Momentum space anisotropy in doped Mott insulators

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We study the single hole $tt't''J$-model numerically to address the momentum space anisotropy found in doped Mott insulators. A simple two band picture to understand how the doped hole is screened by the spin background in states of different momenta is proposed. In this picture, the disparity between the nodal and antinodal regions, observed by experiments in the underdoped cuprate superconductors, follows from local energetic considerations and amounts to the distinction between well defined quasiparticle behavior and spin-charge separation related phenomenology.

**Introduction** - It is known, both experimentally and theoretically, that doped Mott insulators can be significantly anisotropic in momentum space. Explaining this behavior is relevant to understanding the properties of metals close to the Mott insulating state, like the pseudogap regime in high-T$_c$ superconductors. 1, 2

The pseudogap measured by ARPES is the energy difference between the one-electron spectral features at the nodal $[\mathbf{k} = (\pm \frac{\pi}{2}, \pm \frac{\pi}{2})]$ and antinodal points $[\mathbf{k} = (\pi, 0), (0, \pi)]$. 3 This difference, which increases as both the temperature and the level of doping in the CuO$_2$ layers are reduced, is accompanied by the anisotropic behavior in $k$-space present in various experimental observations. 2, 3, 4, 5, 6, 7, 8, 9 Indeed, the deeply underdoped regime shows a clear nodal-antinodal dichotomy as low energy quasiparticle peaks exist around the nodes while there is no evidence of quasiparticle-like behavior near the antinodal points. 2, 4, 5 In electron underdoped cuprates, low energy spectral weight appears around $(\pi, 0)$ instead as the pseudogap is pushed toward the zone diagonal. 10 Interestingly, Raman spectroscopy 11 and the violation of the Wiedemann-Franz law 12 in electron doped materials suggests the presence of chargeless excitations around $(\frac{\pi}{2}, \frac{\pi}{2})$. Hence, the pseudogap in the one-particle dispersion appears to strongly reduce the electronic character of excitations in the pseudogap region.

Strongly correlated materials close to the Mott insulator transition are notorious for the near degeneracy of different ordered states, some of which have been argued to provide a scattering mechanism that reduces quasiparticle features in the pseudogap region. 2, 3, 4, 5, 13, 14 In this letter, we propose a different scenario to understand the observed momentum space anisotropy. In particular, we argue that states close to $(\frac{\pi}{2}, \frac{\pi}{2})$ and $(\pi, 0)$ are different because, due to the competition between the spin exchange energy and the hole kinetic energy, spins surrounding the hole in states near $(\frac{\pi}{2}, \frac{\pi}{2})$ behave differently from the spins surrounding the hole in antinodal states. 13, 14 The nodal-antinodal dichotomy then reflects the existence of two distinct ways in which the lattice spins screen the doped holes.

The 2D $tt't''J$-model, which is the simplest model to study doped Mott insulators as of relevance to the cuprate systems, reproduces the experimental pseudogap dispersion and accounts for anisotropic behavior in $k$-space. 15, 16, 17, 18, 19 Below, we employ the exact diagonalization (ED) and the self-consistent Born approximation (SCBA) techniques to study the single hole $tt't''J$-model and to address how the hole is screened by the local spins in different regions of momentum space. We find that the single hole states can be understood as the superposition of two distinct states, namely a hole-like quasiparticle state and a state where the hole strongly distorts the surrounding spins. Due to their different properties, these states predominate in different parts of $k$-space in the pseudogap regime, thus leading to the disparity between the nodal and antinodal regions. Our results are valid for both hole and electron doped materials – for our purposes, the main distinction between the two regimes is that in the former the pseudogap opens in the antinodal region while in the latter it opens in the nodal region.

**Model** - The single hole 2D $tt't''J$ Hamiltonian is

$$H_{tt't''J} = - \sum_{\langle ij \rangle, \sigma} t_{ij} \left( c_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} + H.c. \right) + \sum_{\langle ij \rangle} J_{ij} S_i \cdot S_j \quad (1)$$

where $t_{ij}$ equals $t$, $t'$ and $t''$ for first, second and third nearest neighbor sites respectively and vanishes otherwise. $\tilde{c}_{i,\sigma}$ is the constrained operator $\tilde{c}_{i,\sigma} = c_{i,\sigma} (1 - n_{i,\sigma})$. The exchange interaction only involves nearest neighbor spins for which $J_{ij} = J$. We only consider $0.2 < J < 0.8$ (units are set so that $t = 1$). Unless otherwise stated, all our results come from the ED of $H_{tt't''J}$ on a $4 \times 4$ lattice. Since we want to analyze how the hole affects the local configuration of the surrounding spins we believe that the study of such a small lattice is relevant. We also present results from the SCBA approach to the $tJ$ model 20, 21, 22 on a $16 \times 16$ lattice to further support the ED analysis.

We start by considering the $t', t'' = 0$ case. In particular, we use the ED technique to determine the lowest energy state for each momentum, denoted by $|\psi_k, J\rangle$, for both $J = 0.2$ and $J = 0.6$. Quite surprisingly, we find that if we perform the same calculation for different values of $J$ the resulting states $|\psi_k, J\rangle$ have almost complete overlap with the Hilbert space $\{|\psi_k, J = 0.2\rangle, |\psi_k, J = 0.6\rangle\}$.
satisfied if the quasiparticle spectral weight vanishes for \( J < J_{\text{dec}} \). The SCBA technique, which is described in Table I, leads to the same result. Therefore, for \( 0.2 < J < 0.8 \), the wave function \( |\psi_{\text{ED}}(t)\rangle \) for different \( J \) and the SCBA results are shown for \( t = 0.2, t = 0.8 \) in Fig. 1. Note that \( |\psi_{\text{ED}}(t)\rangle \) is the Hilbert space spanned by \(|Q_k\rangle\) and \(|U_{\tilde{k}}\rangle\). A physically sensible choice, though, comes from requiring that \( q(t) \) increases with \( t \) while \( f(t) \) decreases.

### Table I: Square of the overlap of \( U(t) \) and \( \psi(t) \)

| \( t \) | SCBA | ED |
|---|---|---|
| 0 | 0.999 | 0.999 |
| 0.1 | 0.996 | 0.996 |
| 0.2 | 0.994 | 0.994 |
| 0.3 | 0.993 | 0.993 |
| 0.4 | 0.992 | 0.992 |
| 0.5 | 0.991 | 0.991 |
| 0.6 | 0.990 | 0.990 |
| 0.7 | 0.989 | 0.989 |
| 0.8 | 0.988 | 0.988 |

FIG. 1: Average value of the staggered magnetization on the holes for \( J \in [0.4, 0.8] \). The model was used instead.
Table II: $\sum_q n_k^U(q, -\frac{1}{2}) \equiv \sum_q (\tilde{U}_k | e^{-\frac{1}{2} \sum_a \frac{J_a}{2} - a/2} | \tilde{U}_k)$. $q = (0, 0)$ results involve sum over $q = (0, 0)$, $q = (\pm \frac{\pi}{2}, 0)$ and $q = (0, \pm \frac{\pi}{2})$. $q = (\pm \frac{\pi}{2}, \pi)$ and $q = (\pi, \pm \frac{\pi}{2})$. $J = 0.4$.

Q states, $(\tilde{e}^{\uparrow})^n S^Q_k(i)$, for different $k$, $t'$ and $t''$. Since these states have a well defined quasiparticle character, the doped hole coexists with the AF spin pattern inherited from the undoped system. For the same reason, the hole momentum distribution function $n_k^U(q, -\frac{1}{2})$ is peaked at $q = k$ while a smaller peak is also observed at $q = k + (\pi, \pi)$ due to the strong AF correlations.

U states have no quasiparticle weight and display quite different behavior. Indeed, Figs. 11(b), 11(d) and 11(f) show that in $|U_k\rangle$ the AF spin pattern of the undoped system is destroyed and the staggered magnetization around the hole [given by $(\tilde{e}^{\uparrow})^{n} S^Q_k(i)$] is very close to zero and even negative. Moreover, the hole momentum distribution function $n_k^U(q, -\frac{1}{2})$ peaks around $q = (\pi, \pi)$ for all momenta $k$ [Fig. 12(a)]. The same real and momentum space properties were checked for $\tilde{U}$ states [these are the energy eigenfunctions $|\psi_k, J, t', t''\rangle$ when $J < J_c(k, t', t'')$]. This fact is illustrated for $\tilde{U}$ states concerning the parameter regime relevant to both hole doped cuprates ($J = 0.4$, $t' = -0.3$, $t'' = 0.2$) and electron doped cuprates ($J = 0.4$, $t' = 0.3$, $t'' = -0.2$) in Table III [which explicitly shows that in these states the hole density also peaks around $(\pi, \pi)$ independently of the momenta $k$.

According to the above spin density results the extra $S^z = -\frac{1}{2}$ spin introduced by doping spreads away from the vacancy in both $U$ and $\tilde{U}$ states. The resulting loss of spin exchange energy is accompanied by a gain in hole kinetic energy. Indeed, the hole momentum distribution results support that, in these states, the hole always lies around the bare band bottom [which is located at $(\pi, \pi)$]. This evidence resembles predictions from spin-charge separation scenarios. Indeed, within the slave-boson formalism, the electron decays into a charged spinless holon, which condenses at $(\pi, \pi)$, and a chargeless spinon, which describes the delocalized spin-$\frac{1}{2}$ that carries the remaining momentum. We should remark that our calculation involves equal time properties in a small lattice and does not aim to prove the existence of true spin-charge separation. However, it supports that in $U$ and $\tilde{U}$ states the lattice spins screen the hole in conformity with short range aspects of spin-charge separation phenomenology.

Table III: $\Delta E^Q$, $\Delta E^U$, $\Delta E^Q$ and $W_k^Q$ with $k = k' \equiv (\pi, 0)$ and $k = k'' \equiv (\frac{\pi}{2}, \frac{\pi}{2})$ for several $t'$ and $t''$ and $J = 0.4$.

The previous results demonstrate that the local configuration of spins encircling the hole is quite different in Q and U states. In this context, it is important to remark that the influence of $t'$, $t''$ on the hole dispersion is sensitive to the surrounding spin environment. For instance, intrasublattice hopping is not frustrated by AF correlations and, indeed, the hole in Q states (which is surrounded by a spin configuration reminiscent of the undoped AF groundstate) strongly disperses along the AF Brillouin zone boundary (AFBZB) for $t', t'' \neq 0$ (see Fig. 2). The opposite limit occurs, for example, in certain $U(1)$ spin liquids, where the underlying spin correlations inhibit coherent intrasublattice hopping. 27 This limit
is closer to what is observed in U states, as \( t', t'' \) are heavily renormalized by the spin background (whose AF correlations are depleted by the hole nearest-neighbor hopping processes). In fact, Table \( \text{III} \) explicitly shows that \( \Delta E^Q_\pi \equiv E^Q_{(\pi,0)} - E^Q_{(\pi/2,\pi/2)} \) is almost one order of magnitude larger than \( \Delta E^U_\pi \equiv E^U_{(\pi,0)} - E^U_{(\pi/2,\pi/2)} \), where \( E^Q_k \equiv \langle Q_k | H_{tt'J} | Q_k \rangle \) and \( E^U_k \equiv \langle U_k | H_{tt''J} | U_k \rangle \).

**Momentum space anisotropy** - In the \( tt't'' \)-model the intrasublattice hopping parameters \( t', t'' \) control the dispersion \( E_k \equiv \langle \psi_k | H_{tt'J} | \psi_k \rangle \) along the ABZB and, thus, the pseudogap energy as well (this is the energy difference between the antinodal and nodal states \( \Delta E^\psi_\pi \equiv E^\psi_{(\pi,0)} - E^\psi_{(\pi/2,\pi/2)} \)). Indeed, both Fig. 2 and Table \( \text{III} \) show that these parameters set the magnitude of the pseudogap, as well as its location in -space.

Interestingly, \( t', t'' \) also control the difference in the quasiparticle character of \( (\pi,0) \) and \( (\pi/2,\pi/2) \), as supported by the dependence of the overlap integral \( W^Q_k \equiv \langle \psi_k | Q_k \rangle^2 \) on these parameters (Table \( \text{III} \)). The resulting \( t', t'' \)-driven momentum space anisotropy is particularly evident when both \( Q \) and \( U \) states have large overlaps with the eigenstates \( | \psi_k \rangle \), as it is the case for the value of \( J \) which is relevant to the cuprate systems, namely \( J = 0.4 \).

The main message of this letter is that the above roles of \( t', t'' \) can be understood with a simple two band picture of the spins around the hole lost their staggered pattern and, at short distances, the doped spin and charge separate. The resulting nodal-antinodal dichotomy, found to occur in the parameter regimes concerning hole and electron doped cuprates, follows from local energetic considerations and not from the interaction of holes with other holes, an incipient order parameter or disorder. It also agrees with previous numerical evidence for spin-charge separation phenomenology at high energy.

Following our results, a new mean field theory of the \( tt't'' \)-model was recently proposed that describes holes dressed by two different spin configurations. It accounts for the observed momentum space anisotropy and is in good agreement with the doping dependence of ARPES experiments.

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