Checkerboard charge density wave and pseudogap of high-\( T_c \) cuprate

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We consider the scenario where a four-lattice constant, rotationally symmetric charge density wave (CDW) is present in the underdoped cuprates. We prove a theorem that puts strong constraint on the possible form factor of such a CDW. We demonstrate, within mean-field theory, that a particular form factor within the allowed class describes the angle-resolved photoemission and scan tunneling spectroscopy well. We conjecture that the “large pseudogap” in cuprates is the consequence of this type of charge density wave.

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I. INTRODUCTION

After almost two decades of theoretical study, it is known that the high temperature superconductors have the following known ordered states: (i) antiferromagnetic order at very low doping \((x \leq 3\%)\), (ii) the \( d \)-wave superconducting (DSC) order for \( 5\% \leq x \leq 30\%\). While these two orders exist in all families of cuprates, there is a third order, namely, (iii) a four-lattice constant charge and eight-lattice constant spin density wave order, occurring near doping \( x = 1/8 \) in the \( \text{La}_{1-x}\text{Nd}_{x}\text{CuO}_2 / \text{La}_{1-x}\text{Ba}_{x}\text{CuO}_2 \) (LNSCO/LBCO) systems.1 There is a widespread belief that this charge/spin density wave order is anisotropic, i.e., they form stripes.1–4

A significant part of the high-\( T_c \) mystery lies in the behavior of the underdoped systems.5 Based on specific heat,6 nuclear magnetic resonance,7 DC transport,8 optical and Raman spectroscopy,9,10 angle-resolved photoemission (ARPES)11 and tunneling,12–16 Tallon and Loram have made the case that the high-\( T_c \) superconductors possess two energy gaps, a pseudogap and a superconducting gap.6 Recently ARPES experiments on LSCO systems17 and underdoped Bi2212 (Ref. 18) both point to a large pseudogap in the antinodal region and a superconducting gap near the Brillouin zone diagonals. A similar result has also been found in electronic Raman scattering experiment on Hg1201 (Ref. 19). In addition, it is shown that for underdoped Bi2212 a large pseudogap exists in the antinodal region even at temperature \( \approx 3T_c \), while a gapless Fermi arc exists near the nodes.20

Recently, there are clear evidences from the the scan tunneling spectroscopy (STM) studies suggesting the presence of a four-lattice constant checkerboard order in NaCCOC (Ref. 14) and underdoped Bi2212.15,16 Interestingly ARPES study has shown that in Na\( _2\)Ca\( _{12-x}\)Cu\( _x\)O\( _{22-2x} \)Cl\( _2 \), where STM found checkerboard order,14 the Fermi arcs survive.21 In view of these new experimental results we ask the question “can the pseudogap in underdoped cuprates be caused by some kind of checkerboard CDW”? To answer the question, we will look at the effects of the checkerboard CDW on low energy quasiparticles. Since the existence of low energy quasiparticles is an experimental fact, it is reasonable to model the influence of CDW by an effective scattering Hamiltonian of the form

\[
H_{\text{CDW}} = \sum_Q \sum_k \sum_\sigma \left[ f(k, Q) C_{k+Q, \sigma} C_{k, \sigma} + \text{H.c.} \right].
\]

where \( Q \) is the CDW ordering wave vector and \( f(k, Q) \) the form factor.

In the following, we will first explore the symmetry property of the checkerboard CDW form factor using the experimentally observed STM patterns in Sec. II. In Sec. III, we compare the low energy ARPES and STM spectral functions generated by two representatives among the allowed form factors. Section IV is the summary.

II. TWO THEOREMS ABOUT \( f(k, Q) \)

In Fig. 1(a), we reproduce the STM \( dI/dV \) image of Na\( _2\)Ca\( _{12-x}\)Cu\( _x\)O\( _{22-2x} \)Cl\( _2 \) from Ref. 14. This particular image is made at bias voltage \( 30 \text{ mV} \). However, the same checkerboard pattern was seen in a wide bias range \( -150 \text{ mV} \). Experimentally, it was determined that such a checkerboard pattern contains \( \pm Q \), where

\[
Q = (2\pi/4, 0, 0, 2\pi/4)
\]

as its fundamental ordering wave vector. Hence we limit the \( Q \) summation in Eq. (1) to those given by Eq. (2) and \( k \) to the first Brillouin zone. In Fig. 1(b), we reproduce the two-point correlation function of the observed image presented in Ref. 14. From Figs. 1(a) and 1(b) we construct a caricature in Fig. 1(c) to capture the essence of the observed checkerboard. Interestingly, in each \( 4\times4 \) unit cell there are two inequivalent centers about which the checkerboard is symmetric under

\[
C_{4v} = \{ E, C_2, \sigma_x, \sigma_y, C_4, C_4^3, \sigma_{x+y}, \sigma_{x-y} \},
\]

the point group of the square lattice. (Here \( E \) represents identity, and \( C_2, C_4 \) denote 180 and 90 degree rotations, and \( \sigma \) denotes reflection.) In the following, we take this as implying that \( H_{\text{CDW}} \) is \( C_{4v} \) invariant about these two centers.

Theorem I. A CDW that has the ordering wave vectors given by Eq. (2) and possesses a center of \( C_{4v} \) symmetry in its unit cell must have the following properties.

(1) There must exist another inequivalent \( C_{4v} \) center in the unit cell. This second center is displaced from the first by the
FIG. 1. (Color online) STM dI/dV map (a) and the autocorrelation image of $|E|<100$ meV LDOS maps (b) from Hanaguri et al. (Ref. 14) on NaCCOC, showing the $4 \times 4$ ordering. (c) Caricature of the observed image shown in (a). (d) Possible LDOS pattern which exhibits six independent intensities in the $4 \times 4$ unit cell. In panels (c) and (d), two nonequivalent $s$-symmetry centers are indicated by arrows. In panel (d), the $d$-symmetry centers are indicated by the ellipses.

(2,2) translation or its equivalent. About these two centers $f(k,Q)$ has $s$ symmetry.

(2) There must exist two other centers around which $H_{\text{CDW}}$ remains invariant under $C_{2v}$, the subgroup formed by the first four elements of $C_{4v}$, but changes sign under $C_{4}, C_{4}', \sigma_{x'y'}, \sigma_{x'y}$. Spatially these two new centers must be displaced from the two $C_{4}$ centers by the (2,0) and (0,2) translation or their equivalents. About these two centers $f(k,Q)$ has $d$ symmetry.

Proof. Let us assume $H_{\text{CDW}}$ is invariant under $C_{4v}$ at the origin, i.e., $R'H_{\text{CDW}}R^{-1}=H_{\text{CDW}}$ where $R \in C_{4v}$. This implies

$$f(Rk,RQ) = f(k,Q)$$

from Eq. (1). After a translation $t$ the form factor changes to

$$f(k,Q) \rightarrow g(k,Q) = f(k,Q)e^{iQ\cdot t},$$

where $t$ can be any one of the 16 possible displacements within the unit cell

$$t = (m,n), \quad m,n = 0,1,2,3.$$  

Due to the fact that $Q$ only takes one of the four possible values given in Eq. (2), it can be easily checked that for $t=(2,2)$

$$g(Rk,RQ) = g(k,Q) \forall R \in C_{4v},$$

and for $t=(2,0), (0,2),

$$g(Rk,RQ) = g(k,Q) \forall R \in C_{2v},$$

where $C_{4v}-C_{2v} = \{C_{4}, C_{4}', \sigma_{x'y'}, \sigma_{x'y'} \}$. Q.E.D.

Theorem 1 implies that any 90-degree rotationally symmetric CDW with $(\pm 2\pi/4,0),(0, \pm 2\pi/4)$ ordering wave vectors must simultaneously possess $s$-symmetry centers and $d$-symmetry centers. The presence of both symmetry centers is a necessary consequence of the CDW being rotationally symmetric. Conversely any four lattice constant CDW that does not possess both symmetry centers must break rotation symmetry. In addition, it can be shown easily that a rotationally symmetric CDW discussed above possesses six inequivalent sites in the unit cell, hence allowing six different values of $dI/dV$. This is shown in Fig. 1(d).

Theorem 2. If $H_{\text{CDW}}$ is time reversal invariant, $f(k,Q)$ must be real if one chooses either $d$- or $s$-symmetry center as the origin.

Proof. Time reversal symmetry requires

$$f^*(k,Q) = f(-k,-Q).$$

Since $f(k,Q)$ is invariant under the 180 degree rotation about the $s$ and $d$ centers we have

$$f(k,Q) = f(-k,-Q).$$

As a result,

$$f^*(k,Q) = f(k,Q),$$

i.e., $f(k,Q)$ is real. Q.E.D.

III. EFFECTS OF THE CDW ON ARPES AND STM SPECTRA

In this section we apply the two theorems proven above and take the input from a previous renormalization group calculation to guess the plausible form of $f(k,Q)$. We then investigate the effect of the checkerboard CDW on the STM and ARPES spectral functions of the low energy quasiparticles. We stress that the purpose of this section is not to prove that the ground state of certain microscopic Hamiltonian has CDW order. Rather, we take a phenomenological approach by assuming its existence and look at its consequences that are observable by STM and ARPES.

In Ref. 23 it was shown that, with the help of electron-phonon interaction, a class of electron-electron scattering is enhanced at low energies. This class of scattering involves (momentum conserving) scattering of a pair of quasiparticles near the antinodes. For example, consider a pair of quasiparticles lying on the opposite sides of the almost nested Fermi surface near the $(\pi,0)$ antinodes as shown in Fig. 2(a). After the scattering these two quasiparticles switch sides. The momentum transfer in such a scattering is the “nesting wave vector” of the antinodes. For systems such as NaCCOC (Ref. 21) and underdoped Bi2212 (Ref. 24) it has been shown that such nesting wave vectors are approximately given by Eq. (2). Interestingly, Ref. 23 also shows that accompanying each such scattering there is a related process, whose scattering amplitude has opposite sign, where one of the quasiparticle scattering takes place near the $(0,\pi)$ rather than the...
The above considerations lead us to the following ansatz for realization of Eq. 16 and Fermi surface. In addition, Eq. 16 plus the continuity condition requires
\[ f(k, Q) = 0 \text{ for } k \text{ along } \hat{x} \pm \hat{y}. \tag{15} \]

The above considerations lead us to the following ansatz for the CDW form factor
\[ f(k, Q) = \sum Q \langle \cos k_x - \cos k_y \rangle = \sum Q f_0(k), \tag{16} \]

where \( S(Q) > 0 \). In the following we shall pick a simple realization of Eq. 16 and focus on \( k \) lying close to the Fermi surface.

In general the CDW couples each \( k \) to other 15 \( k \) points in the first Brillouin zone. However, most of these 16 \( k \)'s lie far away from the Fermi surface, hence can be omitted in the low-energy theory. This suggests that one only needs to keep a few close neighbors for each \( k \). Another important consideration guiding our construction of \( H_{CDW} \) is the requirement that a robust antinodal CDW gap exists for reasonable change of doping. It turns out that this requirement is satisfied as long as the nested scattering across the antinodal Fermi surface is the dominant scattering process.

Put all the constraints together we consider the following quasiparticle Hamiltonian in the absence of superconducting pairing
\[ \mathcal{H} = \sum_k \Psi^\dagger_{\alpha}(k) A(k) \Psi_{\alpha}(k), \tag{17} \]

where
\[ \Psi^\dagger_{\alpha}(k) = (e_{k_{x},x} + e_{k_{y},y} + e_{k_{z},z} + e_{k_{w},w})^\dagger, \]

and
\[ A(k) = \begin{pmatrix} \epsilon_k & S_0 f_0(k) & S_1 f_0(k) & S_2 f_0(k) \\ S_0 f_0(k) & \epsilon_{k+Q_1} & 0 & 0 \\ S_1 f_0(k) & 0 & \epsilon_{k-Q_2} & 0 \\ S_2 f_0(k) & 0 & 0 & \epsilon_{k-Q_2} \end{pmatrix}. \tag{19} \]

In Eq. 19
\[ Q_1 = -\text{sign}(k_x)(2\pi/4), \quad Q_2 = (2\pi/4) \text{ for } |k_x| > |k_y|, \]

as shown schematically in Fig. 2(c). In addition, we expect \( S_0 \) to be stronger than \( S_1 \) and \( S_2 \). For the normal state dispersion, we use \( \epsilon_k = \epsilon_{t_0} + t_{1}\lambda \cos(k_x) + \cos(k_y)) / 2 + t_2 \cos(k_x) \cos(k_y) + t_3 \cos(k_x + 2k_y) + \cos(2k_y) / 2 \lambda + \lambda_2 \cos(2k_y) \times \cos(k_x) + \cos(2k_y) \cos(k_x) / 2 + t_5 \cos(2k_y) \cos(2k_y), \) with the hopping constants (in eV) \( t_1, \ldots, t_5 = (-0.5951, 0.1636, -0.0519, -0.1117, 0.0510). \]

In the following, we will compare the effects of the CDW for the two cases where the Fermi surface is nested/not nested by the \( Q \) given by Eq. (2). (We adjust \( t_0 \) to control the degree of nesting.) As to the CDW order parameter, we choose
\[ S_0 = \Delta, \quad S_1 = s \Delta, \quad S_2 = s \Delta, \tag{20} \]

We first discuss the case with Fermi surface nesting. In Figs. 3(a) and 3(c) we present the real space \( dI/dV \) image at bias voltage 20 mV and the ARPES intensity map at the Fermi level. These results are calculated with \( s = 0.2 \) in Eq. (20). The primary effect of changing \( s \) is (1) change the intensity variation in the black perimeter in each unit cell in Fig. 3(a); and (2) affect the strength of shadow band in Fig. 3(c) (see later). Except these changes, the main features of both results are preserved. In Fig. 3(b) we show the \( dI/dV \) image resulting from Eq. (17) where the \( f_0(k) \) in Eq. (19) is replaced by \( \cos k_x - \cos k_y \). (Of course, after such a choice the \( d\)-symmetry center becomes the \( s\)-symmetry center.) The purpose of this figure is to demonstrate the sensitivity of the real space image on the sign of \( f_0 \). Indeed, while the ARPES
image is completely unaffected by such a change, the real space $dV/dN$ is strongly modified. Upon a comparison with the checkerboard pattern observed in Na$_2$Ca$_2$CuO$_2$Cl$_2$ (Ref. 14), it is clear that the form factor $\cos k_x - \cos k_y$ [Fig. 3(a)] produces the real space description best. To better understand the Fermi arc present in Fig. 3(c) we note that in the presence of CDW, the new Fermi surface is determined by
\[
\text{det}[A(k)] = 0. 
\] (21)

Since $\text{det}[A(k)]$ is real [because $A(k)$ is Hermitian] $\text{det}[A(k)]=0$ yields a single equation with two unknowns ($k_x$ and $k_y$). Generally, one expects the solutions to form closed one-dimensional curves. Since $f_\parallel(k)$ vanishes at the node, it is natural to expect the Fermi surface to be practically unaffected in its vicinity. Such an unaffected piece of the Fermi surface and its CDW shadows form a closed contour. The reason that in Fig. 3(c) only a Fermi arc is visible is due to the CDW coherence factor.\textsuperscript{26} In Fig. 3(c), the strongest shadow band effect shows up near the end of the Fermi arcs. Note that such a shadow band position is very different from that expected from antiferromagnetism. Presently there is no report of seeing such shadow bands.\textsuperscript{20,27} The reason may be: (1) the CDW correlation length as observed by STM experiment is not sufficiently long (it is typically of 10 nanometers); (2) in the pseudogap regime, the superconducting pairing still persists. In all cases we studied, the superconducting pairing is very effective in weakening the shadow band effect. When moving away from the zero binding energy, we find that the main changes in the ARPES intensity map are: (1) the intensity in the antinodal regions increases, and (2) the Fermi arcs shrink and move toward the origin of the first Brillouin zone.

By considering all panels of Fig. 3, it is obvious that it is the checkerboard CDW with $f_\parallel(k)=\cos k_x - \cos k_y$ that reproduces both the ARPES and STM phenomenology well. Therefore, we will only consider this kind of form factor in the rest of the paper.

Now, we turn to the case without Fermi surface nesting. In this case, using the checkerboard CDW with an order parameter of the same magnitude as that in Fig. 3, we obtain a weaker fragmentation of the Fermi surface as shown in Fig. 4(a). As to the real space pattern (not shown), the only difference with Fig. 3(a) is a slight increase in the intensity variation in the dark perimeter region.

Next, we turn on a DSC pairing and ask what is the signature of the checkerboard CDW and superconducting pairing coexistence in STM. In this case the Hamiltonian becomes
\[
\mathcal{H} = \sum_k \Phi^\dagger(k) \mathcal{H}(k) \Phi(k), 
\] (22)

where
\[
\Phi^\dagger(k) = (\Psi^\dagger_i(k), \Psi^\dagger_j(-k)), 
\] (23)

and
\[
\mathcal{H}(k) = \begin{pmatrix} A(k) & B(k) \\ B^*(k) & -A(-k) \end{pmatrix}. 
\] (24)

In the above equations
\[
B_{ij}(k) = 0 \text{ for } i \neq j.
\]

For $d$-wave superconducting (DSC) pairing $\Delta_k = \Delta_\parallel(\cos k_x - \cos k_y)/2$. In the presence of inversion symmetry $[A(-k) = A(k)]$ the Hamiltonian in Eq. (24) can also be written
\[
\mathcal{H}(k) = A(k) \otimes \sigma_3 + B(k) \otimes \sigma_1. 
\] (26)

In that case because $\mathcal{H}(k)$ anticommutes with $I \otimes \sigma_z$, the eigenspectrum is particle-hole symmetric. Under such condition the zero-energy eigenvectors are also eigenvectors of $I \otimes \sigma_z$. As a result, the locus of zero energy satisfies
\[
\text{det}[A(k) \pm iB(k)] = 0. 
\] (27)

Since this determinant is complex, setting its real and imaginary parts to zero gives two equations for the two unknown $k_x$ and $k_y$. Consequently, one expects the solutions to be isolated points in the Brillouin zone. Thus with the DSC pairing the Fermi arc produced by checkerboard CDW is reduced to point gap nodes.

In Figs. 4(b) and 4(c) we consider the case where a 60 meV checkerboard CDW order parameter coexists with a $\Delta_\parallel = 40$ meV DSC pairing. Figure 4(b) shows the spatial averaged local density of states (LDOS). Note that the CDW feature on the negative bias side is much weaker than that of the positive side. This is because it is overwhelmed by the density of states due to the van Hove singularity. The two peaks on the positive bias side are the original antinodal coherence peak split by the CDW order. We have checked that the energy separation between these peaks is proportional to the CDW order parameter. Another way to determine the strength of the CDW order is to Fourier transform LDOS at the CDW ordering wave vector. In Fig. 4(c), the real part of the $q=(\pi/2,0)$ component of LDOS is shown. The two peaks on the positive bias side of Fig. 4(b) now appear as a peak and an antipeak. Again, the distance between them is proportional to the CDW order parameter. Thus we propose that by studying the Fourier transformed LDOS, it is possible to extract the strength of CDW ordering.

In Fig. 5(a), we show several ARPES momentum distribution curves (MDC) along the momentum cut ($-\pi/2, \pi$) between them is proportional to the CDW order parameter.
are the same as those in Fig. 3. The presence of two nondispersive MDC peaks separated by the CDW ordering energy gap are below the CDW gap. The presence of two checkerboard CDW state.

The ARPES MDC along the momentum cut \(-\pi/2, \pi\) \rightarrow (\pi/2, \pi) for the checkerboard CDW. All energies considered here are below the CDW gap. The presence of two nondispersive MDC peaks separated by the CDW ordering wave vector is apparent. This is very similar to that observed in Ref. 21.

In Fig. 5(b), we present the energy gap along the normal state Fermi surface for a pure checkerboard CDW state (dashed curve) and a state with coexisting CDW and DSC order (solid curve). The purpose of this figure is to illustrate the effect of DSC pairing in the pseudogap state. It shows how the Fermi arc is replaced by a gap node. With thermal phase fluctuations, this explains why Fermi arcs shrink to four points as temperature approaches zero as observed recently.\(^{20}\) Given these results, we feel quite tempted to associate the larger checkerboard CDW gap with the large pseudogap and the smaller pairing gap on the Fermi arc with the small pseudogap.

In the literature it is widely believed that the pseudogap is a consequence of the short-range antiferromagnetic correlation.\(^{2}\) Thus it is natural to ask what is the relation between the checkerboard CDW discussed above and such physics. On a microscopic level the CDW presented in this paper represents the modulation in the hopping (or antiferromagnetic exchange) integrals. Consequently, it is a kind of spin Peiers distortion which, of course, is compatible with the spin singlet pairing tendency of a quantum antiferromagnet. In addition to the above remarks we note that in a recent paper\(^{28}\) it is found that checkerboard CDW is a self-consistent solution of a $t$–$J$–like model at mean-field level, again testify that checkerboard CDW does not contradict the superexchange physics.

IV. CONCLUSION

In this paper, we present a symmetry constraint on the form factor of a 90 degree rotationally symmetric, commensurate, checkerboard charge density wave. Further guided by a previous renormalization group study\(^{23}\) we construct a simple model describing the scattering of the low energy quasiparticles by the CDW. We then calculate the low energy ARPES and STM spectra using this simple model. The results compare favorably with the existing experiments. In particular, the results show a spatial $dI/dV$ pattern similar to the one observed in Na$_{x}$Ca$_{2-x}$CuO$_{2}$Cl$_{2}$ and underdoped Bi2212 by STM (Refs. 14 and 16). Moreover, in the momentum space it produces Fermi arcs resembling those observed by ARPES (Refs. 17 and 21). In the presence of a d-wave superconducting pairing, the Fermi arcs of the checkerboard CDW are reduced to four gap nodes.\(^{20}\) Therefore, this study supports the notion that the large antinodal pseudogap in underdoped cuprates is generated by the checkerboard charge density wave\(^{29-31}\) conjectured at the beginning of the paper.

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5For a review, see, e.g., P. A. Lee, N. Nagaosa, and X. G. Wen, Rev. Mod. Phys. 78, 17 (2006).
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