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Generalized flux phases: Hubbard versus t-J model

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Kinetic and magnetic energies are calculated for the two-dimensional Hubbard model using the variational Monte Carlo method and including a fictitious flux phase. In contrast to earlier results for the two-dimensional t-J model, we found all the flux phases studied lie higher in energy than the paramagnetic or the antiferromagnetic states. Near half filling, the t-J model with no double occupancy on a lattice site is dominated by the magnetic energy, while the Hubbard model with partial double occupancy is dominated by the kinetic energy. When flux phases are introduced into the Hubbard model, the decrease in the magnetic energy is not nearly enough to offset the cost in kinetic energy.

A common feature of all the high-T_c oxide superconductors is the existence of CuO_2 layers. It has been proposed that the t-J model,[1,2] which is derived from the large-U limit of the Hubbard Hamiltonian ($J=4t^2/U$ in two dimensions),[3] is a reasonable starting point to describe the properties of these materials. In order to understand the mechanism of high-temperature superconductivity, many exotic quantum-spin-liquid states have been proposed as the ground state for this model. Anderson *et al.*[4] were the first to propose that the ground state is a d-wave resonating-valence-bond (RVB) state, which is supported by several numerical studies of the t-J model. Alternatively, early mean-field calculations have shown that the ground state of the Heisenberg model evolves in a fictitious, internal magnetic field with $\frac{1}{2}$ flux quantum per plaquette, called the π phase.[5,6] This has been generalized to states with arbitrary flux quantum per plaquette,[7,8] as well as to a staggered flux phase, in which equal but oppositely directed flux is enclosed between neighboring plaquettes.[9,10] Time-reversal symmetry is broken if the flux is not a half-integral or integral multiple of the flux quantum. It has been shown that the generalized flux phase is similar to the fractional quantum Hall effect, with anyon excitations obeying fractional statistics.[11,12] At half filling, it has been shown that both the d-wave RVB states and the commensurate or the staggered flux phases converge to the antiferromagnetic state.[13]

Using the variational Monte Carlo method on the t-J model, Liang and Trivedi[8] found that the commensurate flux phase (CFP) is stabilized for $t \leq J$, at 10% doping, while Lee and Chang[10] showed that away from half filling the staggered flux phase (SFP) has the lower energy, although its energy is still higher than that of the superconducting d-wave state. Uniform and staggered chiral order have also been investigated for a 4×4 cluster in the t-J model using Lanczos algorithm.[14] The cluster calculation[14] suggests that staggered chiral phase may be important in the low-energy physics of the t-J model, while there is no evidence in favor of uniform chiral state. Since the t-J model is derived from the large-U limit of the Hubbard Hamiltonian, it is interesting to see if these conclusions remain valid in the Hubbard model.

We have carried out variational Monte Carlo simulations for the two-dimensional Hubbard model on a square for a wide range of electron density, flux phases, and U. In contrast to earlier results for the t-J model,[8-10] we find that the nonsuperconducting ground state is either paramagnetic or antiferromagnetic. The discrepancy can be understood from the choice of variational wave functions: The t-J model, being derived from the large-U limit of the Hubbard model, employs a Gutzwiller projection operator to eliminate any possibility of doubly occupying a site, while in the Hubbard model, the fraction of doubly occupied sites is a variational parameter. In agreement with the earlier calculations for the t-J model,[8-10] we find the presence of flux in the wave function leads to an increase of the kinetic energy and a drop in the Coulomb energy. However, the cost in the kinetic energy near half filling is significantly lower in the t-J model than that in the Hubbard model (the kinetic energy of the t-J model vanishes at half filling). In the Hubbard case, the decrease in magnetic energy is not nearly enough to offset the cost in kinetic energy.

The nearest-neighbor Hubbard model is given by

$$H=-t\sum_{\langle i,j,\sigma\rangle} c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_i U n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where $\langle i,j\rangle$ denotes a sum over the nearest-neighbor pairs. The simplest trial state is the Gutzwiller wave function:

$$|G\rangle=\prod_i[1-(1-g)n_{i\uparrow}n_{i\downarrow}]|\Psi\rangle\,, \tag{2}$$

which projects out some fraction of doubly occupied sites, with the parameter g determined variationally. The state $|\Psi\rangle$ is an independent-particle state which can contain additional variational parameters. For the antiferromagnetic state,

$$|\Psi\rangle=\exp\left(h\sum_i \pm (n_{i\uparrow}-n_{i\downarrow})\right)|\Psi_0\rangle\,, \tag{3}$$

where a fictitious magnetic field h serves as a variational parameter to enforce antiferromagnetic order. For the flux phases, $|\Psi\rangle$ is the eigenstate of the tight-binding Hamiltonian for electrons in a uniform magnetic field B:[15]

$$H_0=-\sum_{\substack{\langle i,j\rangle\\ \sigma}} \exp(i\phi_{ij})c_{i\sigma}^{\dagger}c_{j\sigma}\,. \tag{4}$$

For electrons on a lattice in a magnetic field with flux $p/q = Ba^2$ per plaquette in units of the flux quantum, $\phi_{ij} = 2\pi \int_i^j \mathbf{A} \cdot d\mathbf{l}$, where $\mathbf{A}$ is the vector potential, and p, q are integers. In the mean-field limit, Affleck and Marston[5] have shown that the Heisenberg Hamiltonian can be reduced, by a Hubbard-Stratonovich transformation, to a tight-binding model with a nonuniform hopping parameter, the solutions of which include the uniform π phase. In this model, the magnetic field is dynamically generated through the interaction of the hole with the background spins, but does not appear explicitly in the Hamiltonian. The inconsistency of having an external magnetic field in the wave functions but not explicitly in the Hamiltonian leads to a gauge-dependent energy spectrum. To determine the optimal gauge, we follow Liang and Trivedi[8] to exploit an extra degree of freedom in the wave function by introducing additional phases associated with the location of the holes. This procedure is equivalent to a gauge transformation. The resulting kinetic energies resemble the Hamiltonian of the uniformly frustrated classical XY model. The ground state of this model[16] gives the optimal gauge that minimizes the kinetic energy. The Landau levels are rescaled by a factor of $1/\sqrt{2}$ for the $\frac{1}{2}$ flux state and by $\frac{2}{3}$ for the $\frac{1}{3}$ flux state.

The staggered flux phase breaks the lattice up into two interpenetrating square sublattices (i.e., a checkerboard), each of which encloses an equal but oppositely directed flux energy. In this case the optimal gauge is obtained[10] by simply taking all $|\phi_{ij}| = (\pi/2)\varphi$, with opposite sign for the two neighboring plaquettes. The resulting SFP wave functions are identical to that of the CFP for $\varphi = \frac{1}{2}$.

We used a stochastic algorithm developed by McQueen and Wang[17] that maps the Gutzwiller matrix elements onto a statistical model, which can be evaluated in a way similar to finite-temperature Monte Carlo simulations. This approach has been applied successfully to the Anderson model.[18] Our results for the Hubbard model will be presented for the antiferromagnetic state, for the CFP with $\frac{1}{2}$ and $\frac{1}{3}$ flux, and for the SFP with $\frac{1}{3}$ flux.

Introducing a CFP into the variational wave functions effectively renormalizes the band width so that electrons become more localized. This lowers the Hubbard energy (i.e., the probability of double occupancy) at the expense of the kinetic energy. These results can be seen from Fig. 1 which shows (a) the kinetic energy per site and (b) $\langle \sum_i n_{i\uparrow} n_{i\downarrow} \rangle$ per site as a function of g, at half filling, for a 6×6 lattice. (The remaining figures are all for 12×12 square lattices.) The Gutzwiller states are denoted by open squares, the CFP are solid squares ($\varphi = \frac{1}{2}$) and asterisks ($\varphi = \frac{1}{3}$), and the SFP is solid triangles ($\varphi = \frac{1}{3}$). It is interesting to compare them with the recent calculations of Hasegawa *et al.*,[19] who studied the ground-state energy of spinless electrons in two dimensions, in an external magnetic field. The magnetic field splits the parabolic

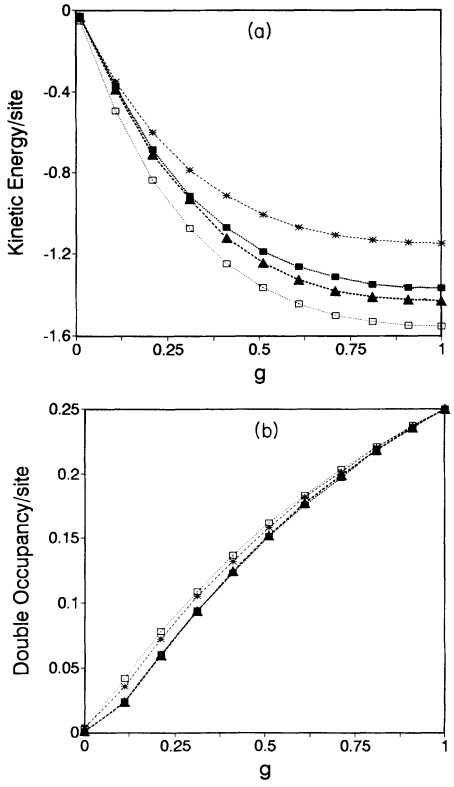

FIG. 1. (a) The kinetic energy per site and (b) $\langle \sum_i n_{i\uparrow} n_{i\downarrow} \rangle$ per site as a function of g, at half filling, for 6×6 lattices. The symbols are open squares (paramagnetic), solid squares (CFP, $\varphi = \frac{1}{2}$), asterisks (CFP, $\varphi = \frac{1}{3}$), and solid triangles (SFP, $\varphi = \frac{1}{3}$). Lines drawn through the points are guides to the eye.

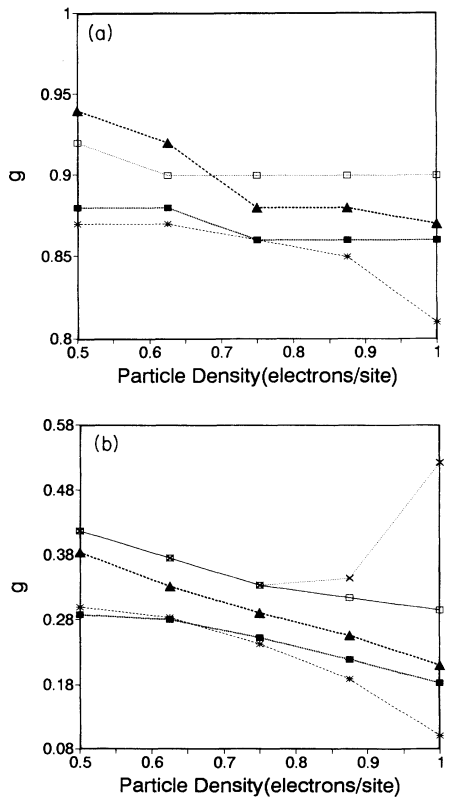

FIG. 2. g as a function of particle density for (a) $U = 0.8t$ and (b) $U = 8t$, for 12×12 lattices. Symbols have the same meaning as in Fig. 1. The crosses represent antiferromagnetic states. Lines drawn through points are guides to the eye.

bands into Landau levels which are φ-fold degenerate. The periodic potential broadens the Landau levels into subbands, and the energy has an absolute minimum if the chemical potential falls in the gap of the Landau subbands. This behavior is similar in spirit to the Peierls instability. For a square lattice, they find the π phase is the ground state at half filling, which is in close agreement with our results. In the Hubbard model, there is some cancellation between the kinetic energy (raised by the flux phases) and the Hubbard energy (lowered by the flux phases), because the magnetic field is hidden within the Hubbard term. The cost in kinetic energy is higher in the CFP than in the SFP, and is the highest in the noninteracting limit ($g=1$), since the flux phases represent a poor variational state when the internal field is missing. Double occupancy is prohibited in the infinite-U ($g=0$) limit, so that the kinetic energies for all flux phases become zero.

Near the half filled limit, the variation of the kinetic energy with respect to g highlights a fundamental difference between the t-J model and the Hubbard model: in the t-J model g is *artificially* set at zero, while in the Hubbard model g is a variational parameter. The density dependence of g is shown in Fig. 2 for (a) $U=0.8t$ and (b) $U=8t$. At half filling, for the paramagnetic ground state, we find $g=0.9$ and 0.29 for $U=0.8t$ and $8t$, respectively. Also included in Fig. 2(b) is the antiferromagnetic states (crosses). At half filling, antiferromagnetic order promotes electron hopping which increases the probability of doubly occupied sites (g is raised from 0.29 to 0.52). However, $\langle\sum_i n_{i\uparrow}n_{i\downarrow}\rangle$ per site is actually lowered at the expense of kinetic energy. The discrepancy can be understood in the mean-field limit:

$$\left\langle\sum_i n_{i\uparrow}n_{i\downarrow}\right\rangle \simeq \sum_i \left\langle\left[n_i+\frac{\Delta n_i}{2}\right]\right\rangle\left\langle\left[n_i-\frac{\Delta n_i}{2}\right]\right\rangle$$

$$\simeq \sum_i \left[\langle n_i\rangle^2-\left\langle\frac{\Delta n_i}{2}\right\rangle^2\right], \tag{5}$$

where n_i and Δn_i are the average density and the spin density at site i, respectively. Thus, antiferromagnetism may lower $\langle\sum_i n_{i\uparrow}n_{i\downarrow}\rangle$ even though the probability of double occupancy is enhanced.

The calculated kinetic energy per site as a function of electron density is shown in Fig. 3 for (a) $U=0.8t$ and (b) $U=8t$. As the density increases, the kinetic energy decreases in case (a), but increases in case (b). The difference arises from the choice of g. In the large-U limit, case (b) is somewhat closer to the t-J model ($g=0$), the kinetic energy of which vanishes in the half filled limit for all phases. The major effect of introducing the flux phases into Gutzwiller wave functions is to raise the kinet-

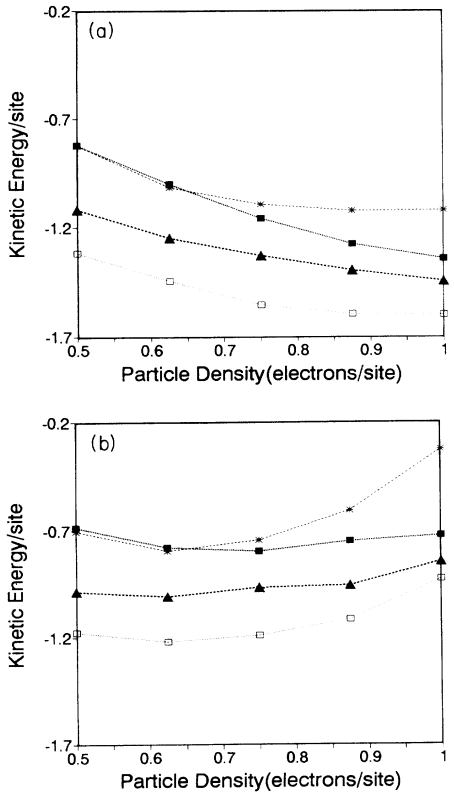

FIG. 3. Kinetic energy as a function of particle density for (a) $U=0.8t$ and (b) $U=8t$, for 12×12 lattices. Symbols have the same meaning as in Fig. 1. Lines drawn through the points are guides to the eye.

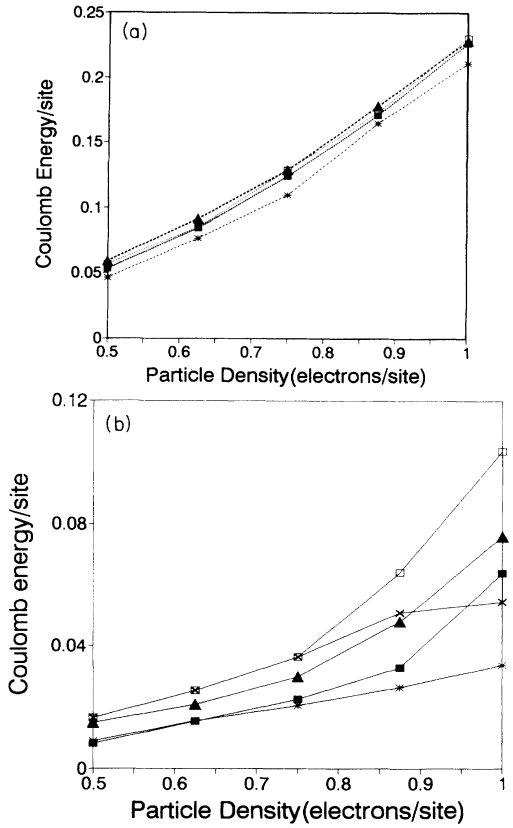

FIG. 4. $\langle\sum_i n_{i\uparrow}n_{i\downarrow}\rangle$ per site as a function of particle density for (a) $U=0.8t$ and (b) $U=8t$, for 12×12 lattices. Symbols have the same meaning as in Fig. 2. Lines drawn through the points are guides to the eye.

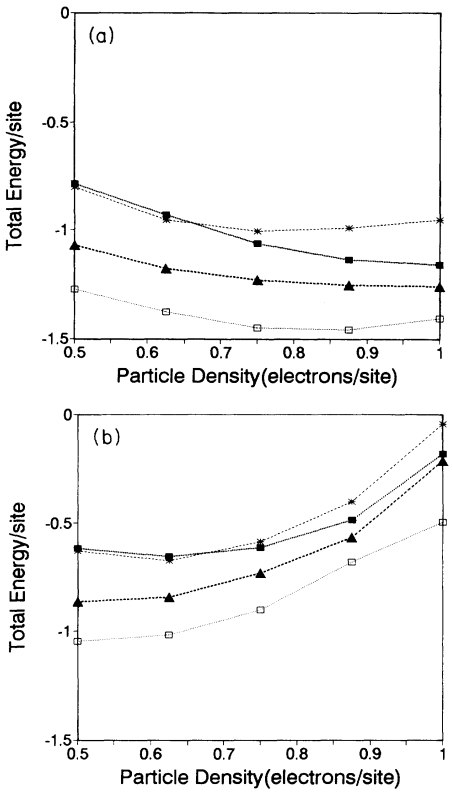

FIG. 5. Total energy per site as a function of particle density for (a) $U=0.8t$ and (b) $U=8t$, for 12×12 lattices. Symbols have the same meaning as in Fig. 1. Lines drawn through the points are guides to the eye.

ic energy for any density due to rescaling of the band width. Accordingly, the corresponding Hubbard energies, shown in Fig. 4, are lowered because electrons hop less frequently. In particular, there is a locking behavior of the flux states with density. We find a minimum in the kinetic energy whenever the Fermi energy lies in a gap between Landau subbands similar in spirit to the Peierls instability. At a given number of electron per site n, the minimum occurs whenever $p/q \sim n/2$. Qualitatively, these results are consistent with those of the t-J model.[8-10]

The total energy as a function of particle density is shown in Fig. 5 for (a) $U=0.8t$ and (b) $U=8t$. In all cases studied, the cost in kinetic energy when flux phases are introduced is so high that the ground state is either paramagnetic, or in the half filled limit, antiferromagnetic. Lee and Chang[10] have shown that the nonsuperconducting ground state is SFP ($\varphi=0.1$) for a lattice of 82 sites with a hole concentration of $\frac{8}{82}$ and $J/t=2$. We have repeated these calculations for the Hubbard model. The energy differences are smaller in this case because the flux is so small. However, the qualitative behavior remains unchanged.

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