Modulation of the local density of states within the $d$-density wave theory in the underdoped cuprates

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The low temperature scanning tunneling microscopy spectra in the underdoped regime is analyzed from the perspective of coexisting $d$-density wave (DDW) and $d$-wave superconducting states (DSC). The calculations are carried out in the presence of a low concentration of unitary impurities and within the framework of the fully self-consistent Bogoliubov-de Gennes theory, which allows local modulations of the magnitude of the order parameters in response to the impurities. Our theory captures the essential aspects of the experiments in the underdoped BSCCO at very low temperatures.

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A fundamental tension in the field of high temperature superconductors is the notion of a competing order parameter in the underdoped regime, which can provide a natural explanation of why the superconducting dome exists and shed light on the nature of the pseudogap. While a charge ordered state is a candidate [1], one of us has proposed, and extensively studied, a new order parameter, which results in circulating currents arranged in a staggered pattern (DDW) [2]. Many experiments are consistent with this order parameter, as demonstrated in studies of the superfluid density, the polarized neutron scattering, the Hall number in pulsed 60 T magnetic field, the angle resolved photoemission spectroscopy (ARPES), the lack of specific heat anomaly at the pseudogap temperature, the transition temperature in multi-layer cuprates, and the infrared Hall angle measurements [3]. So far the clinching direct experiment, the polarized neutron scattering, the Hall number in pulsed 60 T magnetic field, the angle resolved photoemission spectroscopy (ARPES), the lack of specific heat anomaly at the pseudogap temperature, the transition temperature in multi-layer cuprates, and the infrared Hall angle measurements [3].

Here we turn to the intriguing scanning tunneling microscopy (STM) measurements [4] in the underdoped regime. In spite of numerous theoretical analyses of this problem [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24], no comprehensive theoretical picture has yet emerged, although certain aspects are captured by some of them. For example, earlier measurements in the slightly overdoped samples at very low temperatures have been elegantly explained in terms of a quasiparticle scattering interference model, named the octet model [8, 14]. At the same time, an interpretation in terms of dynamic charge fluctuations has also been advanced [11]. The focus here, however, is on an extensive set of experiments as a function of doping in BSCCO at very low temperatures [8]. The exciting finding of these experiments is the emergence of a new order, present along with the $d$-wave superconductivity (DSC). The salient signature is a sudden development of a relatively non-dispersive incommensurate wave vector, $q^*$, at higher energies in the underdoped regime.

In this Letter we explain the experiments by adopting a view that is orthogonal to the notion of charge order and consider DDW. At first sight, this would seem impossible, as STM is not sensitive to currents. The key to this puzzle lies in the presence of disorder (inevitable in these materials) that leads to variations of the charge density, which in turn can scatter the quasiparticles of the DDW, revealing indirectly the DDW order in the form of an interference pattern. The idea is not as surprising as it may seem, because, after all, this was precisely the basis of the successful octet model. Clearly, DSC corresponds to off-diagonal long range order rather than diagonal long range order and therefore cannot directly affect STM. The general message is that a large class of ordered states can leave their characteristic signatures via the scattering interference of their distinctive quasiparticle spectra. Our analysis is broadly consistent with the conclusions drawn from the recent comparisons of the autocorrelation function of the ARPES spectra and the STM spectra [23, 24].

A single-impurity $T$-matrix calculation in the coexisting DDW and DSC state [12, 13] was unable to recover the salient feature of the experiments, while pin-pointing certain important aspects. We shall show that the fault lies with the method and not intrinsically with the idea that a new order arises in the low temperature underdoped regime, namely the coexisting DDW and DSC order. The problem is that the $T$-matrix approach neither allows the amplitude of the order parameter of the DSC to modulate in response to the impurity potential nor allows a proper treatment of the current conservation in the DDW state in the presence of impurities [25, 26]. Moreover, it excludes not only spatial structures but also the interference of the impurities.

To understand the effect of various competing orders on the local density of states (LDOS), all we need to know
are the corresponding wave functions in the presence of finite concentration of impurities. We accomplish this by choosing the simplest Hamiltonian that yields both DSC and DDW, and coexisting DDW and DSC, states within the Bogoliubov-de Gennes mean field theory. We use this Hamiltonian solely as a crutch to generate the states with the broken symmetries that we wish to study. In general, deep within the superconducting dome, that is, at very low temperatures, there is good evidence of the existence of quasiparticles. The experiments that we address here are precisely in the regime in which our theory is expected to be valid. The corollary to these observations is that a straightforward finite temperature extension of our theory cannot be applied to the experiments of Ref. [10] because the simple picture of quasiparticles may not be valid at higher temperatures and above the superconducting dome.

The Hamiltonian is \( \mathcal{H} = \mathcal{K} + \mathcal{H}_{\text{int}} + \mathcal{H}_{\text{dis}} \), where \( \mathcal{K} = \sum_{ij} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \text{h.c.} \). The operator \( c_{i\alpha}^\dagger \) (\( c_{i\alpha} \)) creates (destroys) an electron at the site \( i \) with spin \( \alpha \), and \( t_{ij} \) is the hopping matrix element to the nearest \((-0.273t)\) neighbor. The interacting part consists of

\[
\mathcal{H}_{\text{int}} = J \sum_{<ij>} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) - W \sum_{<ij>,\alpha,\beta} n_{i\alpha} n_{j\beta},
\]

which is identified by two parameters \( J \) and \( W \). \( \mathbf{S}_i \) is the spin operator at the site \( i \) and \( n_{i\alpha} \) is the density operator. Disorder is introduced through \( \mathcal{H}_{\text{dis}} = \sum_{i\alpha} (V_i - \mu) n_{i\alpha} \), at each site \( i \), is an independent random variable, which is either \(+V_0\) (repulsive) with a probability \( n_{\text{imp}} \) (impurity concentration) or zero, and \( \mu \) is the chemical potential of the system.

We solve the above model within the self-consistent framework of BdG mean field theory, which amounts to decoupling the interaction terms, resulting in a \( \mathcal{H}_{\text{eg}} \) that leads to the local order parameters: DSC order \( (\Delta_i) \), DDW order \( (\chi_i) \) and also the local Hartree and Fock shifts. The details can be found in Ref. [29]. The chemical potential \( \mu \) is obtained by fixing the average density of electrons, \( \langle n \rangle = \sum_i \langle n_i \rangle / N \), at the desired value \( (N \) being the system size).

We concentrate on the results at \( T = 0 \) for parameters \( J = 1.6, \ W = 0.6 \) in units of \( t \) (all energies will be expressed in this unit and all lengths will be expressed in terms of the lattice spacing), and \( \langle n \rangle = 0.9 \) (equivalently 10\% hole doping) on square lattices with a unit cell of size \( N = 30 \times 30 \). Larger unit cells result in negligible improvements at the cost of computer time; the dimensionality of the matrices for which all the eigenvalues and the eigenvectors must be repeatedly obtained is \( 2N \times 2N \), that is, 1800 \times 1800. These parameters result in \( \chi_0 = 0.33 \) and \( \Delta_0 = 0.12 \) in a disorder free system in the coexisting DDW and DSC phases, where \( \chi_0 \) is defined through \( \chi_k = \chi_0 (\cos k_x - \cos k_y) / 2 \) and similarly for \( \Delta_0 \). Results for systems with solely DDW or DSC order will also be discussed for slightly different parameters: \( J = 1.4, \ W = 0.5 \). We choose \( V_0 = 100 \), close to the unitary limit, and results are averaged over 8-10 different realizations (8 for the DDW and the DSC orders by themselves, but 10 for the coexisting DDW and DSC) of the random potential. For better statistics we use the repeated zone scheme [26, 29] in which a super-cell is constructed by replicating the \( 30 \times 30 \) unit cell 10 times along the \( x \)-direction and 10 times along the \( y \)-direction. This provides a denser set of energy eigenvalues.

![FIG. 1: Density plots on a linear scale of the FT-LDOS within the first Brillouin zone in the \( k_x - k_y \) plane.](image-url)

The panels (a) through (f) correspond to different energies, \( \omega \), for the coexisting DDW+DSC phase. Here \( n_{\text{imp}} = 0.01 \) and \( V_0 = 100 \). Peaks at \( q^* \approx 0.15(2\pi) \) are clear in panels (a) through (d). At smaller energies, panels (e) and (f), \( q^* \)-peaks are absent and a broad peak appears near \( q = 0 \), whose width decreases with increasing \( |\omega| \). The strength of the peak at \( (0,0) \) is reduced for the clarity.

In the presence of impurities, both orders become spatially inhomogeneous. However, at \( n_{\text{imp}} = 0.01 \), the (disorder) averaged DDW order degrades much less \((\chi^2 \approx 0.95 \chi_0)\) compared to the DSC order \((\langle \Delta \rangle \approx 0.55 \Delta_0)\), consistent with earlier findings [26]. We define the Fourier
transform \( N(q, \omega) = \sum_r e^{-iq \cdot r} N(r, \omega) \), where \( N(r, \omega) \) is the LDOS at a site \( r \) with energy \( \omega \). The disorder averaged power spectrum \( P(q, \omega) = \langle |N(q, \omega)|^2 \rangle / N \) is calculated and then \( \sqrt{P(q, \omega)} \) is compared with experiments, as this is the theoretical measure [13] of the Fourier transform of the experimentally measured \( dI(V, r)/dV \), where \( I \) is the tunneling current, and \( V \) is the bias voltage \( (\omega = eV) \).

The results in the coexisting DDW+DSC state are shown in Fig. 1. The intensity of the peaks along \((0, \pm 1)\) and \((\pm 1, 0)\) appears as a generic and robust property, more precisely at \( q^* \sim (0.15)2\pi \) for the chosen set of parameters. The \( q^* \) peaks occur for \( |\omega| > \Delta_0 \). At lower energies the FT-LDOS profile looses periodic \( q \)-modulations and a rather broad peak occurs in its Fourier transform at \( q \approx 0 \) (See Figs. 1(e) and 1(f)). Unitary impurity resonances [31] dominate this regime (near \( \omega \approx 0 \)) and wash out the globally periodic LDOS modulations arising from interference. Unitary scatterers do not affect the spectrum at energies larger than \( \Delta_0 \), and hence the LDOS modulations are preserved.

The finite system, \( 30 \times 30 \), allows a \( q \)-resolution of 0.033, which is rather coarse compared to the real data (the super-cell does not introduce any additional independent wave vectors due to the periodicity). Along with the strong peak at \( q = 0 \) mentioned above, the resolution problem prevents us from observing the low energy modulation \( q_1 \), in the terminology of Ref. [3]; it is hidden by the broad peak around \( q = 0 \), whose width decreases with \( |\omega| \). On the other hand, \( q_5 \) is quite visible (at least for \( \omega > 0 \)). It is known from Ref. [3] that the intensities of \( q_2, q_3, q_6, q_7 \) relative to \( q_1 \) and \( q_5 \) fall with decreasing doping and \( q_4 \) is not seen at all [23, 24]. This is consistent with our calculation, which was performed in the underdoped regime.

Because DSC order is already weak in the pure system for our chosen parameters, and it rapidly gets weaker with impurities, it is important to study profiles similar to Fig.1 in the DDW phase without coexisting DSC order with \( n_{\text{imp}} = 0.01 \). The results are presented in Fig.2. The features are similar to those of Fig.1, but the \( q^* \) peaks first emerge for a little smaller value of \( |\omega| \) [see, Fig. 3]. The spectra shown in Fig. 2 are generic, and similar results are obtained for \( n_{\text{imp}} = 0.02 \). We have also studied our model in the DSC-only state in the same underdoped region and have not found \( q^* \) peaks.

An intuitive explanation of \( q^* \) is as follows. It is due to scattering between the tips of the hole pockets and the sharp rise of the pseudogap. In the coexisting DDW and DSC state, the low-energy constant energy contours are “bananas”, essentially from the pure DSC order, except that they are doubled up because of the broken translational symmetry. However, the disorder considerably smears out these scattering events. As the energy increases these bananas coalesce and, then on, the scattering is between the tips of the hole pockets of DDW. Since DDW is less affected by potential scattering than DSC, the signature becomes robust.

![FIG. 2: FT-LDOS as in Fig.1 but for DDW (\( \chi_0 \approx 0.28 \)). DSC order is forced to zero on all sites. Qualitative features are similar to Fig.1 for a wide range of \( \omega \).](image)

The dispersion of the \( q^* \)-peaks is shown in Fig. 3. The dispersion in the top panel of Fig. 3 is somewhat stronger than in Ref. [3] but gets weaker in the DDW-only phase (bottom panel). Similar results are also found for \( n_{\text{imp}} = 0.02 \). The value of \( q^* \sim (0.15)2\pi \) is due to the chosen set of band parameters, which will change with a different choice.

We have repeated our calculations with impurity strengths \( V_0 = 10 \) and \( V_0 = 1 \). The results are essentially the same for \( V_0 = 10 \), while for \( V_0 = 1 \) (non-unitary scatterers) the spectra for negative energy are somewhat different, though the key features are preserved. Thus the robustness of the results found here is heartening. We emphasize, however, that the effects of inhomogeneity and impurity interactions can be very subtle.

The disorder \emph{averaged} DOS, \( N(\omega) \), is shown in Fig. 4. We see that \( N(\omega) \) is asymmetric in the DDW phase, both with and without DSC order. The asymmetry in
the spectrum has the same origin as the asymmetries in Figs. 1 and 2. In the coexisting phase, the remnants of the superconducting density of states peaks can be seen, below which modulation of LDOS dies out. The spectrum is tantalizingly similar to the experimental results of Ref. 3.

To summarize, the inhomogeneous phase of coexisting DDW and DSC captures the essential experimental features seen in the underdoped regime at low temperatures, namely the emergence and the nature of the relatively non-dispersive $q^*$ peaks seen only at higher energies; in contrast, the DSC order alone is inadequate. From our perspective the emergence of $q^*$ is not due to an explicit charge order, fluctuating or otherwise, but due to the current modulations of the DDW. It would be interesting to see if $q^*$ extends to lower energies with purer samples. The interpretation of the experiment in $\text{Ca}_2\text{Na}_x\text{CuO}_2\text{Cl}_2$ is an open issue.

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