Large-N limit of the square-lattice t-J model at $\frac{1}{4}$ and other filling fractions

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We present a mean-field theory of the t-J model on a square lattice that becomes exact in a particular large-N limit. A detailed study of the free-energy manifold is carried out for the case of filling fraction $\nu=\frac{1}{4}$ as a function of t/J. Over the manifold examined, the ground state is either an insulating crystal of an N-hole bound state (for small t/J) or a normal Fermi liquid (for large t/J). For $\frac{1}{4}\leq\nu\leq\frac{1}{2}$, and $t=0^+$, states with the localized holes, and nonzero spin correlations restricted to clusters of 4 or smaller, are global free-energy minima; in particular they are lower in energy than the state with uniform flux $\Phi=\nu$, with staggered flux or a normal Fermi liquid.

I. INTRODUCTION

The t-J model has recently emerged as a viable phenomenological model for the motion of holes in CuO_2 layers of the high-temperature superconductors in the $La_{2-x}Sr_xCuO_4$ family.[1] The constraint prohibiting double occupancy of every site, however, makes the solution of the model highly nontrivial. Considerable progress has been made on understanding the properties of a small number of holes.[1] An alternative approach has been to extend the spin symmetry group of the electrons from SU(2) to SU(N) and to then perform a large-N expansion.[2-5] An advantage of the latter approach is that it is not restricted to filling fractions, ν, near $\frac{1}{2}$. We shall use the large-N method to examine in detail a mean-field theory of the t-J model at $\nu=\frac{1}{4}$. Some results will also be presented for other rational values of ν between $\frac{1}{4}$ and $\frac{1}{2}$. Throughout, our emphasis shall be on determining *global* free-energy minima; this strategy was fruitful in understanding the properties of undoped SU(N) antiferromagnets.[6]

A few comments are in order here on the meaning and validity of the large-N method. By adding biquadratic exchange terms to the Hamiltonian[2] it is possible to obtain a family of SU(N) models all of which have the same SU(2) limit. The particular large-N limit we shall use here has no biquadratic exchange, and is closely related to the "fermionic" large-N limit used by Read and Sachdev[6] for the case of the insulator at $\nu=\frac{1}{2}$; the insulating ground state was found to possess strong spin-Peierls ordering. By changing the representation of the SU(N) spins it is possible to decrease the magnitude of the spin-Peierls ordering until eventually the system undergoes a transition to a Néel ordered phase.[6] The fermionic large-N limit is well away from this transition and thus does not clarify the nature of the destruction of Néel order. However, for the insulator, it captures the correct physics at distances much larger than the spin correlation length.[7] The presumption of this paper is that the fermionic large-N limit continues to do this at values of ν away from half filling. Thus our results will not shed any light on the details of the destruction of Néel order by doping,[8] but hopefully will capture the correct physics at the longest length scales.

The t-J model studied in this paper is described by the Hamiltonian,

$$H=-\frac{t}{N}\sum_{\langle ij\rangle}Pc_{i\alpha}^{\dagger}c_j^{\alpha}P+\text{H.c.}-\frac{J}{N}\sum_{\langle ij\rangle}c_{i\alpha}^{\dagger}c_i^{\beta}c_{j\beta}^{\dagger}c_j^{\alpha}\,, \tag{1.1}$$

where the $c_{i\alpha}$ are fermion annihilation operators, the sums over i,j extend over all nearest-neighbor links on the square lattice, there is an implied sum over repeated spin indices α,β over $1,\ldots,N$ ($N=2$ for the high-temperature superconductors) and P is the projection operator that maintains the constraint

$$c_{i\alpha}^{\dagger}c_i^{\alpha}\leq\frac{N}{2} \tag{1.2}$$

at every site (N even). The Hamiltonian H is clearly invariant under global SU(N) spin rotations, and the fermions transform under the fundamental representation of SU(N). The large-N expansion proceeds[3,4] by introducing a boson b_i at each site that counts the number of holes; thus the constraint (1.2) is replaced by

$$c_{i\alpha}^{\dagger}c_i^{\alpha}+b_i^{\dagger}b_i=\frac{N}{2}\,, \tag{1.3}$$

and the hopping term in H takes the form

$$-(t/N)\sum_{\langle ij\rangle}b_ic_{i\alpha}^{\dagger}c_j^{\alpha}b_j^{\dagger}\,.$$

The filling fraction ν is determined by the global constraint

$$\frac{1}{N_s}\sum_i c_{i\alpha}^{\dagger}c_i^{\alpha}=N\nu\,, \tag{1.4}$$

where N_s is the number of sites on the lattice.

We express the partition function Z associated with H at inverse temperature β as follows:

$$Z\int\mathcal{D}\tilde{Q}\mathcal{D}c\mathcal{D}c^{\dagger}\mathcal{D}b\mathcal{D}\lambda\exp\left[-\int_0^{\beta}d\tau(\mathcal{L}_1+\mathcal{L}_2)\right], \tag{1.5}$$

where

$$\mathcal{L}_1=\sum_i\left[b_i^{\dagger}\frac{\partial b_i}{\partial\tau}+c_{i\alpha}^{\dagger}\frac{\partial c_i^{\alpha}}{\partial\tau}-i\lambda_i\left[c_{i\alpha}^{\dagger}c_i^{\alpha}+b_i^{\dagger}b_i-\frac{N}{2}\right]-\mu(c_{i\alpha}^{\dagger}c_i^{\alpha}-N\nu)\right] \tag{1.6}$$

and

$$\mathcal{L}_2=\sum_{\langle ij\rangle}\left[\frac{N|\tilde{Q}_{ij}|^2}{J}-\tilde{Q}_{ij}c_{i\alpha}^{\dagger}c_j^{\alpha}-\frac{t}{N}b_i c_{i\alpha}^{\dagger}c_j^{\alpha}b_j^{\dagger}\right]. \quad (1.7)$$

We have introduced a chemical potential μ to fix the total number of electrons. The field $\tilde{Q}_{ij}$ arises from a Hubbard-Stratonovich decoupling of the exchange term. Further analysis is simplest in terms of the shifted field $Q_{ij}=\tilde{Q}_{ij}+tb_i b_j^{\dagger}/N$ and the decomposition $b_i=\sqrt{N\delta_i}\exp(i\phi_i)$ whence $\mathcal{L}_2$ takes the form

$$\mathcal{L}_2=\sum_{\langle ij\rangle}\left[\frac{N}{J}[|Q_{ij}|^2-2|Q_{ij}|t\sqrt{\delta_i\delta_j}\cos(\phi_i-\phi_j-a_{ij})+t^2\delta_i\delta_j]-Q_{ij}c_{i\alpha}^{\dagger}c_j^{\alpha}\right]. \quad (1.8)$$

The fictitious gauge field a_{ij} is the phase of Q_{ij}, i.e., $Q_{ij}=|Q_{ij}|\exp(ia_{ij})$.

It is clear now that upon integrating over the fermion fields, the resulting effective action will be multiplied by a prefactor N. In the large-N limit, therefore, the functional integral can be performed in the saddle-point approximation. This procedure is equivalent to determining the mean values of the chemical potential μ and the fields Q_{ij}, δ_i, ϕ_i, and λ_i that satisfy the constraints [(1.3) and (1.4)] on the average and minimize the fermion free energy. We can use the gauge invariance of the action to choose $\phi_i=0$; in this gauge the values of all the a_{ij} (and not just the fluxes on each plaquette) become significant.

We note here that the *physical* electromagnetic gauge field can be introduced by replacing the last term in $\mathcal{L}_2$ by $\exp(iA_{ih})Q_{ij}c_{i\alpha}^{\dagger}c_j^{\alpha}$. The action now has the U(1)×U(1) gauge invariance

$$\begin{aligned} &c_{i\alpha}^{\dagger}\rightarrow c_{i\alpha}^{\dagger}\exp(-i\alpha_i-i\beta_i)\,,\\ &\phi_i\rightarrow\phi_i+\alpha_i\,,\\ &a_{ij}\rightarrow a_{ij}+\alpha_i-\alpha_j\,,\\ &A_{ij}\rightarrow A_{ij}+\beta_i-\beta_j\,. \end{aligned} \quad (1.9)$$

In the large-N limit, the b_i bosons Bose condense, $\langle b_i\rangle=\sqrt{N\delta_i}$, leading to a breaking of the internal U(1) gauge symmetry associated with α_i. The physical electromagnetic gauge symmetry associated with β_i is, however, unbroken. Bose condensation of the b_i bosons therefore does not imply the existence of superconductivity.[9]

Having established our notation, we are now in a position to present the new results established in this paper. The most extensive analysis has been carried out for $\nu=\frac{1}{4}$ and some results have been obtained for other rational $\frac{1}{4}\leq\nu\leq\frac{1}{2}$. We discuss these two cases in turn.

A. $\nu=\frac{1}{4}$

(a) For $t<0.3J$ the global ground state, over the manifold examined, is shown in Fig. 1. We have $a_{ij}=0$, $\delta_i=0.25$, and $Q_2<0.5Q_1$. The state is an insulator with a fermion excitation gap of Q_1-2Q_2. For $t=0^+$, we have $Q_2=0$ and $Q_1=J/4$; each plaquette surrounded by the Q_1 bonds can therefore be interpreted as a *N-hole bound state*. For finite values of t, therefore, an appealing interpretation of the insulating state is that of a crystal of an N-hole bound state.

(b) At $t=0.3J$, the system undergoes a first-order transition to a normal metallic Fermi liquid. The metallic states has $a_{ij}=0, Q_{ij}$ uniform on all the bonds and $\delta_i=0.25$. It is globally stable for all $t>0.3J$.

(c) The commensurate flux state introduced by Hasegawa *et al.*[10] and Lederer *et al.*[11] would correspond to a state with sum of a_{ij} around a plaquette equal to $2\pi\Phi=\pi/2$. Such a state was found as a metastable saddle point of the free energy *only* at $t=0$. For nonzero t the state *immediately* developed a modulation in the values of $|Q_{ij}|$. Moreover the flux distribution becomes nonuniform and is no longer pinned at the commensurate value. Hasegawa *et al.* and Lederer *et al.* have pointed out the existence of a cusp in the total energy as a function of a uniform flux through the lattice; however, there is no such cusp towards variations in $|Q_{ij}|$, thus explaining the instability of the commensurate flux state at nonzero t.

(d) Staggered[2,5] and nonuniform flux states are also found as saddle points of the free energy. It has already been noted in Ref. 2 that the Fermi-liquid state is lower in energy than the staggered flux state at $\nu=\frac{1}{4}$. We find here that the staggered and nonuniform flux states are always higher in energy than all of the states discussed under points (a), (b), and (c).

B. $\frac{1}{4}<\nu\leq\frac{1}{2}$

Because of the complexity of the free-energy minimization problem, our analysis was restricted to $t=0^+$. An

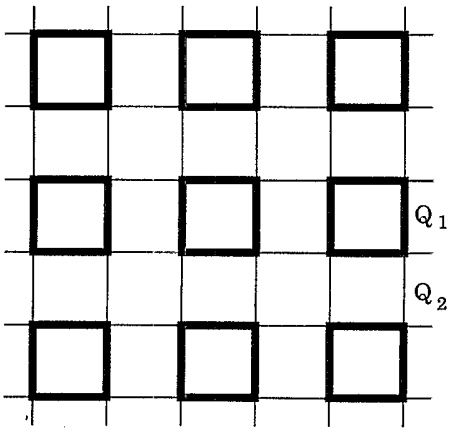

FIG. 1. Insulating crystal ground state for filling factor $\nu=\frac{1}{4}$ and $t<0.3J$. The dark bonds take the real value Q_1, while the light bonds take the value $Q_2<Q_1/2$.

attractive set of saddle points for these values of ν were proposed recently by Hasegawa *et al.*[10] and Lederer *et al.*[11] consisting of states with flux $\Phi=\nu$ piercing each plaquette. We found that these flux states were lower in energy than states with nonuniform or staggered flux. However, *states with a nonuniform charge distribution and localized holes were always found to be the global minima of the energy.* (Note, however, that for the special case of $\nu=\frac{1}{4}$ already considered, the localized-hole state has a uniform charge distribution.) Moreover, the mutual fermion spin correlations in these localized-hole states were zero except those taken on clusters of sizes less than or equal to four sites. Further analysis of the localized-hole states at nonzero values of t is clearly necessary and is currently being carried out (see Sec. IV).

The rest of the paper is organized as follows. In Sec. II we present additional details of the calculations for $\nu=\frac{1}{4}$, while in Sec. III we present details for other values of ν. Finally, in Sec. IV we reiterate the conclusions and present some speculations.

II. $\nu=\frac{1}{4}$

The bulk of the constrained free-energy minimization was carried out using the periodic Q_{ij} configuration shown in Fig. 2. The ansatz shown guarantees that the fermion densities at all sites are equal. For $\nu=\frac{1}{4}$ this immediately fixes $\delta_i=\frac{1}{4}$ and considerably simplifies the constrained minimization problem. Moreover, the unit cell of four sites in Fig. 2 is large enough to allow for states with uniform flux $\pi/2$ per plaquette. The free-energy minimization was carried out using the downhill simplex method[12] as a function of the four complex variables Q_1, Q_2, Q_3, and Q_4. At each step of the minimization the chemical potential μ was varied to fix the filling fraction ν at $\frac{1}{4}$. Several random initial conditions were chosen, making it reasonably certain that the global minimum of the free energy has been found.

For $t<0.3J$, the global ground state had Q_i real, $Q_1=Q_3$, and $Q_2=Q_4$. A schematic of this state is shown in Fig. 1. The fermion dispersion relation can be easily computed to yield the following four bands:

$$\epsilon_k=\pm|Q_1e^{ik_x}+Q_2e^{-ik_x}|\pm|Q_1e^{ik_y}+Q_2e^{-ik_y}| \ . \quad (2.1)$$

TABLE I. Ground-state energy per fermion (E) for the insulating crystal state as a function of t/J. This state is the global ground state for $t<0.3J$. Also shown are values of the effective hopping parameters Q_1 and Q_2.

t/J	E/J	Q_1/J	Q_2/J
0.0	−0.25	0.25	0.0
0.008	−0.254	0.252	0.003
0.012	−0.258	0.254	0.008
0.04	−0.270	0.260	0.019
0.12	−0.313	0.278	0.055
0.20	−0.357	0.294	0.088
0.30	−0.415	0.315	0.126

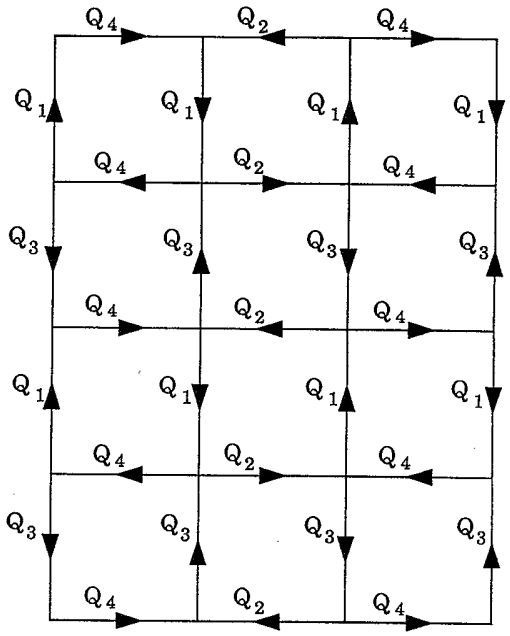

FIG. 2. Ansatz for Q_{ij} configuration used in free-energy minima search at $\nu=\frac{1}{4}$. The variables Q_1, Q_2, Q_3, and Q_4 are independent complex numbers.

At $\nu=\frac{1}{4}$ only the lowest of the four bands is fully occupied. This leads to an indirect fermion band gap of Q_1-2Q_2. The values of Q_1, Q_2, and the ground-state energy are shown in Table I as a function of t/J. Notice that $2Q_2<Q_1$ for all t/J. The band gap is therefore always positive, and the state is insulating. At $t=0$, we have $Q_2=0$; the holes are therefore in decoupled N tuples occupying plaquettes of four sites. It is useful to define a *bond* charge density ρ_{ij} by

$$\rho_{ij}=\langle(c_{i\alpha}^\dagger b_i+c_{j\alpha}^\dagger b_j)(c_i^\alpha b_i^\dagger+c_j^\alpha b_j^\dagger)\rangle \quad (2.2)$$

where i,j are nearest neighbors. The Q_1 bonds will clearly have larger values of ρ_{ij} than the Q_2 bonds. This oscillation in bond charge density leads to a natural interpretation of each Q_1 plaquette as a bound state of N holes. We may therefore consider this minimum as a Bose crystal of an N-hole bound state.

For $t>0.3J$, the global ground state consists of Q_i real and $Q_1=Q_2=Q_3=Q_4$. This is clearly a metallic normal Fermi liquid. An analysis of the optical and charge transport properties of this state has been carried out by Dombre *et al.*[3] A comparison of the energy per particle of the Fermi liquid and insulating crystal states is shown in Fig. 3.

We now turn to a discussion of the various metastable saddle points. The most competitive of these was the commensurate flux state of Hasegawa *et al.*[10] and Lederer *et al.*[11] (see Table II). A commensurate flux saddle point was found for $t=0$ and had flux $2\pi\nu=\pi/2$ through each plaquette. However, for nonzero t, this state *immediately* developed a modulation in the values of $|Q_{ij}|$ and the flux became nonuniform and moved off its commensurate value. Moreover, this saddle point became *unstable* at $t\geq 0.016J$ (Fig. 3).

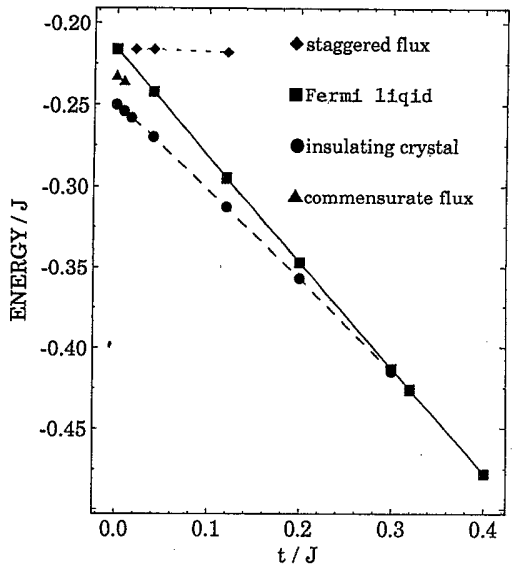

FIG. 3. Energy per particle as a function of t/J at filling $\nu=\frac{1}{4}$. For $t<0.3J$ the insulating crystal state shown in Fig. 1 is the ground state. For $t>0.3J$, the Fermi-liquid state is the ground state. Metastable saddle points corresponding to a staggered flux state and commensurate flux states ($\Phi=\nu$) exist only for a *small* range of t/J. A nonuniform flux state discussed in Sec. II and Table II has not been shown for clarity.

Another saddle point shown in Table II is the nonuniform flux state; this state has flux π in half the plaquettes and flux 0 in the remaining half. Again this state was found to be unstable at all $t \geq 0.008J$.

Finally, we also found saddle points with a staggered arrangement of flux[2,5] that had the Q_i complex but with $Q_1=Q_2=Q_3=Q_4$. At $t=0$ this state had zero flux and was degenerate with the Fermi-liquid state. A metastable state was found for $0<t/J\leq 0.12$ with a nonzero flux (see Fig. 3).

III. $\frac{1}{4}<\nu\leq\frac{1}{2}$

An important factor that considerably simplified the constrained minimization calculations at $\nu=\frac{1}{4}$ was the use of the ansatz shown in Fig. 2. This ansatz guaranteed a uniform charge density and at the same time was general enough to include the commensurate flux state. Such an ansatz is no longer possible for $t\neq 0$ and $\frac{1}{4}<\nu<\frac{1}{2}$. Our results will therefore be restricted in this paper to $t=0$. Further analysis of the nonzero t case is in progress. All the subsequent discussion in this section implicitly refers to $t=0$.

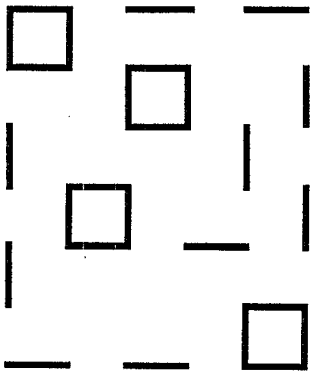

FIG. 4. A typical ground state at $t=0$. The effective hopping parameter Q_{ij} take the values $J/2$ on ever dimer, $J/4$ on the bonds surrounding the plaquettes and 0 everywhere else. Each dimer has N fermions, and each plaquette has a total of N fermions. The state shown has a total of $14N$ fermions on 42 sites. A periodic continuation of this state over the infinite lattice would therefore correspond to a filling factor of $\nu=\frac{1}{3}$.

The global ground-state manifold was found to have a large degeneracy at $N=\infty$. For all $\frac{1}{4}\leq\nu\leq\frac{1}{2}$, the ground-state energy was $-0.25J$ per electron. A typical ground state is shown in Fig. 4. It consists of an arbitrary arrangement of empty sites, dimers, and plaquettes. All the Q_{ij} are chosen real. The dimer bonds have $Q_{ij}=J/2$; the bonds around a plaquette have $Q_{ij}=J/4$ while all other $Q_{ij}=0$. Each dimer or plaquette has exactly N electrons on it. The ratio of the number of dimer, plaquettes, and empty sites must be chosen to fix the filling factor at ν.

The most competitive metastable states were again the commensurate flux states of Hasegawa *et al.*[10] and Lederer *et al.*[11] We show in Fig. 5 the difference in energy between these states and the ground state as a function of ν. They never become the lowest energy state. As was the case for $\nu=\frac{1}{4}$, it is expected that for $t\neq 0$ these states will immediately develop oscillations in $|Q_{ij}|$ and lose the pinning of the flux to a rational value. The staggered flux state was also examined and was always found to be higher in energy than both the localized hole and commensurate flux states.

IV. CONCLUSIONS

The large-N expansion offers one of the few controlled approximations for analyzing strongly correlated systems. It has been successfully used to understand the

TABLE II. Comparison of the ground-state energy per fermion (E) for various saddle points of the free energy at $t=0$ and $\nu=\frac{1}{4}$. At $t=0$, the values of Q_i are clearly arbitrary up to gauge transformations.

State	E/J	Q_1/J	Q_2/J	Q_3/J	Q_4/J
Insulating crystal	-0.25	0.25	0.0	0.25	0.0
Fermi liquid	-0.216	0.164	0.164	0.164	0.164
Commensurate flux	-0.233	$0.171e^{i\pi/8}$	$0.171e^{i\pi/8}$	$0.171e^{-i3\pi/8}$	$0.171e^{-i3\pi/8}$
Nonuniform flux	-0.230	0.169	0.169	$0.169e^{i\pi/2}$	$0.169e^{i\pi/2}$

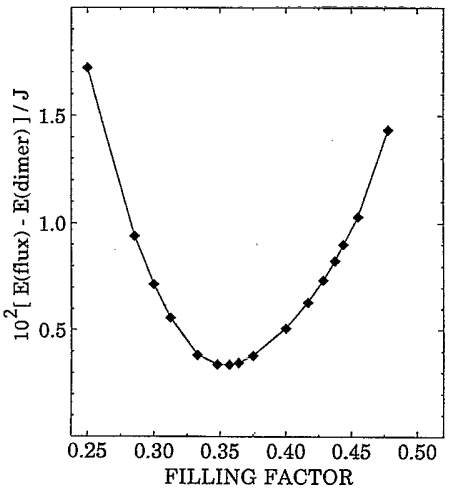

FIG. 5. Difference in energy per fermion between the commensurate flux states with $\Phi=\nu$ and the global ground state (the localized hole or the "dimer" state) as a function of filling factor ν at $t=0^+$. The ground-state energy per fermion is $E_g=-0.25J$. The staggered flux state was always higher in energy than both these states ($E>-0.236J$) off scale.

properties of insulating two-dimensional quantum Heisenberg antiferromagnets.[6] It now appears that the columnar spin-Peierls state found in the large-N limit, also appears in frustrated SU(2) antiferromagnets.[13] This paper has presented the results of a large-N mean-field theory of the t-J model on a two-dimensional square lattice. As was the case at half filling, the emphasis has been on the determination of the global ground states of the mean-field theory.

Our most extensive results have been obtained for the case of filling fraction $\nu=\frac{1}{4}$. Over the manifold of states examined, we found that the global ground state for $t<0.3J$ was an insulator consisting of a crystalline arrangement of an N-hole bound state. At $t=0.3J$, the system undergoes a first-order transition to a normal Fermi liquid. The Fermi liquid is stable at $N=\infty$ for all $t>0.3J$, and its properties have been analyzed by Dombre *et al.*[3]

The analysis for $\frac{1}{4}<\nu<\frac{1}{2}$ was considerably more complicated. The results in this paper are restricted to the case $t=0$. The ground-state manifold had a large degeneracy with a macroscopic entropy. We found that states with two fermion spin correlations nonzero only small (four sites or less) clusters to make up the ground-state manifold. The most interesting issue touched upon in this paper is the precise manner in which this degeneracy is lifted at nonzero t. An attractive possibility is that the holes will form the bound states appearing at $\nu=\frac{1}{4}$; the bound states can in turn Bose condense (N is even) or form a regular crystalline arrangement. The commensurate flux states introduced by Hasegawa *et al.*[10] were never found to be the global ground state for all $\frac{1}{4}\leq\nu\leq\frac{1}{2}$. Since these commensurate flux states are designed to maximize the exchange energy,[11] the prognosis for them becoming the global ground state at nonzero values of t is not good.

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