Breakdown of the Nagaoka phase in the two-dimensional t-J model

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(Received 30 August 2001; revised manuscript received 29 November 2001; published 26 March 2002)

In the limit of weak exchange J at low hole concentration δ the ground state of the two-dimensional t-J model is believed to be ferromagnetic. We study the leading instability of this Nagaoka state, which emerges with increasing J. Both exact diagonalization of small clusters, and a semiclassical analytical calculation of larger systems show that above a certain critical value of the exchange, $J_{cr} \sim t\delta^2$, Nagaoka's state is unstable to phase separation. In a finite-size system a bubble of antiferromagnetic Mott insulator appears in the ground state above this threshold. The size of this bubble depends on δ and scales as a power of the system size N.

DOI: 10.1103/PhysRevB.65.134437 PACS number(s): 75.10.Lp, 75.30.Kz

Recently, much interest was focused on the behavior of strongly correlated electron systems, which cannot be explained by weak-coupling perturbation theory. A variety of unusual phenomena such as, e.g., high-temperature superconductivity and quantum magnetism, is believed to require a nonperturbative description.[1] An important paradigm for the study of strongly interacting electrons in general, is the Hubbard model for interacting particles on a lattice. This is probably the simplest possible model that captures some of the behavior of strongly correlated electrons. It is, therefore, widely used to study various correlation driven effects, which are not described by a perturbative approach. These include the metal-insulator (Mott) transition, and the superconductivity of the high-T_c compounds.

The Hubbard model was originally introduced in an attempt to describe quantum ferromagnetism of itinerant electrons in narrow-band metals.[2] However, it is now well known that it is also a model for quantum antiferromagnetism. The effective Hamiltonian that governs the low-energy behavior of the Hubbard model for a nearly half-filled band in the $U \to \infty$ limit is the t-J model of itinerant fermions on the lattice

$$H^{t-J} = -t \sum_{\langle ij \rangle \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + \text{c.c.} + J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right). \tag{1}$$

The occupation number of each site $n_i = a^{\dagger}_{i\uparrow} a_{i\uparrow} + a^{\dagger}_{i\downarrow} a_{i\downarrow}$ can be either 0 (a hole) or 1 (a spin), since double occupancy is forbidden by strong on-site Hubbard repulsion. The spin operators $\mathbf{S}_i$ are given in terms of the Pauli matrices $\sigma_{\alpha\beta}$

$$\mathbf{S}_i = \frac{1}{2} \sum_{\alpha\beta} a^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} a_{i\beta}. \tag{2}$$

Since the spin-exchange coupling constant $J \approx 4t^2/U$ is positive, the on-site Hubbard interaction translates to an antiferromagnetic (AFM) superexchange, which favors an AFM correlated ground state.

Nevertheless, in one extreme case this model has a ferromagnetic (FM) ground state, known as the Nagaoka state.[3] A fully polarized state minimizes the total energy of a single hole in an otherwise half-filled band, at least in the limit $J \to 0$. This is due to the hole kinetic energy that favors FM ordering. The nature of the ground state for finite J is, therefore, determined by the competition of this FM tendency with the AFM exchange.

In this work, we study the ground state of the 2D t-J model for low concentration of holes, as a function of the AFM interaction strength J. We aim to identify the leading instability of the Nagaoka state, i.e., the state that minimizes the energy for not fully polarized states. Based on numerical evidence, we claim that the leading instability is towards the creation of an AFM bubble, while the holes are confined to the FM region. The transition between Nagaoka state and this ''bubble'' state is a first-order transition,[4] including a jump $\Delta S \gg 1$ in the total spin. We will concentrate on the t-J model, Eq. (1). However, our study is focused on the small J regime, and thus our considerations apply equally to the Hubbard model.

We start by summarizing in some detail what is known and conjectured about the nature of the t-J model ground state. For half-filling, where each site is occupied by one electron, no hopping is possible, and the Hamiltonian reduces to the quantum Heisenberg Hamiltonian with AFM spin exchange. Although the two-dimensional (2D) Heisenberg model cannot be solved analytically, there is strong numerical evidence, (obtained from exact diagonalization and Quantum Monte Carlo simulations) that the ground state has long-range AFM correlations at zero temperature.[5,6]

The presence of holes makes the picture more complicated. Each hole hopping creates changes in the spin configuration, unless the spin polarization is uniform. The resulting excitations in the system inhibit the hopping, since the hopping probability is reduced by a factor proportional to the overlap between the original and final spin-wave functions. This effect results in narrowing the kinetic-energy band, thus increasing the kinetic contribution to the energy. The bandwidth is maximized in the fully polarized state for which the spin configuration is unaffected by permutations of different spins. Thus, while the J term in the Hamiltonian favors an AFM ordering, the kinetic t term favors a FM state. The competition between these terms depends on the hole density and interaction strength J/t, and determines the physical properties of the t-J model.

The question of charge-carrier dynamics on an AFM background was extensively studied using the string picture, self-consistent Born approximation, and numerical studies.[6] For $J \gg t$ a single hole is unable to alter its AFM surrounding, and its kinetic energy comes only through coupling to the quantum fluctuations of the spin system. For moderately large J ($J/t \approx 5-10$) the hole develops a spin polaron around itself. Within this polaron, the AFM order is suppressed by hole hopping. The size of the polaron increases with decreasing J/t. The ''string'' picture emerges when this size is much larger than the lattice constant. In this picture, the hole acts as a particle with mass $1/t$ subject to an effective potential resulting from the string of flipped spins created by its hopping. This effective potential is a linear potential with slope J. Accordingly, the size of the polaron scales as $(J/t)^{-1/3}$. In this regime the hole movement scrambles its surrounding spins, thus suppressing the local AFM order parameter, but does not yet create a local magnetic moment larger than the spin 1/2 of a single hole.[7,8]

As soon as J/t decreases beyond some critical value ($J_c < 0.1$), the nature of the ground state changes.[9] It turns out that lower energy is achieved by creating a FM polaron,[10] where not only the AFM ordering is destroyed, but also FM correlations and a larger magnetic moment are formed in the vicinity of the hole. The radius of the polaron in this regime scales as $(J/t)^{-1/4}$. In the limit $J \to 0$, the kinetic energy that favors FM ordering dominates the tendency towards AFM coupling of neighboring spins represented by the J term, and the size of this polaron diverges. As a result, the ground state becomes fully polarized. This statement was rigorously proven in the the celebrated paper of Nagaoka[3] for a single hole case. It was shown that Nagaoka FM phase survives for sufficiently small density of holes, even in the thermodynamic limit.[11]

Thus, this apparently simple model exhibits a ferromagnet-antiferromagnet transition at zero temperature, as the interaction strength J increases. Very little is known about the properties of the system in the transition region. Even the dependences of the magnetization curve on J and the hole concentration δ are yet to be determined. In the following, we try to understand some features of the transition. We focus on the boundary regime of Nagaoka's phase, i.e., the transition from full to partial polarization.

Naturally, the question of the stability of the Nagaoka fully polarized state with respect to switching on the AFM exchange term, as well as finite hole density δ, attracted much interest. Several variational wave functions were suggested in order to yield bounds for the Nagaoka stability region in δ-U plane (See Ref. 12, and references therein). Most of these estimates were based on the belief that the transition from Nagaoka state is continuous at $T=0$.[12] In other words, it was implicitly assumed that the leading instability of Nagaoka's state is a single spin flip (SSF). According to this picture, the transition to the AFM singlet ground state with increasing J/t occurs gradually, through small incremental $\Delta S = 1$ changes in the total spin. However, it was suggested that for sufficiently low δ a phase-separation instability, rather than a SSF one, might be relevant.[13,14]

Many authors have discussed the possibility of phase separation in the Hubbard and $t-J$ models.[4,13,15–18] For high concentration of holes (low electron density), phase separation does occur for J sufficiently large.[4,16] However, the small J/t case is still under debate. Some groups argue that the ground-state phase separates for all values of J/t for sufficiently low concentration of holes.[4,17] Others claim that there exists a critical value J_{ps} (estimates for its value vary between $J_{ps} \sim 0.4t$ and $J_{ps} \sim 1.4t$), such that for $J < J_{ps}$ the ground state is uniform even for vanishing hole density.[18]

In the following, we present evidence that the leading instability for low densities is indeed a phase-separated state. We, therefore, claim that phase separation does occur for small values of J/t, given that δ is sufficiently small. We further show that for a finite-size sample the transition in the ground state between the Nagaoka phase and the phase-separated state is discontinuous,[4] including a large change in the total spin $\Delta S \gg 1$. Thus this transition cannot be captured by the SSF variational studies. It is, therefore, reasonable to assume that better bounds for Nagaoka stability might require considering many simultaneous, rather than sequential, spin flips.

We start by examining at the single hole case. It is straightforward to show that J_{cr}, the J value needed to destabilize Nagaoka's state, for two spin flips *is smaller* than for one spin flip.[13] This can be demonstrated by deriving an effective Hamiltonian of a single hole and flipped spins, in the background on the FM Nagaoka state. Since the number of flipped spins is presumably small, it is convenient to describe the system in terms of the two types of ''particles''—the hole and the flipped spins. The kinetic part of the Hamiltonian induces hopping of the hole to its nearest neighbors, with an effective mass $1/(2t)$. The nondiagonal part of the exchange interaction induces hopping of the flipped spins to their nearest neighbors, with an effective mass $1/J$. The ratio between the effective masses of the spin and the hole is, therefore, $J/2t$, which is small around J_{cr}. Therefore, one can assume that the spin is static for calculating its effect on the hole energy, i.e., use Born-Oppenheimer-like adiabatic approximation. The diagonal part of the exchange term contributes the energy $-J/2$ per flipped spin. In addition to these terms, one should take into account the constraint that each site can be occupied by no more than one ''particle'' (hole or flipped spin). For that purpose, one can introduce effective, infinitely strong, on-site repulsion between the particles. There are other terms in the effective Hamiltonian resulting from nearest-neighbors interaction between the particles, but they do not contribute to the energy in the leading order in J/t. The Nagaoka state is destabilized as soon as the $O(J)$ magnetic energy gained by the flipped spins overcomes this kinetic-energy gain.

For a state with two spin flips, the kinetic-energy increase depends on the distance between the spin flips. When they are far apart, the kinetic energy lost by the excluded area is about twice the value for a single flip. However, as the two spin flips get closer, the effective excluded area for the hole decreases. When the distance is small compared to the hole wavelength, the excluded area is not changed much, and the kinetic-energy increase is about the same as for one flip.

TABLE I. Exact diagonalization results for the breakdown on Nagaoka's state for the case of one hole. ΔS is the jump in the ground-state spin at the transition.

Cluster	ΔS	J_{cr}	Cluster	ΔS	J_{cr}
2×8	3	0.0225	4×4	4	0.0629
2×10	4	0.0134	4×5	6	0.0398
2×12	5	0.0086	4×6	6	0.0269

Thus, there is an effective attraction between the flipped spins, and they bind together, with total energy similar to that of a single flip. On the other hand, the magnetic energy is simply proportional to the number of spin flips, and does not depend on the distance between the spin flips, as long as they are not nearest neighbors. Thus the magnetic energy for two flipped spins, bound or not, is twice as much as the energy for a single flip. Therefore, J_{cr}, for which the magnetic energy balances the kinetic-energy increase, is lower for a state with two flipped spins. One concludes that, for a single hole, the transition between the maximum spin Nagaoka state and a lower spin state involves a spin jump $\Delta S>1$.

In order to describe the leading instability of the Nagaoka ferromagnet with respect to switching on the J term one should, therefore, determine the number of spin flips that minimizes J_{cr}. We start with presenting results of exact diagonalization for small rectangular $a\times b$ clusters. We choose periodic boundary conditions when the large axis of the cluster has even number of sites $(a=2n)$, and antiperiodic boundary conditions otherwise $(a=2n+1)$. Under these conditions the $J=0$ ground state is always fully polarized. For each of the following clusters we diagonalize exactly the full many-particle Hamiltonian, for different spin sectors and various J values. We determine J_{cr} and the value of the ground-state spin for $J=J_{cr}+$. It was already pointed out,[19] based on exact diagonalization results, that for big enough clusters, large number of spins may flip together. We present here a more systematic study of finite clusters, showing a large spin jump $\Delta S>1$. For the one hole case, the biggest cluster studied was a 6×4 torus. The effective size of the full Hilbert space can be substantially reduced by excluding the doubly occupied states and using spin and translational symmetry. For 6×4 torus, this reduces the problem to the diagonalization of a $1\,352\,078\times1\,352\,078$ matrix. We employed the Lanczos algorithm to carry out this diagonalization. The results for the different clusters are summarized in Table I. Extension of these exact diagonalization studies to larger systems or more than one hole is limited by the size of the Hilbert space.

We did repeat the calculation for two holes on the above clusters. It is well known that for two holes on a torus the ground state is a singlet even for $J=0$.[19,20] This is due to the fact that a slowly varying, locally polarized, spin background creates the effect of a fictitious flux, which minimizes the kinetic energy of the two holes.[21] As it was done for one hole, we chose the boundary conditions to overcome this effect. However, in all cases studied, a ground state with small nonzero spin was never observed. We always dealt with an abrupt transition to the singlet $S=0$ state, ΔS being as large as the largest possible spin, S_{max}, even larger than the jump in the spin for the one hole case. This, however, is a particular feature of systems with two holes, which might not be relevant for the behavior of large systems.

These exact results show that the number of spins that flip at the transition is significantly larger than one, and it increases with the system size. They indicate that the breakdown of Nagaoka phase might indeed occur through an abrupt spin change. It looks interesting to understand how ΔS scales with system size. Besides, it is not clear to what extent are the results specific for a particular small number of holes (1 or 2), i.e., extension of the results to more holes is required. Clearly, exact diagonalization is not an adequate tool to clarify these questions.

To get an insight into the behavior of larger systems, we use the spin-hole coherent-state path-integral formalism. We follow the derivation presented in Ref. 22. A semiclassical approximation for the ground state is obtained through the formal large S expansion. In the classical limit, $S\rightarrow\infty$, the spins are frozen (i.e., the spin part of the coherent-state path integral is time independent). The energy is determined solely by the interplay between hole dynamics and the classical AFM interaction between the spins. In essence, this limit deals with a classical spin field, interacting with the quantum holes. Clearly this approximation cannot capture the full complexity of the exact wave function, as it ignores dynamical corrections to the spin background as introduced by, e.g., the dressed holes. Thus, some of the exotic phases suggested for the t-J model are essentially not taken into account in this approximation. However, in some cases the instability towards these phases can be described within the semiclassical approximation. For example, the incommensurate MAF, or spiral phase,[19,20] with dressed holes, supercedes the Nagaoka phase for two holes. Within the semiclassical approximation, ignoring the dressing of the holes, the incomensurate AFM background becomes degenerate with the Nagaoka phase. Thus one can expect to find signs for the emergence of complex spin structures even within this simplified approach. The same approach was previously used to study the formation of the FM polaron. Here we use the same technique to study the extreme low J case $J=J_{cr}+$, at the breakdown of Nagaoka phase, where the FM region occupies most of the system. We use a Monte-Carlo algorithm to find the spin configuration that minimizes the sum of the energy of the holes and the magnetic energy of the (classical) spin field.

We study different lattice sizes (up to 16×16) and various number of electrons close to half-filling ($0<\delta<0.12$). In all cases, we find the same behavior: (a) all the spins align colinearly (b) we do not see any signature suggesting the emergence of exotic spin configurations (spiral, canted, etc.) for these small values of J, and most importantly (c) the uniform Nagaoka's state breaks down into a phase-separated state, with a hole-rich FM region and an AFM bubble with no holes inside. The size of the bubble at the transition is large relative to the lattice constant, giving a big jump in the spin. As an example we present in Fig. 1 results for a 16×16 lattice with 25 holes. These results, for different lattice sizes and densities, suggest that Nagaoka state breaks down by

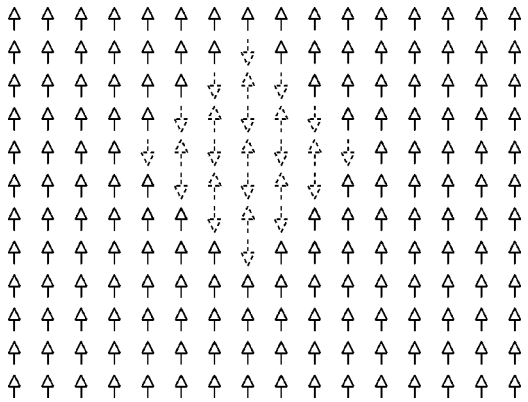

FIG. 1. The spin configuration of the leading instability as obtained from a semiclassical calculation. The hole density is 25/256. 16 spins flip in a slanted square configuration. The hole density vanishes inside the AFM bubble, while being approximately constant in the FM region.

forming an AFM bubble, whose size is large compared to the lattice constant. Contradicting evidence were recently presented regarding the existence of phase separation for small J.[17,18] We find that the above described phase-separated state seems to be stable even for $J \ll t$, provided that the hole density δ is sufficiently small, in agreement with Refs. 4 and 17. The stability of the phase-separated state for larger J, and its relation to the above discussed phase, is beyond the scope of this study.

Motivated by these results, we turn to study the stability of the Nagaoka phase with respect to phase separation. That is, we compare the energy of the Nagaoka state with that of a system with an AFM ordered domain. To first approximation, the AFM domain acts as an infinite potential barrier, i.e., the holes are confined to the FM region. Due to this confinement, the kinetic energy of the holes increases with the size of the AFM domain. On the other hand, the AFM domain contributes a magnetic term to the energy, which also increases with its size. We estimate the magnetic energy per site in the AFM domain by the value obtained in an infinite Heisenberg system,

$$E_{\mathrm{mag}} = -\alpha J(\mathcal{S} + \mathcal{P}/2), \tag{3}$$

where $\mathcal{S}$ is the area (number of sites) of the AFM domain, $\mathcal{P}$ is its perimeter, and α is the energy per site of the ground state of the 2D Heisenberg model (spin-wave theory gives $\alpha = 1.1705$, which is in a good agreement with the numerical result[5]) $\alpha = 1.169$. An estimate to the increase in the kinetic energy of holes for a large system is obtained through the well-known Weyl formula for the density of states. The number of levels up to an energy E for a free particle in a continuous 2D domain with area $\mathcal{A}$ and boundary perimeter $\mathcal{P}$ is given by

$$\langle N(E) \rangle \sim \frac{1}{4\pi}(\mathcal{A}E - \mathcal{P}\sqrt{E} + \mathcal{K}), \tag{4}$$

where Dirichlet boundary conditions are assumed, and $\mathcal{K}$ is a constant term containing information on the geometry and topology of the domain.[23] The units are chosen such that $\hbar = 2m = 1$. Equivalently, for the Hubbard (or $t-J$) model, the same formula holds near the bottom of the band, where the energy is in units of t and the bottom of the band is taken as the energy zero. In the following t is taken as the unit of energy, and the lattice constant is taken as the unit of length. The average $\langle \rho(E) \rangle$ of the density of states (DOS) $\rho(E) \equiv \partial N(E)/\partial E$, is thus given by

$$\langle \rho(E) \rangle \sim \frac{\mathcal{A}}{4\pi} - \frac{\mathcal{P}}{8\pi\sqrt{E}}. \tag{5}$$

In the Nagaoka FM state, the available domain for the holes is the whole torus $\mathcal{A} = N$. The DOS is, therefore, just the familiar $\mathcal{A}/4\pi$ term and the energy is given by

$$E_{\mathrm{Nag}} = 2\pi N \delta^2 = 2\pi N_h^2/N, \tag{6}$$

where N_h is the number of holes and N is the total number of sites. As soon as the AFM bubble is formed, the energy increases due to two reasons. First of all, the available area is reduced to $\mathcal{A} = N - \mathcal{S}$, and, therefore, the denominator in Eq. (6) decreases. Due to this fact, the total energy increases by the factor $N/(N-\mathcal{S})$. Another contribution comes from the boundary term that reduces the DOS even further. Bearing in mind to compare the energy increase with the magnetic energy that is $O(\mathcal{S})$, we realize that the increase due to the boundary term $O(\mathcal{P})$ divided by $\mathcal{S}$ becomes singular $(\sim \mathcal{S}^{-1/2})$ for small $\mathcal{S}$. We will see below that the transition occurs for $\mathcal{S}$ values much smaller than the system size. As a result, boundary terms are important even for large N. The topological $\mathcal{K}$ term also changes due to the AFM barrier. However, it can be checked explicitly that it does not affect the $N \to \infty$ asymptotic behavior.

Using the above averaged DOS, one can calculate the total energy of holes as a function of their density. Adding the magnetic energy, the total energy relative to the Nagaoka energy is given by

$$E(\delta, s) = 2\pi\delta^2 N\left(\frac{s}{1-s} + \frac{2p}{3\sqrt{\pi\delta N}(1-s)^{3/2}}\right) - \alpha J N\left(s + \frac{p}{2\sqrt{N}}\right), \tag{7}$$

where we introduced the normalized quantities

$$p \equiv \mathcal{P}/\sqrt{N}, \quad s \equiv \mathcal{S}/N. \tag{8}$$

It follows from the dimensional analysis that $p = C\sqrt{s}$, where C is a dimensionless constant depending on the shape of the bubble. Although we deal with a lattice problem, in the limit we are considering of low doping and large bubbles, the perimeter term from the hole kinetic energy dominates. Since the dispersion relation for low-energy holes is asymptotically isotropic, this produces an isotropic perimeter energy so the lowest energy bubbles are circular $(C = 2\sqrt{\pi})$. It is straightforward to see that given the grand canonical potential $G = E(\delta, s) - N\mu\delta$ with a fixed chemical potential μ, the system goes through a first-order phase transition. This transi-

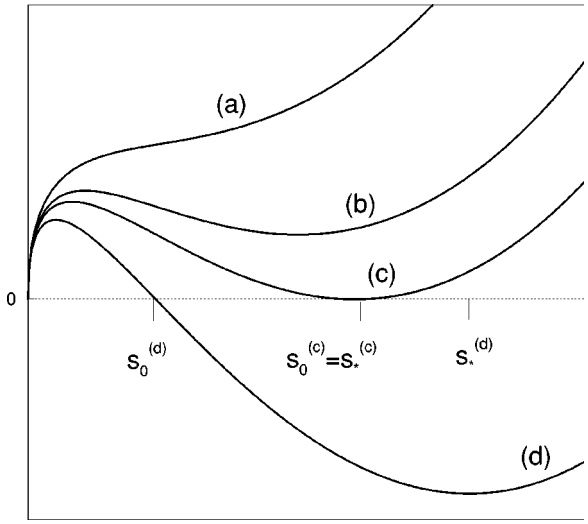

FIG. 2. An illustration of the total energy (7) for different values of j. (a) No metastable state. (b) A metastable state appears. (c) The transition point. (d) $J>J_{\rm cr}$.

tion occurs at $J_{\rm cr}=\mu^2/(8\pi\alpha)$, where the density jumps from $\delta_-=\mu/(4\pi)$ at $J=J_{\rm cr}-$ to $\delta_+=0$ at $J=J_{\rm cr}+$. In the same time s jumps from $s=0$ (Nagaoka phase) below the transition, to $s=1$ (antiferromagnet) above the transition. If the density is instead held between these two values, the ground state, ignoring surface terms, is a phase-separated state, which is a mixture of the two phases. In the following we study the formation of the AFM bubble in a finite system, given the surface terms. The energy (7) as a function of s is presented in Fig. 2 for various values of J. At the origin, $E(0)=0$, and the energy increases with s. For sufficiently large J, the function has a maximum at which the energy is positive and a (local) minimum at $s=s_*$ [see Fig. 2 curve (b)]. When J increases beyond a critical value $J>J_{\rm cr}$, the value of the energy at this minimum becomes negative, the local minimum at s_* becomes the global minimum of the function. The function crosses the x axis at $s=s_0<s_*$ [see Fig. 2 curve (d)]. For $s>s_*$ the function again increases. Therefore, as long as $J<J_{\rm cr}$, the global energy minimum is obtained at $s=0$, corresponding to Nagaoka FM state, although a metastable state with an AFM bubble does exist for a range of J near, but below $J_{\rm cr}$. As J increases beyond $J_{\rm cr}$, the global minimum shifts to s_*. It is convenient to introduce the variable j

$$j=\frac{J-J_0^{\rm cr}}{J_0^{\rm cr}},\quad J=2\pi\delta^2/\alpha(1+j)\equiv J_0^{\rm cr}(1+j). \tag{9}$$

$J_0^{\rm cr}$ is the value of $J_{\rm cr}$ for an infinite size system. Thus, j measures the relative distance of J from the value of $J_{\rm cr}$ obtained ignoring boundary terms. In terms of this variable, one can express the large N asymptotics of s_0 (the value of s where the energy vanishes) and s_*, which minimizes the energy.

$$s_0=C^2(A/j-1)^2/4N;\quad A=4/(3\sqrt{\pi\delta})-1 \tag{10}$$

$$s_*=1-\frac{1}{\sqrt{1+j}}. \tag{11}$$

Note that A depends only on the hole density δ. Thus, for $j>0$, the minimal size of the droplet needed to destabilize Nagaoka's state remains finite in the $N\to\infty$ limit [$S_0\equiv s_0N=O(1)$], while the global minimum is obtained when the droplet is of macroscopic size [$S_*\equiv s_*N=O(N)$]. Comparing these two expressions, one immediately sees that the transition occurs for $j\sim O(N^{-1/3})$.

In this regime s_0 and s_* are connected with j via the equations

$$j=2s_*+\frac{CA}{4\sqrt{Ns_*}}, \tag{12}$$

$$j=s_0+\frac{CA}{2\sqrt{Ns_0}}. \tag{13}$$

The last equation has a solution provided that $j>j_{cr}=3(C^2A^2/16N)^{1/3}$. The transition point $J_{\rm cr}$ is, therefore,

$$J_{\rm cr}=\frac{2\pi\delta^2}{\alpha}\{1+3[(CA)^2/16N]^{1/3}\}. \tag{14}$$

Beyond the transition point $J>J_{cr}$, and for some s the energy of the bubble is negative and, therefore, the FM state is unstable. At the transition point, the area of the optimal AFM bubble is

$$\mathcal{S}_0=Ns_0=Ns_*=(CAN/4)^{2/3}. \tag{15}$$

For $j<j_{cr}$ Eq. (13) has no solution and the energy is minimized by Nagaoka state. However, the energy function does have a local minimum at s_* for $j>j_{\rm ms}=2^{-1/3}j_{cr}$, and thus a large metastable bubble can be created. The size of the metastable bubble at $j=j_{\rm ms}+$ is

$$S_*=s_*N=(CAN/16)^{2/3}. \tag{16}$$

In fact, it can be shown that the $N^{2/3}$ power law follows from a very general argument. Whenever phase separation occurs between two phases, with densities δ_1 and δ_2, the fraction of the first phase in the phase-separated ground state of an infinite system at a fixed density $\delta_1<\delta<\delta_2$ is given by $(\delta_2-\delta)/(\delta_2-\delta_1)$. Thus, for densities very close to δ_2 the size of the bubble of the first phase is arbitrarily small. However, the surface energy term raises the energy of the phase-separated state as compared to the uniform state, and thus finite-size corrections arise. The energy cost to create a boundary between the two phases, is proportional to (in d dimensions) $V^{(d-1)/d}$, where V is the size of the bubble. This energy makes it favorable to retain the uniform phase even at densities slightly smaller than δ_2. The formation of a bubble becomes energetically favorable when the density is shifted away from the (infinite system) transition point, such that the difference in the volume energy of the uniform state as compared to the phase-separated state overcomes the surface term. In the generic case, this difference is proportional to

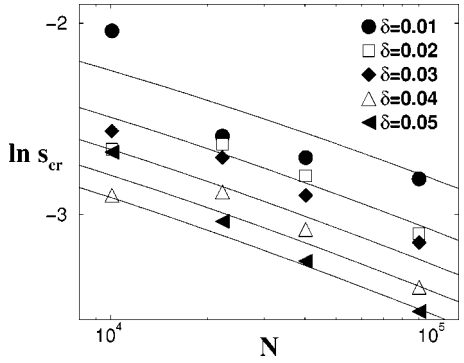

FIG. 3. The area of the AFM bubble at the transition point s_{cr} normalized by system size, as a function of N for various N values. The solid lines are the asymptotic expansion up to order N^{-1} for the same five densities (top to bottom).

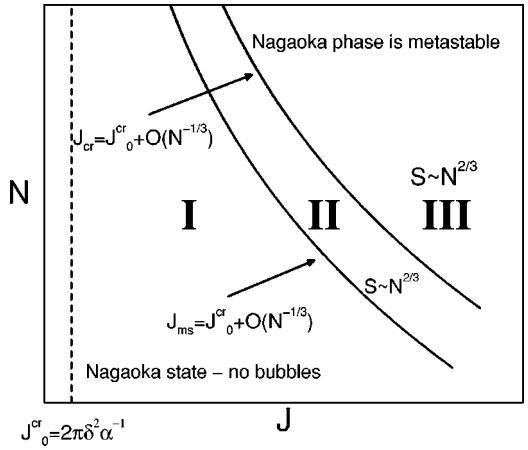

FIG. 4. Schematic phase diagram in the vicinity of the breakdown of Nagaoka phase. Region I, Nagaoka phase is stable. Region II, bubbles bigger than the critical value are metastable. Region III, bubbles bigger than the critical value are stable.

V^2/N where N is the system size, and V is the size of the optimal bubble. Comparing the two energies, one observes that at the transition $V \sim N^{d/(d+1)}$.

We performed a numerical study to validate the above calculations. The single-particle spectrum of a tight-binding square lattice model with periodic boundary conditions and an excluded domain, was calculated for different sizes of the excluded domain. We then calculated the ground-state kinetic energy (which is the sum of the lowest m eigenvalues, where m is the number of holes), and compared the increase of kinetic energy as a result of the excluded bubble with the gain in magnetic energy. For each size of excluded domain, a minimal value of J is needed to balance the increase of kinetic energy, thus stabilizing the AFM bubble. J_{cr} is determined as the minimum of these J values, i.e., the lowest value of J that allows for a stable bubble. The size of the bubble at this minimum is S_0. The area of the stable bubble at $J=J_{\mathrm{cr}}+$ is presented in Fig. 3 as a function of δ and N. It turns out that the leading asymptotic dominates only for a very big system, beyond numerical capabilities. We, therefore, calculated the subleading corrections $O(N^{-2/3})$ and $O(N^{-1})$ and compared the numerical results with this asymptotic expansion. The agreement with the analytical result is quite good for sufficiently large lattices, and it seems that the results converge to the asymptotic estimate as the system size increases, indicating that corrections due to deviations from the free particle band shape are not important for $\delta \leqslant 0.05$.

The picture emerging from these calculation is as follows (see also Fig. 4). At $J=J_{\mathrm{cr}}$ [Eq. (14)] the Nagaoka state breaks down and one large AFM bubble with the area of order of $O(N^{2/3})$ is formed [Eq. (15)]. As the size of the bubble scales only sublinearily with system size, the magnetization per site is continuous in the thermodynamic limit. In the vicinity of the transition point, only these large bubbles are stable, and, therefore, a large fluctuation is needed to destroy the Nagaoka phase. It is, therefore, a metastable phase. For larger J, s_0, the critical size for a stable bubble, decreases, and for $j \sim O(1)$ (i.e., $J-J_{\mathrm{cr}} \sim J_{\mathrm{cr}}$) it becomes finite and system-size independent. This behavior is typical for a first-order phase transition, where a domain of a new phase has to be large enough to survive. However, the jump in the magnetization is not extensive.

Why does not the system create many more bubbles, once the first bubble is formed, thus reducing the magnetization even further? The reason is, as can be shown in Eq. (7), that the kinetic energy is not a linear function of s. Therefore, the energy cost to create two bubbles is more than twice the cost to create one. On the other hand, the magnetic energy gain, is linear in s, and, therefore, it would just double by the creation of the second bubble.

There is an ongoing discussion in the literature regarding the existence of a striped ground state in the Hubbard and t-J models. Experimentally, there is evidence for stripe modulations in doped cuprates,[24] which are generally believed to be described by the t-J model. Some authors found that the t-J model ground state is indeed striped for a wide range of doping,[25] while others claim that uniform or phase-separated states have lower energy.[26] According to the latter view, the origin of the experimental observation is attributed to the competition between the local tendency for phase separation and the long-range Coulomb interaction, which is missing in the t-J model.[27]

In this study, we compared the energy of a striped state with the the energy of a phase-separated state with an AFM bubble. Within our approach, the kinetic energy increases in the striped phase due to the higher surface energy, with nothing else to compensate for this increase. Accordingly, the striped state energy is higher, suggesting that the long-range Coulomb repulsion is needed in order to create a striped ground state for $J/t \ll 1$. Our approach cannot rule out the possibility of a striped ground state of the t-J model at $J \sim t$.

In conclusion, we presented analytical arguments, exact diagonalization results, and semiclassical calculations of the 2D t-J model, which suggest that at small hole concentration δ and rather weak AFM coupling J the Nagaoka ferromagnetic state becomes unstable towards the creation of an AFM bubble. In this phase-separated state, the holes are confined to the FM regime. At the transition only a single large $O(N^{2/3})$ bubble is (meta)stable. Thus, the magnetization is

continuous at the transition in the thermodynamic limit. However, the jump in magnetization per unit area in a system with finite number of sites N, scales as $N^{-1/3}$. This dependence of the critical bubble size, and thus of the magnetization, on the size of the system is a typical finite-size effect in a phase-separated ground state.

ACKNOWLEDGMENTS

We thank S.A. Brazovskii, A.V. Chubukov, Y.M. Galperin, and S.A. Kivelson for helpful discussions and comments. The work at Princeton University was supported by the ARO and DARPA.

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