) = \rho(Q_\mu, -E, \{\phi(x)\}) \),

\[
\rho(Q_\mu, E, \{\phi\}) = -\rho(Q_\mu, -E, \{\phi\}) \tag{6}
\]

where \( Q_\mu \cdot L_\mu = 2\pi \). In a pseudogap state where the phase coherence is destroyed, we must carry out a weighted average over all of the classical phase configurations. We assume that to a good approximation the probability distribution \( P(\{\phi(x)\}) \) is invariant under translation, i.e. \( P(\{\phi(x)\}) = P(\{\phi(r + L_\mu/2)\}) \) (e.g. XY-model). We thus conclude that the symmetry \( \hat{H} \) survives in the presence of the classical phase fluctuations.

Now in contrast to CDW, we consider the case of pair-density-wave. In the case of the periodic pairing potential with periodicity \( L_d \) and zero uniform chemical potential, \((-1)^{x+y}(-v_n^*(r), u_n^*(r))\) is an eigenstate with energy \( E_n \), which makes the Fourier transform of the LDOS an even function of energy

\[
\rho(q, E, \{\phi(x)\}) = \rho(q, -E, \{\phi(x)\}), \tag{7}
\]

where \( q \) is an arbitrary wave vector.

In the presence of modulation of both chemical potential and d-wave pairing potential, the above arguments do not hold in general. However, in the special case of the chemical potential oscillating with \( Q_\mu = (2\pi/4a, 2\pi/8a) \) and pairing potential with \( Q_d = (2\pi/4a, 0) \) and \((0, 2\pi/4a)\), one can show that the phase averaged LDOS satisfy \( \bar{\rho}(Q_d, E) = \bar{\rho}(Q_d, -E) \) while \( \bar{\rho}(Q_\mu, E) = \bar{\rho}(Q_\mu, -E) \). We believe that this case is relevant for the actual experiments in BSCCO.

The dichotomy of the local and non-local modulation serves as our point of departure in analyzing perturbations which break particle hole symmetry. If the departure from the symmetry is not too large, the above arguments are still useful as the odd or even character of \( \rho(Q, E) \) is true approximately. An immediate check is the tunneling density of states at the wavevector corresponding to the BSCCO superstructure. We expect it to enter
as a local periodic scattering potential, making \( \rho(Q_\mu, E) \) odd under \( E \rightarrow -E \). On the other hand, the charge density wave of d-wave bosons (see Fig.3 of Ref 24) should serve as an effective periodic pairing potential that is inherently non-local. Thus \( \rho(Q_\mu, E) \) should be even under \( E \rightarrow -E \).

We shall now turn to the numerical solutions of the BdG equations 1 for the superconducting state with uniform phase. The effect of phase fluctuations will then be described later in the text. We set \( t = 0.125eV \) such that \(\Delta = 40meV\), which is relevant for slightly underdoped BSCCO. In Fig.1, we plot the results for a pair-density-wave with \( \Delta V(Q_d) = 0.2V_0 \) with \( Q_d = (2\pi/4a, 0) \) and \( (0, 2\pi/4a) \). As expected, \( \rho(Q_d, E) \) are even functions of energy. At low temperature compared to the mean-field transition temperature \( T_c^{MF} \), \( \rho(Q_d, E) \) shows peaks at the energy within the superconducting gap and zero crossings at energies above the gap, which is consistent with the experimental data of Howald et al. 21. At higher temperature, \( T = 0.86T_c^{MF} \), \( \rho(Q_d, E) \) has a peak at zero energy and decreases as the energy increases. Again, this is consistent with the experiment 1. In the case of the periodic chemical potential with \( \Delta \mu(Q_\mu) = 4meV \) and \( Q_\mu = (2\pi/4a, 0) \), \( \rho(Q_\mu, E) \) plotted in Fig.2(a) as a solid line. As expected \( \rho(Q_\mu, E) \) is an odd function of energy. As discussed later, this feature enables us to exclude the modulation of chemical potential as the direct cause of the observed peak around \((2\pi/4a, 0)\).

So far, our calculation and symmetry arguments assume the particle-hole symmetry. As an illustration of the effects of weak symmetry breaking, in Fig.2 we display \( \rho(Q, E) \) for a finite chemical potential \( \mu = -20meV \). In Fig.3 we include finite next-nearest neighbor hopping term \( t' = -0.3t \) and a chemical modulation around a finite average with a wavevector \((2\pi/10a, 2\pi/10a)\) corresponding a periodicity about \( 7a \) in the \((\pi, \pi)\) direction. In both plots, remnants of the expected symmetry are clearly visible. In particular, in the case of the periodic \( \mu(r) \), \( \rho(Q_\mu, E) \) has odd number of zero-crossings below the gap energy, while in the case of pair-density-wave \( \rho(Q_d, E) \) has even number of zero-crossings at energies close to the gap.

We now include the effect of the phase fluctuations within the model of Franz and Millis 31, where the
the new peak picks up as the pseudogap opens. Our work ing data has confirmed that the new non-dispersive peak tional CDW state. The preliminary analysis of the exist-

where $\Omega^\alpha_{r\eta}$ is just the Doppler energy shift due to the presence of a uniform supercurrent and $P(\eta)$ is the probability distribution of $\eta$ that can be calculated within 2D XY Hamiltonian to yield

$$P(\eta) = \sqrt{2\pi W(T)} e^{-\eta^2/2W^2(T)}$$

with $W(T)$ a temperature-dependent parameter of the order of magnitude of the pseudogap. Since $P(\eta)$ is translationally invariant, the argument regarding the symmetry of the LDOS is still valid. In Fig.4, we plot the LDOS calculated from Eq.8 and Fig.2 for $Q_\parallel = (2\pi/4a, 0)$ and $(0, 2\pi/4a)$. Here, $\Delta \approx 40\text{meV}$ is the pseudogap. The solid dots are the experimental data of $(2\pi/4.7a, 0)$ peak of Vershinin et al.[1].

LDOS of a pseudogap state $\rho(r, E)$ can be calculated as an average over the phase fluctuations that are slowly varying in space

$$\rho(r, E) = \int d\eta P(\eta)\rho(r, E - \eta), \quad (8)$$

In conclusion, we show that the Fourier transform of the tunneling density of states recently obtained from the STM experiments, $\rho(Q, E)$, contains sufficient information to distinguish the pair-density-wave state from the conventional CDW state. Near the doping level of $x = 1/8$, the pair-density-wave has a rotationally invariant periodicity of $4a \times 4a$, which is close to the experimental observation. We are able to reproduce the most salient future of the non-dispersive peak as shown in Fig.2C of Vershinin et al.[1], namely, the intensity of the new peak picks up as the pseudogap opens. Our work also makes an experimentally testable prediction about the behavior of $\rho(Q, E)$ for $E < 0$, which is the opposite behavior for the pair-density-wave state and the conventional CDW state. The preliminary analysis of the existing data has confirmed that the new non-dispersive peak is spatially particle-hole symmetric[32], as predicted here. The pair-density-wave state therefore offers a unified theoretical explanation of the STM experiments both near the vortex core[24] and in the pseudogap state. This state plays an essential part in understanding the zero temperature global phase diagram of the high Tc cuprates[33], and our current work shows that it is also the dominant competing order in the pseudogap state. This state could be favored in the pseudogap regime of underdoped cuprates because of the combination of the low superfluid density and strong pairing, which is consistent with the previous theoretical ideas[3,34].

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