Quasi-one-dimensional dynamics and nematic phases in the two-dimensional Emery model

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We consider the Emery model of a Cu-O plane of the high-temperature superconductors. We show that in a strong-coupling limit, with strong Coulomb repulsions between electrons on nearest-neighbor O sites, the electron dynamics is strictly one dimensional, and consequently a number of asymptotically exact results can be obtained concerning the electronic structure. In particular, we show that a nematic phase, which spontaneously breaks the point-group symmetry of the square lattice, is stable at low enough temperatures and strong enough coupling.

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Immediately following the discovery of high-temperature superconductivity in the cuprates, it was realized[1,2] that the novel physics of these materials is dominated by the strong, short-range repulsion between electrons. However, there has been considerable debate over what is the simplest ''paradigmatic'' model that captures the essential physics of the problem. Despite the fact, pointed out early on by Emery[2] and by Varma and co-workers,[3] that the minimal model which captures the essential local chemistry of the doped copper-oxide planes is the three-band copper-oxide or Emery model (defined below), it has generally been the accepted practice among theoreticians to, instead, consider the single-band Hubbard or *t-J* model—certainly reasonable models for studying the interplay between the localized quantum antiferromagnetism of the undoped system and the charge delocalization produced by doping. Moreover, since none of these strongly interacting models can be solved in two dimensions (2D), any theoretical results that can be established with an acceptable degree of rigor can shed light on the observed physics of the actual materials.

In this paper we show that there exists a limit (which is not wildly unphysical) of the Emery model about which a number of exact statements are possible. Specifically, despite the fact that the model itself possesses the symmetries of the square lattice, the electron dynamics is quasi-one-dimensional in this limit. It is also possible to establish the existence of various electronic liquid crystalline phases,[4] including especially an Ising-nematic phase[5] which spontaneously breaks the fourfold rotational symmetry of the underlying lattice.

I. THE MODEL

We consider a model defined on the copper-oxide lattice, shown in Fig. 1; the corresponding Hamiltonian operator is written explicitly in the Appendix. The copper sites define a simple square lattice at lattice positions $\vec{R}$ with lattice constant a, while the oxygen sites sit at the center of the nearest-neighbor bonds on this lattice, and so define a second square lattice, rotated by 45° relative to the Cu lattice, with lattice positions $\vec{R}+(a/2)\hat{e}_x$ and $\vec{R}+(a/2)\hat{e}_y$, which we will call site $(\vec{R},x)$ and $(\vec{R},y)$, respectively. The vacuum is defined as the state in which all the O p orbitals and Cu d orbitals are full. The relevant Fock space is constructed by adding holes (removing electrons) from the Cu $3d_{x^2-y^2}$ and O $2p_\sigma$ orbitals (i.e., the $2p_x$ orbital associated with the oxygens at $\vec{R},x$ and the $2p_y$ for the oxygens at $\vec{R},y$). The corresponding hole creation operators are $d^\dagger_{\vec{R},\sigma}$ and $p^\dagger_{\vec{R},a,\sigma}$.

The various interactions in the model (also shown in Fig. 1) are defined as follows: The repulsion between two holes on the same site is U_d and U_p, respectively, for a copper and an oxygen site, while the repulsion between two holes on an adjacent copper and oxygen or a nearest-neighbor pair of oxygens are V_{pd} and V_{pp}. All further neighbor interactions are neglected. The hopping matrix elements which transfer a hole between a nearest-neighbor O-Cu pair are $t_{pd}\equiv t$, while those between nearest-neighbor O's are t_{pp}, and the difference between the energies of an electron on an O and a Cu site is $\epsilon>0$. The signs of the various hopping matrix elements are determined by the symmetry of the relevant d and p orbitals. However, a simple gauge transformation with wave vector $\vec{\pi}\equiv(\pi/a)(1,1)$ changes the signs so that all the relevant hopping matrix elements are positive.

The insulating parent state of the undoped cuprates has

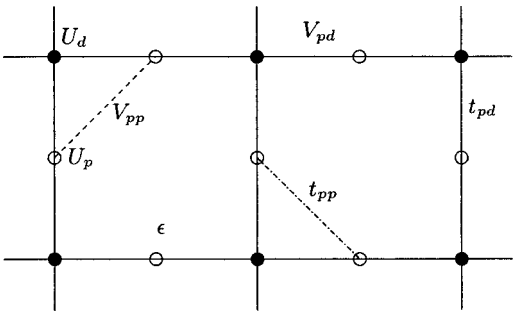

FIG. 1. Schematic representation of the Cu-O lattice. The full circles represent Cu sites and the open circles are O sites. The various terms in the Emery-model Hamiltonian are represented, as discussed in the text.

one hole per unit cell which, because $\epsilon > 0$, live preferentially on the Cu sites. Additional doped holes, whose concentration per unit cell we denote x, go preferentially on O sites because $U_d \gg \epsilon$.

II. THE STRONG-COUPLING LIMIT

We start by defining the ''strong-coupling limit'' of this model, in which the interaction strengths are large compared to the one-electron energies. Here we discuss the salient features of this regime. In the Appendix we present details and prove that the statements we make here are asymptotically exact in this limit.

By the strong-coupling limit we formally mean that we consider the model in the limit $U/t \to \infty$, where all the interactions $U_p, U_d, V_{pd}, V_{pp} \sim U$ and the hopping matrix elements $t_{pd} \equiv t$ and $t_{pp} \sim t$. Even in this limit, the physics depends on the finite ratios of the various interaction strengths. In particular, we will always assume that the following inequalities are satisfied: $U_d > \epsilon > 0$ and $U_d > U_p > V_{pd} > V_{pp} > 0$, consistent with chemical intuition. (Somewhat more restrictive inequalities must be assumed in order to prove all the stated results, as is discussed explicitly in the Appendix.) Finally, since the hopping matrix elements depend exponentially on separation, we set $t_{pp}/t \to 0$. This final assumption may not be well satisfied in the actual materials, where cluster calculations[6] suggest that $t_{pp}/t \sim 1/3$. We will study this model as a function of x and for arbitrary ratio of ϵ/t.

For the undoped system, $x = 0$, the ground-state has zero energy and is 2^N-fold degenerate, with one hole on each copper. Of course, this degeneracy is resolved for finite interaction strengths when antiferromagnetic superexchange interactions, with $J \approx 8t^4/U_p V_{pd}^2$, are included. However, in the strong-coupling limit, this (and most of the other spin physics we will encounter) involves energy scales that vanish as t/U and $t/V \to 0$; we will therefore ignore this physics at first, and then return to it when we consider ''t-J-like'' physics that arises from low order corrections to the strong-coupling limit.

Neglecting the spin degeneracy, the first excited state is an exciton, shown in Fig. 2(a), with a large energy $E_{ex} = V_{pd} + \epsilon + O(t)$, and so can be ignored at low energies and temperatures.

Now, consider one additional doped hole. Since $U \gg V$, adding one hole means increasing the number of occupied sites by 1, and so necessarily costs a minimum energy of $\mu \equiv 2V_{pd} + \epsilon$. Some possible representative states are shown in Figs. 2(b)–2(d): (b) shows the bare hole state, which to zeroth order in t has energy μ; (c) shows a hole-exciton bound state, with zeroth-order energy $\mu + \epsilon$; (d) shows a hole broken into two charge $e/2$ solitons separated by $L = 4$ sites, with zeroth-order energy $\mu + L\epsilon$; (e) shows a bent hole-exciton bound state which is the lowest energy state which involves a disturbance outside of this row and has zeroth-order energy $\mu + V_{pp} + \epsilon$, and so can be neglected in the strong-coupling limit.[7]

The most salient point to notice is that if the doped hole is added to an oxygen on a given row, all states with energy near μ involve disturbances which are confined to the same row. Any state which involves a noncollinear disturbance, such as the bent-hole exciton in 2(e), costs infinite energy in the strong coupling limit.

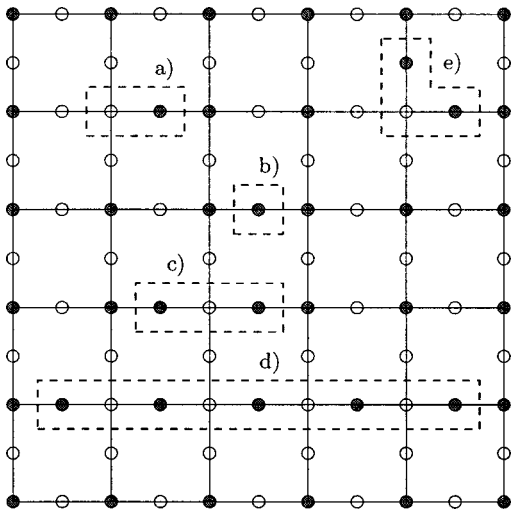

FIG. 2. Schematic representation of various states discussed in the text. The dark circles are Cu and O sites occupied by a hole; the open circles are sites not occupied by holes.

In this limit, therefore, the number of holes on each row and each column of the lattice are separately conserved quantities, and the charge dynamics is purely one dimensional. More precisely, in the Appendix we show that, to leading order in the strong-coupling expansion and for $t_{pp} = 0$, each row p has a conserved quantity X_p and each column q a conserved quantity Y_q, which qualitatively correspond to the number of hole quasiparticles on that row or column. Indeed, doped holes on distinct parallel rows do not interact with each other. However holes on rows and columns do interact with each other (where they meet). We will show below that these interactions play a crucial role. Of course, when we back off from the strong-coupling limit, or if we include a small but nonzero t_{pp}, small effective interactions which violate these conditions will be generated.

III. THE 1D DYNAMICS

Consider a system in which we add a fixed number of doped holes to one and only one row of the lattice. Because the number of electrons in each row is conserved, none of these holes can leak out onto other rows or columns, which thus remain undoped. Indeed, the electron dynamics along this row is exactly equivalent to those of the 1D Cu-O model, which was analyzed previously in Ref. 8:

$$H_{row} = -t \sum_{j,\sigma} [c^\dagger_{j,\sigma} c_{j+1,\sigma} + \text{H.c.}] + \sum_j \epsilon_j \hat{n}_j + \sum_j [U_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} + V_{pd} \hat{n}_j \hat{n}_{j+1}], \quad (1)$$

where even numbered sites are Cu sites and odd numbered sites are O, $\epsilon_{2j} = 0$, $\epsilon_{2j+1} = \epsilon$, $U_{2j} = U_d$, $U_{2j+1} = U_p$, $\hat{n}_{j,\sigma}$

$=c^{\dagger}_{j,\sigma}c_{j,\sigma}$, and $\hat{n}_j=\Sigma_\sigma \hat{n}_{j,\sigma}$. In the strong-coupling $U_j\to\infty$ limit, the charge degrees of freedom can be treated as spinless fermions,[8] with effective Hamiltonian

$$H_c=-t\sum_j\,[c^{\dagger}_j c_{j+1}+\text{H.c.}]+\sum_j\,[\epsilon_j\hat{n}_j+V_{pd}\hat{n}_j\hat{n}_{j+1}], \tag{2}$$

while again the dynamics of the spin degrees of freedom are obtained only when corrections to the strong-coupling limit of order xt^2/U_j are included. The density of spinless fermions per site is simply $(2N)^{-1}\Sigma_j\hat{n}_j=1+x$.

Manifestly, for $x=0$, the system is insulating, with one hole on each copper site and a charge gap $\Delta_c=2V_{pd}+O(t)$. For small, positive x, the *doped holes* are dilute and can be treated within the context of an effective-mass approximation, as free spinless fermions with creation energy Δ_c and effective mass m^*. In particular, the ground-state energy per site (with $W\equiv\hbar^2\pi^2/6m^*$) is

$$E=E_0+\Delta_c x+Wx^3+O(x^5). \tag{3}$$

Both Δ_c and W are continuous functions of ϵ/t: $\Delta_c=2V_{pd}+\epsilon F_\Delta(\epsilon/t)$ and $W=(8\pi^2/3)ta^2F_W(\epsilon/t)$. For $\epsilon\gg t$, $F_\Delta=1+O(t/\epsilon)^2$ and $W=8(t/\epsilon)[1+O(t/\epsilon)^2]$. In the opposite limit, $\epsilon/t\to 0^+$, the fermions fractionalize to form twice as many charge $e/2$ solitonic fermions. However, the ground-state energy has the same x dependence, but with $F_\Delta=-4(t/\epsilon)[1+O(\epsilon/t)]$ and $W=1+O(\epsilon/t)$. An important qualitative point to recognize here is that the Fermi pressure is a decreasing function of ϵ/t which vanishes as $\epsilon/t\to\infty$. Various correlation functions can be accurately estimated, as well, from the well-known theory of the 1D Luttinger liquid.

For $x=1$, the system is again insulating, with one hole on each site. Expanding about this limit, for $1-x$ small, yields a result similar to those obtained for small x. Other interesting states occur in the vicinity of various commensurate values of x. For instance, $x=1/2$ corresponds to commensurability 2 in the spinless fermion problem, where an incompressible charge-density wave state is the ground state of this strongly interacting problem.

Indeed, given the large number of exact, or well controlled approximate, results that can be obtained for the 1D electron gas, and the ease with which quantum Monte-Carlo simulations can be employed to flesh out the analytic results quantitatively, we consider the problem of a single Cu-O row to be a solved problem. This also means that a large number of "fully nematic" states can also be completely characterized. A fully nematic state is defined to be one in which doped holes are placed only on rows (or only on columns). Since holes on neighboring rows do not interact at all (unless we were to add longer range interactions to the model), the dynamics of the holes on each row are determined by the same 1D Hamiltonian we have just analyzed. This does not constitute a complete solution of the problem, since states in which some doped holes lie on rows, and others on columns are still complicated and require additional analysis to characterize. However, we will show below that, under many circumstances, the ground state is fully nematic.

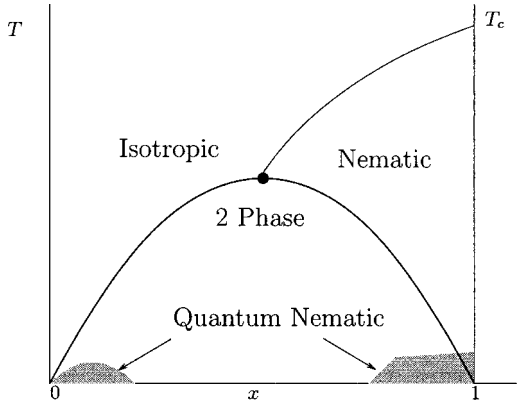

FIG. 3. Schematic phase diagram as a function of temperature and doped-hole concentration in the strong-coupling limit (with magnetic ordering suppressed). Only the classical phase boundaries are shown; thick (thin) line, discontinuous (continuous) transitions; circle, tricritical point; shaded regions, nematic phases stabilized at $t/\epsilon>0$.

IV. THE NEMATIC PHASE

We now move from the analysis of the hole dynamics along a single row or column to study the phases of the full two-dimensional model.

A. The nematic insulator, $x=1$

At $x=1$ there are two holes per unit cell, and in the ground state each Cu and O site along each row is occupied by exactly one hole, while the O sites along columns are empty. The energy per unit cell of this state is $2V_{pd}+\epsilon$. There is a second, degenerate, ground state obtained by exchanging rows and columns. Each ground state spontaneously breaks the 90° rotational invariance of the square lattice but is translationally invariant since all unit cells are equivalent. Furthermore these strong-coupling ground states at $x=1$ have a charge gap. Hence this phase is a nematic insulator.

B. The "classical limit," $\epsilon/t\to\infty$

In this limit (still with $U_d>\epsilon$) the *charge* degrees of freedom define a classical lattice gas which can be mapped precisely to an antiferromagnetic Ising model on the oxygen lattice with exchange coupling $V_{pp}/4$. Here spin up indicates an occupied state and spin down an unoccupied state. Under this mapping, the magnetization of the Ising model is $m=1-x$ and the Néel state is the insulating nematic state.

The phase diagram of this model, shown in Fig. 3, is well known.[9] For $x\lesssim 1$, there is a continuous finite temperature transition from a high-temperature disordered phase to the low-temperature Néel phase. However, at a critical $x=x_c$, there is a tricritical point, such that for $x<x_c$ the transition is discontinuous. At low temperatures, for any $0<x<1$, there

is two-phase coexistence between a ferromagnetic ($x=0$ Mott insulating) and a Néel ($x=1$ insulating nematic) phase.

At elevated temperatures, this classical phase diagram is relatively insensitive to the addition of perturbations to the Hamiltonian. Specifically, even for $t/\epsilon>0$, the phase diagram is hardly altered by quantum effects so long as $T \gg t/\sqrt{t^2+\epsilon^2}$. However, at low temperatures, additional longer range interactions, either added explicitly to the model or induced by quantum fluctuations, can affect the nature of the stable phases substantially. For instance, even at the classical level, including the effect of weak Coulomb repulsion between holes on second-neighbor O orbitals will stabilize an electronic crystalline phase in a narrow range of x near 1/2 and at low enough temperatures. Here the doped holes form a period 2 (Wigner crystal) density wave along each row, while the O's along vertical bonds remain undoped. More generally, at low T and intermediate x, the phase diagram is complex and dependent on details. However, for x near 0 or 1, we will see that quantum effects generically stabilize homogeneous quantum nematic phases, shown as shaded areas in Fig. 3.

C. Quantum effects, $t/\epsilon>0$, for $x\ll 1$ and $1-x\ll 1$

At low temperatures, $T\ll t/\sqrt{t^2+\epsilon^2}$, quantum effects are important, even for small t/ϵ. We start by addressing the nature of the low-temperature phase for $x\ll 1$.

Since the doped holes are fermions, one would generally expect an associated Fermi pressure which tends to favor a uniform state. As shown in Eq. (3), the 1D dynamics of the doped holes imply that the Fermi pressure $\sim Wx^3$, rather than the stronger Wx^2 dependence of a 2D Fermi gas. However, absent any attractive effective interactions between doped holes the Fermi pressure is always sufficient to stabilize a uniform phase at small x. (Effective attractions can arise from magnetic fluctuations but are negligible at strong coupling.)

More specifically, an upper bound to the ground-state energy per site, $E(x)$, at all x is given by the energy of the fully nematic state, $E_{nem}(x)$, i.e., the ground-state energy of the 1D Emery model computed from Eq. (1) or (2). It can easily be imagined that there is an isotropic state (or a less nematic state) that has lower energy. However, while the properties of such an isotropic state cannot be computed exactly, a simple estimate shows that for $x\ll 1$, the ground state is always nematic.

To see this, we compare the energy of the nematic phase with that of an isotropic version of this phase. If we ignore the interactions between doped holes on rows and columns, the isotropic phase would have lower energy, since there are twice as many 1D systems each with 1/2 the density of doped holes, resulting in a factor of 4 reduction in the Fermi pressure. Now, for x small enough, the contributions to the ground-state energy from the V_{pp} coupling between holes on crossing Cu-O rows and columns is a regular function of x, free of infrared divergences. In particular, when two doped holes approach each other at the intersection of a row and a column, the repel each other strongly, and the probability of such an interaction is proportional to x^2. Thus, the energy per site of the nematic state is $E_{\rm nem}=E_0+\Delta_c x+Wx^3+\cdots$, while that of the isotropic state is $E_{\rm iso}=E_0+\Delta_c x+(1/4)Wx^3+V^{\rm eff}x^2+\cdots$, where $V^{\rm eff}$ is an effective repulsion between holes on intersecting rows and columns. Manifestly, at small enough x, the nematic state has lower energy.

The Fermi pressure similarly stabilizes the uniform phase for $x\lesssim 1$. Here the nematic character of the resulting uniform phase is considerably more obvious: the nematic phase consists of an array of Luttinger liquids (one per row) with an effective Luttinger charge parameter K_c and an effective charge velocity v_c.

V. CORRECTIONS TO THE STRONG-COUPLING LIMIT

Low-order corrections to the strong-coupling limit resolve the spin degeneracies we have neglected, and produce other important changes in the physics, which we will discuss elsewhere; here we comment on a few salient features.

A. Magnetic interactions

In the undoped Mott insulator at $x=0$, the most obvious induced interaction[2] is the superexchange interaction between nearest-neighbor Cu spins, which to leading (fourth) order in t is $J=8t^4/[(V_{pd}+\epsilon)^2(U_p+2\epsilon)]\{1+(U_p+2\epsilon)/(2U_d)\}$. However, unlike the one-band model, under some circumstances, for the strong-coupling limit of the Emery model other higher-order interactions can be comparable in magnitude to this interaction. Thus, there is a four-spin ring exchange interaction on a plaquette generated at eighth order, which does not vanish for $U\to\infty$. [For $U_d=U_d=\infty$ and $V_{pd}=V_{pp}=V\gg\epsilon$, we get $J_4=(23/2)t^8/V^7$ while the leading order contribution to J is $J\sim t^4 t_{pp}/V^4$.] Thus, whereas the Mott insulating ground state at $x=0$ of the single band model is inevitably magnetically ordered, the Emery model has, in addition, quantum disordered (likely dimerized) phases.

B. 2D charge dynamics

For any of the conducting phases discussed above, the corrections to strong coupling not only resolve the spin degeneracies but also lead to important changes in the charge dynamics at asymptotically low energies. In particular, under most circumstances, we expect that the peculiar non-Fermi-liquid behavior resulting from the strictly 1D dynamics of the strong-coupling limit will be destroyed at vanishing temperatures by induced interactions (either proportional to t_{pp} or t^2/V_{pp}) which permit holes to hop from a row to a column. These couplings will either lead to a crossover to Fermi-liquid behavior at low temperatures, or to a broken symmetry ground state. However, so long as these interactions are weak, they cannot restore the point-group symmetry, so the nematic character of the resulting states should be robust.[10,11] Moreover, as is characteristic of quasi-1D systems, the non-Fermi-liquid character will still be manifest at nonzero temperatures, energies, or wave vectors.

C. Coulomb interactions

The fact that the model considered has regions of two-phase coexistence, and others where various susceptibilities (including the compressibility) are large, means that the low-temperature physics can be strongly modified by the effect of even weak additional interactions. Of these, the most obvious is the long-range Coulomb interaction, which always frustrates phase separation and instead results in various locally inhomogeneous phases such as stripe and bubble phases.

D. Particle-hole asymmetry

At least at strong coupling, the Mott insulating state at $x=0$ is strongly particle-hole asymmetric: added electrons ($x<0$) remove holes from the Cu sites; these ''doped electrons'' have no local tendency to be dynamically confined to rows or columns.

VI. CONCLUSIONS

It has long been accepted that the Emery model provides a reasonable description of the relevant electronic degrees of freedom in the cuprates. In this paper, we have obtained theoretically well controlled results in a strong-coupling regime of this model. Although cluster calculations suggest that this limit may not be entirely appropriate in the real materials, the insights obtained here may nevertheless capture important features of the physics.

Perhaps the most salient feature of the results obtained here is the existence of a strongly nematic phase in a significant portion of the phase diagram. This contrasts with the behavior of the same model in the weak-coupling limit, where it behaves in similar fashion to the single band Hubbard model in which such a phase, if it occurs at all, is confined to special fillings associated with the proximity to Van Hove singularities.[11,12] Experimental evidence of the existence of a nematic phase[4] in the cuprates was recently reviewed in Ref. 13. The other feature of the phase diagram is the existence of a large region of two-phase coexistence—phase separation. This may be the simplest example of a generic tendency of highly correlated systems to form inhomogeneous states.[14]

ACKNOWLEDGMENTS

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APPENDIX: DETAILS OF THE DERIVATIONS

In this appendix, we formalize the statements concerning the strong-coupling limit. The Cu sites are labeled by the Bravais lattice vectors $\vec{R}$ and the *hole* density on the Cu is $n(\vec{R})$. The hole densities on the two O sites in the same unit cell are labeled $n_{\pm x}(\vec{R})$ and $n_{\pm y}(\vec{R})$, respectively. [Notice that $n_{-x}(\vec{R})=n_x(\vec{R}-a\hat{x})$, and $n_{-y}(\vec{R})=n_y(\vec{R}-a\hat{y})$.] In the strong-coupling limit, the Hamiltonian for the model described in Fig. 1 can be written as the sum of two terms, $H=H_0+H_1$, with

$$\begin{aligned}H_0=&\frac{U_d}{2}\sum_{\vec{R}} n(\vec{R})[n(\vec{R})-1]+\frac{U_p}{2}\sum_{\vec{R}} \{n_x(\vec{R})[n_x(\vec{R})-1]\\&+n_y(\vec{R})[n_y(\vec{R})-1]\}+V_{pd}\sum_{\vec{R}} [n(\vec{R})-1][n_x(\vec{R})\\&+n_{-x}(\vec{R})+n_y(\vec{R})+n_{-y}(\vec{R})-2]\\&+V_{pp}\sum_{\vec{R}} [n_x(\vec{R})n_y(\vec{R})+n_y(\vec{R})n_{-x}(\vec{R})\\&+n_{-x}(\vec{R})n_{-y}(\vec{R})+n_{-y}(\vec{R})n_x(\vec{R})]\end{aligned} \tag{A1}$$

and

$$\begin{aligned}H_1=&-t\sum_{\vec{R},\sigma} [d^\dagger_{\vec{R},\sigma}p_{\vec{R},x,\sigma}+d^\dagger_{\vec{R},\sigma}p_{\vec{R}-a\hat{x},x,\sigma}+d^\dagger_{\vec{R},\sigma}p_{\vec{R},y,\sigma}\\&+d^\dagger_{\vec{R},\sigma}p_{\vec{R}-a\hat{y},y,\sigma}+\text{H. c.}]+\epsilon\sum_{\vec{R}} [n_x(\vec{R})+n_y(\vec{R})],\end{aligned} \tag{A2}$$

where $\sigma=\pm$ is the spin label. As discussed in the text, we set direct O-O hopping amplitude t_{pp} to zero.

To begin with we consider just the effect of the unperturbed Hamiltonian H_0. To make the proofs simpler, we will consider the case in which the following inequalities are satisfied:

$$U_d>2V_{pd},\quad U_p>2V_{pd},\quad V_{pp}>\frac{V_{pd}}{2}. \tag{A3}$$

In this case, H_0 is positive semidefinite, as we will now demonstrate. It is apparent from the structure of the Cu-O lattice, that for every Cu site $\vec{R}$ it is possible to define four triangles, located, respectively, northeast (NE), northwest (NW), southwest (SW), and southeast (SE) of the Cu site, and each having the Cu site and two adjacent O sites for its vertices (see Fig. 1). We will label a triangle $\{\vec{R},s,s'\}$ according to its Cu vertex $\vec{R}$ and by a pair of labels $s=\pm$ and $s'=\pm$, where $\{s,s'\}=\{+,+\}$ corresponds to the triangle NE of $\vec{R}$, $\{s,s'\}=\{+,-\}$ to the triangle NW, etc. We denote by $n_{ss'}(\vec{R})$ the total hole occupancy of triangle $\{\vec{R},s,s'\}$:

$$n_{ss'}(\vec{R})=n(\vec{R})+n_{sx}(\vec{R})+n_{s'y}(\vec{R}). \tag{A4}$$

By using this notation we can equivalently write H_0 in terms of the hole occupancy of each triangle and of the occupancy of the Cu and O sites:

$$H_0=\left(\frac{U_d}{2}-V_{pd}\right)\sum_{\vec{R}} n(\vec{R})[n(\vec{R})-1]+\left(\frac{U_p}{2}-V_{pd}\right)$$
$$\times\sum_{\vec{R}} \{n_x(\vec{R})[n_x(\vec{R})-1]+n_y(\vec{R})[n_y(\vec{R})-1]\}$$
$$+\frac{V_{pd}}{2}\sum_{\vec{R},s,s'} [n_{ss'}(\vec{R})-1][n_{ss'}(\vec{R})-2]$$
$$+\left(V_{pp}-\frac{V_{pd}}{2}\right)\sum_{\vec{R}} \{n_x(\vec{R})n_y(\vec{R})+n_y(\vec{R})n_{-x}(\vec{R})$$
$$+n_{-x}(\vec{R})n_{-y}(\vec{R})+n_{-y}(\vec{R})n_x(\vec{R})\}. \quad \text{(A5)}$$

Since each operator appearing in this expression is individually positive semidefinite, so is H_0, so long as all the inequalities of Eq. (A3) are satisfied.

(Strictly, in the strong-coupling limit, violating the inequalities of Eq. (A3) can lead to major restructuring of the ground state. For instance, for $V_{pp}<V_{pd}/2$, the system phase will separate for any $x>0$, albeit if t is not infinitesimal, quantum effects may lead to inhomogeneous ordered states. Indeed, close to the ''fully frustrated'' point $V_{pp}=V_{pd}/2$, interesting forms of quantum order-from-disorder effects can arise. We will not consider these interesting issues further in this paper.)

Thus, provided the inequalities of Eq. (A3) are satisfied, the Hilbert space of (generally degenerate) zero energy states consists of the set of configurations in which (a) the Cu and the O sites are either empty or singly occupied (by holes), (b) each triangle is either singly or doubly occupied (also by holes), and (c) nearest-neighboring O sites are not simultaneously occupied by holes. All other states are separated from these zero energy states by a finite energy gap. This is the low-energy Hilbert space of states that we will consider here.

Hence, so long as $1\geqslant x\geqslant 0$, there exist zero energy ground states and an extensive ground-state degeneracy. Here, the density of ''doped holes,'' x, is defined in terms of the total hole density per site,

$$1+x\equiv\frac{1}{N}\sum_{\vec{R}} \{n(\vec{R})+n_x(\vec{R})+n_y(\vec{R})\}, \quad \text{(A6)}$$

which is, of course, a conserved quantity. (N is the total number of Cu sites on this lattice.)

To analyze the strong-coupling limit to lowest order in perturbation theory, we confine our attention to the zero energy subspace of the full Hilbert space. Thus, the effective Hamiltonian H_{eff} is obtained by simply taking matrix elements of the perturbing Hamiltonian H_1 defined in Eq. (A2) between states in this subspace. Higher-order terms in the perturbative expansion can be obtained, as is done in deriving the t-J model from the large U limit of the Hubbard model, by including the effects of virtual transitions to the finite energy states of the unperturbed Hamiltonian. For the present purposes, we discuss only the first-order problem, i.e.,

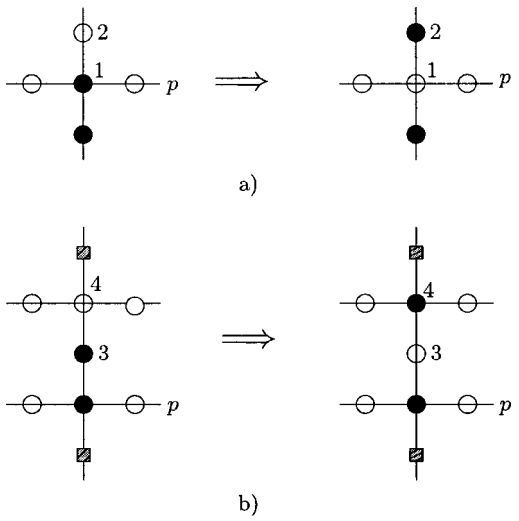

FIG. 4. Conservation of X_p. Shown is a schematic of a segment of the pth row of Cu-O sites and its immediate neighborhood. Cu sites are located at the intersections of the lines; O sites are half way between two Cu sites. Filled (empty) circles are occupied (empty) sites. Empty squares are sites that can either be occupied or empty. In (a) we consider the change in the state produced when a hole hops between a Cu site labeled 1 in the row and the O site labeled 2. In the initial state, the Cu site must be occupied by a hole and the O site must be empty. In order that both the initial and final states survive projection with P_0, the O sites to the left and right must be empty and the O site just below must be occupied. Thus, this process necessarily decreases $n(pa\hat{x})$ by 1, increases $N_x(pa\hat{x})$ by 1, and hence leaves X_p unchanged. In (b) we illustrate the same considerations for applied to the state in which a hole hops from the O site labeled 3 to the Cu site labeled 4, and the notation is the same. The state of the O sites with squares is not uniquely determined. In this case, this process leaves unchanged $n(pa\hat{x})=1$ and $N_x(pa\hat{x})=0$, and so does not change X_p. Clearly, the same considerations imply that the inverse processes and the processes involving sites immediately below the pth row conserve X_p. All other processes in H_1 trivially commute with X_p.

$$H_{\text{eff}}=P_0H_1P_0, \quad \text{(A7)}$$

where P_0 is the projection operator onto the subspace of zero energy eigenstates of H_0 (see Fig. 2).

For $x=0$, there is a threefold orbital degeneracy of the unperturbed ground state, in addition to the 2^N-fold spin degeneracy (which is only lifted, as discussed in the text, when high-order superexchange processes are included). Any $\epsilon>0$ eliminates this orbital degeneracy, and uniquely chooses the ground state with one hole on each Cu site; there are no nonzero matrix elements of the hopping term between states in the ground-state manifold.

For $x=1$, there is a twofold orbital degeneracy of the ground state, as already discussed in the text. As the two states involved are related by a symmetry operation of the Hamiltonian (rotation by $\pi/4$) this degeneracy is not lifted in any order of perturbation theory—this is the nematic insulating phase discussed in the text.

For $\epsilon\gg t$, we perform a second perturbation expansion, which we refer to in the text as the ''classical'' limit: To first

order in ϵ, the ground-state degeneracy is reduced to the subset of states which have precisely xN holes on O sites, i.e., the fewest number possible. Since the term proportional to t in H_1 changes the number of holes on O sites, there are no matrix elements between these states to first order in t. However, to order t^2/ϵ, it is possible for holes to move without violating this constraint.

For intermediate values of x and t/ϵ, the effective Hamiltonian is generally fairly complicated and we have not obtained a general solution. However, we will now prove that under the dynamics of H_{eff}, there are conserved quantities X_p and Y_p corresponding to the number of ''quasiparticles'' in each row or column:

$$X_p \equiv \sum_q \{n(q,p)+n_x(q,p)+N_x(q,p)\}, \tag{A8}$$

where (q,p) is the Cu site $qa\hat{x}+pa\hat{y}$ and $N_x(\vec{R})$ is an operator defined by

$$N_x(\vec{R}) = \begin{cases} 1 & \text{if } n_y(\vec{R}) = n_{-y}(\vec{R}) = 1, \quad n(\vec{R}) = 0 \\ 0 & \text{otherwise.} \end{cases} \tag{A9}$$

Explicitly, since doubly occupied sites are anyway suppressed by U_d and U_p,

$$N_x(\vec{R}) = [1-n(\vec{R})]n_y(\vec{R})n_{-y}(\vec{R}). \tag{A10}$$

The first two terms in the sum in Eq. (A8) count the number of holes along the pth row. The third term, as we shall see, properly accounts for the finite transverse width of the actual quasiparticle excitations by counting the number of vacant Cu sites along the row which have an occupied O site *both* above and below. The column operators Y_p and the associated operator $N_y(\vec{R})$ are defined analogously.

To show that each of these quantities is conserved, we first compute the commutator $[H_1, X_p]$ and then (since $[P_0, X_p]=0$) sandwich the resulting expression between projection operators. X_p trivially commutes with all terms in H_1 except those that hop a hole between a Cu site in row p and the O site immediately above [Fig. 4(a)] or below it, or between a neighboring O site and the next Cu site immediately beyond it [Fig. 4(b)]. In general, the application of these terms changes the value of X_p. However, as can be seen in the figure, and is explained in the caption, if we enforce the condition that the initial and final states after the application of H_1 are still zero energy eigenstates of H_0, only processes which conserve X_p survive. This completes the proof.

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