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Origin of the checkerboard pattern in scanning tunneling microscopy maps of underdoped cuprate superconductors

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The checkerboard pattern in the differential conductance maps on underdoped cuprates appears when the scanning tunneling microscopy is placed above the O sites in the outermost CuO2 plane. In this position the interference between tunneling paths through the apical ions above the neighboring Cu sites leads to an asymmetric weighting of final states in the two antinodal regions of \( k \) space. The form of the asymmetry in the differential conductance spectra in the checkerboard pattern favors asymmetry in the localization length rather than a nematic displacement as the underlying origin.

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I. INTRODUCTION

The large scale detailed maps of the tunneling density of states (DOS) in underdoped cuprates obtained recently by scanning tunneling microscopy (STM) have aroused great interest.1 This surface sensitive technique to date has been limited to strongly disordered BSCCO and \( \text{Ca}_{2-x}\text{Na}_{x}\text{CuO}_{2}\text{Cl}_2 \) samples. An analysis of these DOS maps found a local breaking of the square symmetry of the underlying lattice to form a checkerboard pattern. The presence of this checkerboard pattern in these two different underdoped cuprates has been interpreted as evidence for the presence of an intrinsic bond-centered electronic glass with unidirectional domains as a key characteristic of the pseudogap phase in underdoped cuprates.2 A number of different interpretations of this pattern have also been suggested in the literature.3-9 In our study we re-examine possible origins for this pattern in light of very recent STM experiments.10

The new STM data taken in the superconducting state at low temperatures show that the checkerboard pattern appears most prominently at voltages where the tunneling processes are predominantly into antinodal regions in \( k \) space. At lower voltages the spatial pattern of the DOS maps is quite different. The low-energy pattern in the superconducting state was successfully analyzed as arising from interference generated by the scattering of propagating Bogoliubov quasiparticles in the presence of weak disorder.11 Kohsaka et al.10 found that a rapid change in the spatial pattern in the DOS maps occurred at the tunneling voltage corresponding to the energy of nodal centered arcs of Bogoliubov quasiparticles at their end points on the diamond formed by the lines in \( k \) space connecting the antinodal points. Thus the checkerboard pattern which appears at higher voltages is formed by the tunneling of electrons and holes into pseudogap state located in the antinodal regions of \( k \) space. The key question to be answered is the origin and interpretation of this checkerboard pattern.

The checkerboard pattern is characterized by a local symmetry breaking which reduces the square \( C_4 \) symmetry of the Cu-O-Cu bonds in a (CuO4) square plaquette to \( C_2 \) symmetry leading to a unidirectional pattern of domains with a glassy short-range order on the length scale of \( 4a \) (\( a \): lattice parameter). This short-range order with local symmetry breaking has led to proposals that a static spin-charge stripe glass coexists with the superconductivity.12-16 Another set of proposals3,4,7 are based on the existence of static fluctuations in an order parameter which breaks both translational and \( C_4 \) symmetry leading to strong scattering of the Bogoliubov quasiparticles consistent with the observations. At this point we should comment on the difficulties associated with an explanation based on an intrinsic symmetry breaking. While it is true that the STM experiments were performed on the highly disordered cuprates, BSCCO and \( \text{Ca}_{2-x}\text{Na}_{x}\text{CuO}_{2}\text{Cl}_2 \), because of their good surfaces. Not all underdoped cuprates are disordered, for example, the two members of the YBCO family, \( \text{YBa}_2\text{Cu}_4\text{O}_8 \) and \( \text{YBa}_2\text{Cu}_3\text{O}_{6.5}\text{-ortho-II} \), are well ordered and intrinsically strongly underdoped with hole concentrations estimated to be \( x=0.14 \) and 0.1, respectively. Indeed samples of these cuprates are of sufficient quality to allow the observation of quantum oscillations at high fields and low temperatures.12 Zero-field experiments on these well-ordered samples show no evidence of static broken translational symmetry in nuclear-magnetic-resonance (YBa2Cu4O8) (Ref. 13) or neutron-scattering (YBa2Cu3O8.5-ortho-II) experiments.14 This lead us to conclude that the translational symmetry breaking observed by STM in the BSCCO and \( \text{Ca}_{2-x}\text{Na}_{x}\text{CuO}_{2}\text{Cl}_2 \) samples results from the strong disorder associated with random doping a short-range spin liquid in these cuprates.

In this paper we propose that the checkerboard pattern observed by STM is caused by the local disorder in the CuO2 planes. Our explanation goes back to the observation by Chen, Rice, and Zhang (CRZ) (Ref. 15) that when the STM tip is centered above the planar O sites, it couples to two tunneling paths through apical Cl ions above the neighboring Cu sites and as a consequence interference between these paths plays an important role. This interference leads to a different tunneling matrix elements for electrons into hole states which are bonding (antibonding) upon reflection about the central O site of the Cu-O-Cu bond.15 CRZ considered the dilute limit and examined the localized states of a single hole bound to a Na+ acceptor in a \( \text{Ca}_{2-x}\text{Na}_{x}\text{CuO}_{2}\text{Cl}_2 \) sample. The Na+ acceptor sits above the center of a (CuO4) square plaquette. They found a doubly degenerate acceptor bound
In their recent paper, Kohsaka et al. discussed the conditions that enhance the checkerboard pattern in the tunneling maps. They find that the pattern emerges most clearly in $Z$ maps which plot the ratio of differential conductances $g(r,V)$, at opposite bias, i.e.,

$$Z(r,E=eV) = g(r,+V)/g(r,-V).$$

Further the checkerboard pattern is most pronounced when the voltage $V$ is adjusted locally to the local pseudogap value. This value varies strongly across the field of view in the STM measurements. This is typically $40\alpha \times 40\alpha$ and the typical length scale of the variation in the local value of the pseudogap is roughly $4\alpha$, similar to the length scale of coherent checkerboard patterns.

In this paper we examine possible sources of local symmetry breaking from $C_4$ to $C_2$ symmetry in the STM patterns in the presence of strong local disorder, combining the CRZ theory for STM tunneling with the Yang, Rice, and Zhang (YRZ) (Ref. 16) phenomenological form for the single electron propagator in the underdoped pseudogap phase.

II. YRZ-PHENOMENOLOGICAL SINGLE PARTICLE PROPAGATOR

YRZ based their propagator on a generalization of the form of the propagator for a lightly doped array of two-leg Hubbard ladders derived by Konik et al.\textsuperscript{17} They introduced a self-energy, $\Sigma_0(k,\omega,x)$, which diverges at $\omega=0$ on a surface spanned by elastic particle-particle umklapp scattering analogous to the behavior of the ladder model. In the two-dimensional square lattice this umklapp surface is a diamond connecting antinodal points on the Brillouin-zone boundary. Note this umklapp surface appears as the energy-gap surface also in the case of wider Hubbard ladders with more than two legs.\textsuperscript{18} YRZ took over the form of $d$-wave RVB gap function $\Delta_0(k,x)=\Delta_0(x)(\cos k,_{-}\cos k)$ from the renormalized mean-field theory (RMFT) of Zhang et al.\textsuperscript{10} Using their Gutzwiller renormalization factor $g_0(x)$ for longer range hopping, YRZ proposed a form for the coherent part of the single-particle propagator $G^0(k,\omega,x)$ in the pseudogap state,

$$G^0(k,\omega,x) = \frac{g_0(x)}{\omega - \epsilon(k) - \mu + \Sigma_0(k,\omega,x)} = g_0(x) \sum_i \frac{Z_{i,k}^0}{\omega - E_{i,k}^0},$$

where $\epsilon(k)$ only includes the nearest-neighbor (NN) renormalized hopping contribution, meanwhile $\epsilon(k)$ includes both the NN and longer range renormalized hopping contributions.

The YRZ propagator fits well the quasiparticle dispersion $E_{i,k}^0$ and their weight $Z_{i,k}^0$ seen in angle-resolved photoemission (ARPES) experiments on the pseudogap phase.\textsuperscript{16,20} It has also been used successfully to interpret a number of other experiments on the cuprate superconductor, i.e., Raman scattering,\textsuperscript{21} optical properties,\textsuperscript{22} and specific heat.\textsuperscript{23} Recently Yang et al.\textsuperscript{20} showed that it also accounts well for the particle-hole asymmetry in the quasiparticle properties open-
ORIGIN OF THE CHECKERBOARD PATTERN IN…

PHYSICAL REVIEW B 80, 174505 (2009)

IV. INTERFERENCE IN TUNNELING SPECTRA WITH THE STM TIP ABOVE O SITES

The detailed STM maps showing the checkerboard patterns were taken on two compounds, Dy-doped BSCCO and Ca$_2$-Na$_4$CuO$_2$Cl$_2$. In BSCCO samples the outmost surface layer is a BiO plane with the Bi ions located directly above the Cu sites in the CuO$_2$ plane. Assuming the STM tips couple predominantly to the empty 6$s$/6$p$ Bi orbitals, the analysis presented below will apply also to BSCCO. We shall restrict ourselves to the former which has a simpler structure. At this point it is useful to recap the CRZ analysis, which discussed the role interference between neighboring tunneling paths in the STM maps. Meanwhile, we focus on the antinodal quasiparticles. With the STM tip centered at position $r$, the differential conductivity at $T=0$ and voltage $V$, is following Tersoff and Hamann,

$$\frac{dI}{dV} \approx \sum_{\sigma, m} |\langle m| a_{r,\sigma}^+ |\Psi_0 \rangle|^2 \delta(\omega - E_m + E_0),$$

where $a_{r,\sigma}^+$ is the electron creation operator at position $r$, $|m\rangle$ are final eigenstates with energy $E_m$, and $\omega = eV$, $|\Psi_0 \rangle$ is the ground state with energy $E_0$. The outermost surface layer is composed of Cl ions which sit directly above the Cu ions in the topmost CuO$_2$ layer so that the STM tip couples primarilly to their 3$p_z$ states (see Fig. 1). When the STM tip is scanned from above the Cl ion at $i$ to a NN Cl-ion site, $i + \tau = (\pm 1, 0)$ or $(0, \pm 1)$, we have

$$a_{r,\sigma}^+ = \langle i, Cl | r \rangle p_{Cl,i,\sigma}^+ + \langle i + \tau, Cl | r \rangle p_{Cl,i+\tau,\sigma}^+,$$

$$p_{Cl,i,\sigma}^+ = \sum_{r'} \langle i + \tau', Cl | i, Cl \rangle c_{i+\tau',\sigma}^+ - \frac{1}{2} \sum_{r'} (-1)^{r'} c_{i+\tau',\sigma}^+,$$

where $(-1)^{r'}$ is from the $d_{z^2}$ symmetry of the Cu orbital, $p_{Cl,i,\sigma}^+$ is the electron creation operator at site $i$ Cl, and $c_{i,\sigma}^+$ is the electron creation operator for the $d$-$p$ hybridized orbital centered on the Cu site at $i$. The integrated current up to a positive voltage $V$ (electron injection) is then
\[ I(r, \omega) = \sum_{\sigma, m} \left| \langle m \rangle \sum_{\sigma'} \langle \bar{\tau}' | (iC_l| \bar{r}) c_{i+\bar{r}', \sigma', \sigma}^+ + (i \bar{r}') C_l| \bar{r} \rangle \right|^2 \Theta(\omega - E_m + E_0), \]

where \( \Theta \) is the Heaviside step function. CRZ pointed out that, when the tip is positioned above the O ion at \( i + \bar{r}'/2 \) lying halfway between the two Cu ions at \( i \) and \( i + \bar{r}' \), the integrated current will be sensitive to the relative phase of the hole states centered at the NN Cu ions. Note the orthogonality of the CI \( 3\bar{r}' \) states to the \( d_{x^2-y^2} \) symmetry of the hole states centered on the Cu site underneath leads to a dominant hybridization with the hole states centered on the four NN Cu sites. Finally, we arrive at the result for the tunneling currents when the STM tip lies halfway between NN CI sites, i.e., above the O sites in the \( x/y \) oriented Cu-O-Cu bonds \( f^{O_{x+y}}(r + \bar{r}'/2, \omega) \) and \( f^{Cu}(r, \omega) \) when the STM tip lies above a Cu site:

\[ f^{O_{x+y}} = \Theta(\omega - E_m + E_0) \left| \langle m \rangle \sum_{\sigma', \sigma} \langle \bar{r}' | (1 + (-1)^{\bar{r}'}) c_{i+\bar{r}', \sigma', \sigma}^+ + c_{i+\bar{r}', \sigma, \sigma} \rangle \right|^2 \Theta(\omega - E_m + E_0), \]

\[ f^{Cu} = \Theta(\omega - E_m + E_0) \left| \langle m \rangle \sum_{\sigma', \sigma} \langle \bar{r}' | (1 + (-1)^{\bar{r}'}) c_{i+\bar{r}', \sigma', \sigma}^+ + c_{i+\bar{r}', \sigma, \sigma} \rangle \right|^2 \Theta(\omega - E_m + E_0). \]

CRZ considered the case of a single hole bound to a Na\(^+\) acceptor which they showed may well have a doubly degenerate ground state. This degeneracy in turn splits in the presence of a quadrupole electric field into states with reflection symmetries with respect to the \( x \) and \( y \) axes. The tunneling current is enhanced due to the interference effect, as schematically shown in Fig. 1. As a result any local perturbation which breaks the symmetry between the two antinodal regions of \( k \) space will lead to a lower \( C_2 \) symmetry in the tunneling current. This makes us then to look at various sources that can give rise to such local symmetry breaking in this highly random system. To proceed further it is useful to examine the nature of the anisotropy observed in the tunneling spectra more closely.

V. MEASURED ANISOTROPIC STM TUNNELING SPECTRA

Kohsaka et al.\(^1\) found that the checkerboard pattern emerges most clearly in \( Z \) maps which plot the ratio of differential conductances \( g(r, V) \), at opposite bias, when the voltage \( V \) is chosen to be at the local value of the antinodal energy gap. In an earlier publication by the same group, individual spectra \( g(r, V) \), where plotted for a series of tip positions placed above O sites in a small area with a pronounced checkerboard modulation.\(^2\) This is illustrated in the checkerboard modulation which shows up clearly in the R map in Fig. 3 which is reproduced from their Fig. 4(b).\(^2\) The R ratio measures the ratio of the integrated currents \( I(r, V) \), at positive and negative voltages

\[ R(r, E = eV) = I(r, + V)/I(r, - V). \]

The map reproduced in Fig. 3 shows the R pattern taken at an energy \( E = 150 \) meV, with clear modulations when the tip...
is above the O sites with a local $C_2$ symmetry but almost no modulations are observed over the Cu sites (denoted by black crosses). The value of the R ratio over the O sites ranges from 0.9 (shown as white) to 0.5 (black).

The individual differential conductances taken above a series of O and Cu sites were also shown in their Fig. 5(b). We have extracted the individual tunneling spectra $g(r,V)$ above the O sites in this typical small area with a pronounced checkerboard pattern in the R map [shown in Fig. 5b of Ref. 2]. All spectra on these underdoped samples show a substantial asymmetry between negative and positive voltages,\textsuperscript{30,31} The negative voltage spectra, which correspond to electron extraction or hole injection, show little structure and has the larger differential conductances. Since a hole can easily exchange positions with a neighboring occupied site while an electron can only hop onto the unoccupied neighboring sites, the tunneling processes that accompany an injected hole are much stronger than those for an electron, as shown by Anderson and Ong\textsuperscript{30} and by Randeria et al.\textsuperscript{31} Within the renormalized mean-field theory of Zhang et al.,\textsuperscript{10} the asymmetry is largely due to the incoherent tunneling process in the hole injection. In the approach we use here based on the YRZ normal-state propagator, only coherent parts of the tunneling processes are included and the particle-hole asymmetry appears at finite voltages which involves tunneling into quasiparticle states away from the chemical potential. The positive voltage spectra show a clear peak around an energy of order 100 meV. Such a peak appears in the density of states calculated for the YRZ propagator by Yang et al.\textsuperscript{16} The YRZ propagator is an ansatz to describe coherent quasiparticles moving in a RVB background and so should agree better for positive voltage due to the weaker contribution of inelastic processes which accompany electron injection. In the subsequent discussion we will focus on the positive voltage spectra and normalize the spectra to be the same in the negative voltage region. In Fig. 4 we show a series of the differential conductances with the tip above O sites in the $x/y$ oriented Cu-O-Cu bonds. The difference from the lower $C_2$ symmetry is clearly visible.

VI. POSSIBLE SOURCES OF THE ANISOTROPY IN THE TUNNELING SPECTRA

We now discuss a number of physical effects which could cause an anisotropy in the tunneling spectra.

A. Intrinsic $C_2$ asymmetry due to nematic or Pomeranchuk order

An asymmetry between the two antinodal regions near $k_{\alpha,y}=(\pi,0)$ and $k_{\alpha,y}=(0,\pi)$ suggests that an intrinsic instability which breaks the $C_2$ symmetry may be present in these samples. The possibility of such an instability has been discussed extensively in the literature. One set of these proposals focuses on a quantum electronic liquid crystal with nematic order.\textsuperscript{32-35} A second on a Pomeranchuk instability which splits the two Van Hove singularities.\textsuperscript{36,37} Recent neutron-scattering measurements of the low-frequency spin fluctuations in YBCO samples have been interpreted as evidence for such intrinsic instabilities.\textsuperscript{38} In the presence of intrinsic asymmetry the NN hopping matrix elements in the $x$ and $y$ directions $t_x$ and $t_y$ will be slightly different. Assuming that the intrinsic asymmetry in the self-energy in the YRZ propagator is small, the change in NN hopping integrals $t_{xy}$ leads to a relative displacement of the reference energy for the
RVB splitting at $k_{A,x}$ and $k_{A,y}$. This in turn leads to a shift in the position of the energy gaps $\Delta_{g}(k_{A,x},y)$, relative to the constant chemical potential. This is apparent in Fig. 5 which shows the predicted anisotropy arising from a uniform hopping asymmetry.

The density of states, $N(E)$, observed by putting the STM tip above $O_{12}$ and Cu sites takes the following form from Eq. (7):

$$N^O_{12}(E) \approx \sum_{i,k} Z^O_k \cos^2 \frac{k_{12}}{2} (\cos k_x - \cos k_y)^2 \delta(E - E^O_{12}) - \Delta(E_{12} - E^O_{12}),$$

$$N^{Cu}(E) \approx \sum_{i,k} Z^i_k (\cos k_x - \cos k_y)^2 \delta(E^i - E),$$

(11)

where $(\cos k_x - \cos k_y)^2$ is the interference factor due to the hybridization with the hole states centered on the four NN Cu sites discussed earlier.

In a clean well-ordered sample with intrinsic $C_2$ symmetry order large domains should occur but in the highly disordered $Ca_{2-x}Na_xCuO_2Cl_2$ samples there is a strong spatially varying electric field. The linear coupling between the orientation of the domains and the local quadrupole component of a random electric field acts as a random orienting field on the order. Since the symmetry of the order is Ising type, the random orienting field will act similarly to a random field in an Ising model. It is well known that the ground state of this Ising model consists of a random array of domains, consistent with the orientational domains observed in the checkerboard patterns. A word of caution, however, is in order. The local anisotropy in the STM spectra does not seem to be consistent with that predicted for this type local asymmetry order. Since the symmetry of the order is Ising type, the random orienting field will act similarly to a random field in an Ising model. A word of caution, however, is in order.

The theoretical DOS for the STM tip located above Cu and O sites shown in Fig. 5 display considerably sharper structure in both cases, with and without the weighting factor $(\cos k_x - \cos k_y)^2$, than is evident in the experimental conductances in Fig. 4. The theoretical DOS contain two prominent features. One is the approximately linear drop from negative to positive voltages leading to the minimum at $\approx 60$ meV. Interestingly this linear feature has been reported in integrated photoemission studies on BSSCO samples by Hashimoto et al., as discussed recently by Yang et al. In the STM spectra there are signs of a minimum at positive voltages in the spectral 2h and 2f in Fig. 4 but at a smaller voltage and faint signs in the other spectra. The second feature is the very sharp peak at $\approx 100$ meV in the theoretical spectra and the much broader peaks at around the same energy in the STM spectra. For both discrepancies a possible remedy could be the much stronger disorder broadening in the local probe in the STM spectra as compared to spatially averaged spectra observed in photoemission.

B. Random electric fields

The random distribution of Na$^+$ acceptors in $Ca_{2-x}Na_xCuO_2Cl_2$ samples generates a random electric field. The local quadrupole component of this field acting on a (CuO)$_2$ plaquette will couple differently to the states at $k_{A,x}$ and $k_{A,y}$. The former is antibonding on the Cu-O-Cu bonds along the x axis and bonding on the Cu-O-Cu bonds along the y axis while the latter has the opposite bonding pattern. These patterns cause opposite quadrupole charge distributions in the two states leading to a potential splitting of the antinodal states in the presence of an external electric quadrupole field. This potential splitting will generate STM spectra similar to those we found for hopping asymmetry and so it also differs from the anisotropy displayed in Fig. 4.

C. Variations in the quasiparticle weight and in the localization length

The tunneling DOS into quasiparticle states is weighted by the quasiparticle weight in the single-particle propagator. In the YRZ ansatz this weight is taken from the RMFT calculations of Zhang et al., and is simply proportional to the hole density, $x$. However the fact that little change in the energy gaps $\Delta_{g}(k_{A,x},y)$ is evident in the spectra shown in Fig. 4 argues against such an explanation. Also the spatial variation in the hole density is longer ranged than the distance between O sites on a (CuO)$_2$. Another possibility is that there is substantial anisotropy in the disorder scattering in k space which causes a local anisotropy in the localization lengths. An anisotropic energy shift and localization length could result, if the potential scattering from the disorder is mainly between opposite antinodal points rather than between $\pm k_{A,x}$ or $\pm k_{A,y}$. An anisotropic energy shift, for example, could remove weight from the energy range (200 meV) covered in the STM experiments. The somewhat longer range of the disorder potential is consistent with this suggestion. The umklapp correlated scattering wave vector for backscattering between the antinodal regions near $\pm k_{A,x}$ or $\pm k_{A,y}$ is much smaller than the wave vector connecting the two antinodal regions, $(\pi, \pi)$. The Fourier transforms of the checkerboard maps show peaks arising from short-range order in the form of 4a wide unidirectional electronic domains. The analysis presented here does not directly address the presence of short-range order on a length scale $\geq a$. Several authors have suggested that the wave vector of this short-range order is approximately equal to the wave vector connecting parallel pieces of the bare band-structure Fermi surface near the saddle points and also the wave vector connecting the turning points of the quasiparticle contours in the normal-state YRZ propagators. The length scale of the domains at $\approx 4a$ is roughly the same as the disorder potential length scale but the interpretation of the short-range order in the checkerboard patterns remains to be an open issue.

VII. CONCLUSION

In this paper we have examined several possible origins for the local checkerboard pattern in the tunneling DOS measured over $O_{12}$ sites. The presence of interference between two tunneling paths centered above the neighboring Cu sites
leads to an anisotropic weighting of the two antinodal regions in $k$ space. Thus the local $C_3$ pattern of the checkerboard can reflect an asymmetry between the two antinodal $k$-space regions. An asymmetric hopping $(t_x, t_y)$ could arise from an intrinsic instability, e.g., toward nematic or Pomeranchuk order. This would split the energies of the pseudogaps at $\pm k_{x,\sigma}$ and $\pm k_{y,\sigma}$. However, an examination of the measured anisotropy in the differential conductance points rather toward an asymmetry in the average magnitude of the conductance, which possibly could result from a difference in the localization lengths at the two antinodal saddle points in the quasiparticle dispersion.


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