Abstract

A numerical scaling analysis is used to show that Nagaoka’s ferromagnetic state in two-dimensional Hubbard model with one hole is superseded by an antiferromagnetic (AF) state with a discontinuous jump in the total spin due to the AF coupling as the Hubbard $U$ is made finite. The same applies to the two-hole system, which has a spiral spin structure. We can show, via the scaling, that the crossover to an AF state is a precursor of a pathological coalescence of states having the minimum spin and Nagaoka’s state at $U = \infty$ in the thermodynamic limit.

PACS numbers: 75.10.Lp, 71.27.+a, 75.30.Ds
To identify a stable itinerant ferromagnetism is one of the longest-standing yet unresolved problems in the physics of strongly correlated electron systems. Nagaoka’s theorem is the first rigorous result, which served as a foundation of subsequent studies. Nagaoka’s problem still holds a fascination as a remarkable manifestation of the correlation effect in the doped Mott’s insulator, where a key concept is interference between the motion of a hole and its surrounding spin configuration. A recurring question on Nagaoka’s ferromagnetism, however, is the singular condition (the half-filled band doped with a single hole with the Hubbard $U = \infty$): Is it possible to extend the ferromagnetism away from the extreme condition down to finite number of holes and/or finite coupling strengths?

There have in fact been many attempts at looking into the possibility of a finite ferromagnetic region in the vicinity of Nagaoka’s limit in the phase diagram. Nagaoka has already shown that the spin-wave excitation in Nagaoka’s ferromagnet is singular in that the spin stiffness vanishes like the inverse of the system size, $N$. If one concentrates on the stability against one-spin flip (1SF) modes having $S = S_{\text{max}} - 1$, however, the ferromagnetic phase seems to extend over a finite area on the parameter space of the density of holes ($\delta = N_h/N$) and the antiferromagnetic (AF) coupling ($J = 4t^2/U$), but these variational (usually Gutzwiller-projected RPA) results should be considered as an upper limit for the ferromagnetic boundary. On the other hand, a recent high-temperature expansion result by Putikka et al. shows that the true ground-state is significantly lower in energy than the fully-polarized state for any hole density. They also argue the possibility of a finite ‘ferrimagnetic’ region, which is identified from the uniform spin susceptibility diverging like the Curie law.

An exact way to explore the problem is the numerical diagonalization of finite systems. A serious point found in early studies is that Nagaoka’s state is sensitive to both the boundary condition and the number of holes, where singlet states can supersede Nagaoka’s state even at $U = \infty$. These results have motivated subsequent investigations. As for the instability of Nagaoka’s state against $J$, Ioffe and Larkin have conjectured that a crossover to an AF phase with a jump in $S$ can possibly occur for increasing $J$. Nature of
the lower-spin states that compete with Nagaoka’s, however, is not fully understood yet.

The purpose of the present paper is (i) to give the low-lying spectrum including both charge and spin excitations, which will serve as a foundation (ii) to obtain the scaling properties of the energy gap and level crossings to actually identify how Nagaoka’s state is superseded for the 2D square lattice. In the formalism for (i), the heavy mass spin-wave, which causes the coalescence of states comes from an interference between the charge (Bloch) momentum and the spin momentum. In (ii) we move on to calculate the low-lying states for every possible total spin (0 or \(1/2 < S < S_{\text{max}}\)) to show that the first state to take over Nagaoka’s as \(U\) is decreased from infinity is indeed an AF state rather than a partially polarized one, which indicates a discontinuous jump in the total spin. The same sudden crossover occurs for the \(S = 0\) ground state at \(U = \infty\) that appears for one hole with the anti-periodic boundary condition (APBC) or for two holes with the periodic boundary condition (PBC), which we identify as a spiral spin structure with a wave-length comparable to the system size. The crossover by an AF state is related, via the scaling, to a pathological degeneracy at \(U = \infty\), where even the lowest-spin states become degenerate with the Nagaoka’s (or spiral) state in the thermodynamic limit \((N \to \infty)\).

In order to grasp the subtleness of Nagaoka’s state, we start with introducing the following formulation. Consider the large-\(U\) Hubbard model on a \(d\)-dimensional hyper-cubic lattice with PBC. An eigenfunction for \(N_e = N - 1\) electrons with one hole can be written

\[
|\phi\rangle = \sum_{\{\sigma_j\}} f(\sigma_1, \ldots, \sigma_{N_e}) C^{\dagger}_{x_1 \sigma_1} \cdots C^{\dagger}_{x_{N_e} \sigma_{N_e}} |0\rangle,
\]

where \(x_h\) is the position of a hole and \(C^{\dagger}_{x_j \sigma_j}\) creates an electron with spin \(\sigma_j\) at \(x_j\). The coefficient, \(f(\sigma_1, \ldots, \sigma_{N_e})\), can be regarded as a spin wavefunction around the hole. Note that we do not sum over the position of each electron: A trick in writing the above formula is that the sequence \((x_1, \ldots, x_{N_e})\) (where no two positions coincide to exclude double occupancies) of the multiplication of creation operators is fixed in such a way that the creation at the same coordinate \textit{relative to} \(x_h\) enters in the same position for each value of \(x_h\). In this
convention \( f \) no longer contains \( x_h \) reflecting the translational symmetry, while the factor \( \exp (i \mathbf{k} \cdot x_h) \) takes care of Bloch’s theorem.

Consider the strong-coupling model, which is derived from the Hubbard model in the second order in \( 1/U \)-expansion. Operating to the above basis we end up with a spin Hamiltonian,

\[
\mathcal{H}_{\text{spin}} = -t \sum_{a=1}^{d} \{ \exp (i \mathbf{k} \cdot \mathbf{u}_a) \mathcal{T}_a + \exp (-i \mathbf{k} \cdot \mathbf{u}_a) \mathcal{T}_a^{-1} \} \\
+ J \sum_{<i,j>} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) \\
- \frac{J}{4} \sum_{a,a'} \{ \exp (i \mathbf{k} \cdot \mathbf{u}_a + i \mathbf{k} \cdot \mathbf{u}_{a'}) \mathcal{T}_a \mathcal{T}_{a'} \\
\times (n \mathbf{u}_a + \mathbf{u}_a \downarrow n \mathbf{u}_{a'} + \mathbf{u}_{a'} \downarrow n \mathbf{u}_a \uparrow - S^+ \mathbf{u}_a + \mathbf{u}_a^+ S^- \mathbf{u}_{a'} - S^- \mathbf{u}_a + \mathbf{u}_a^- S^+ \mathbf{u}_{a'}),
\]

(0.2)

which corresponds to the spin part of the \( t-J \) model (including three-site terms). Here the operation, \( \mathcal{T}_a(a = x, y, \ldots) \), is roughly a translation of the spin configuration along \( a \)-axis except for a spin on \( x_h + \mathbf{u}_a \), which is shifted onto \( x_h - \mathbf{u}_a \) with \( \mathbf{u}_a \) being a nearest-neighbor vector. The last line represents the three-site term, where the summation involves the neighbor \( (\mathbf{u}_a) \) of the hole site and the third site \( (\mathbf{u}_{a'}) \) which is the neighbor of \( \mathbf{u}_a \).

The expression in the first term of Eq. (0.2) suggests the following picture. Since \( \mathcal{T}_a \) is almost a translation, it gives a phase which is roughly the momentum of the spin configuration. To be more precise, we can introduce, in place of \( f(\sigma_1, \ldots, \sigma_N) \) where spins are not allowed to occupy the hole site (i.e. \( x_j \neq 0 \)), another basis, \( g(y_1, \ldots, y_M) \), for \( M \)-spin-flip states on the square lattice. Here \( y_j \), which may be \( 0 \), denotes the position of \( j \)-th down spin. We can then readily construct an eigenstate of the total momentum, \( \mathbf{Q} \). As a penalty for using the extended basis, the operation \( \mathcal{T}_a \) must be redefined: it gives zero if any \( y_j \) equals to \( 0 \) in \( g \). In this representation, the problem becomes a scattering of a spin at the hole site. Because the scattering is a higher-order process of \( O(1/N) \) compared with the translation, we can obtain the asymptotic expansion in \( 1/N \) for the 1SF heavy-mass mode in 2D. The solution exhibits a heavy mass (the band width \( \sim 4\pi t/N \ln N \)), which coincides with the result by Barbieri et al. [20]
The advantage here is that the present formalism enables us to introduce a quasi-momentum \( \tilde{Q} \) defined by \( T_a |\phi\rangle = \exp(i\tilde{Q} \cdot u_a) |\phi\rangle \). Then the asymptotic result indicates that \( \tilde{Q} \) is nearly equal to the momentum, \( Q \), of the incoming state (with \( |\tilde{Q} - Q|^2 \sim O(1/N \ln N) \) for spin-wave excitations). For a solution with \( \tilde{Q}(k) \), the dispersion is given by \( \varepsilon(k) = -2t \sum_{a=1}^{d} \cos(\tilde{Q}_a(k) - k_a) \) for each \( k \). In a finite system we have discrete \( k \)-points (= 0, \( k_1 \), ...) having single-particle excitation energy \( \varepsilon(= 0, \varepsilon_1, ...) \). From this we can predict that the 1SF excitation from Nagaoka’s state should comprise a series of bands, each of which consists of an incoming wave, \( Q = k + k_i \) and has a quasi-momentum \( \tilde{Q} = k + k_i + \Delta k(i = 0, ...) \), which are separated by the single-particle energy, \( \varepsilon_i \), with the band widths vanishing like \( O(t/N \ln N) \). Note that \( \varepsilon_i \) itself vanishes like \( O(t/N) \), which roughly gives the gap between heavy-mass bands.

This picture is in fact confirmed from the numerical diagonalization of a 290-site system in Fig. [1]. Interestingly the above picture also holds for two-spin-flip (2SF) excitations, where the width of the lowest 2SF continuum as well as the width of the lowest 1SF dispersion fit to a size dependence of \( \Delta_{1SF}(\infty), \Delta_{2SF}(\infty) \sim t/N \ln N \ll \varepsilon_1 \sim O(t/N) \) within a finite-size correction (inset of Fig. [1]). The energy of 2SF mode is shown to be approximately twice that of 1SF, so that the spin-waves are nearly free. This is natural because the interaction between spin-waves is a higher-order process than the scattering of a single spin at the hole site.

We now turn to finite \( U \) for a fixed boundary condition in finite systems to probe level crossings between Nagaoka’s state and other states having various total spin. So far Nagaoka’s state is suggested to change to partially polarized ones, then finally to a lowest-spin state after several level crossings in 2D from numerical studies on 10- and 16-site systems. [21,22,23,24]

However, if we increase the size to a 20-site system here, the strong-coupling model (\( t-J \) model with or without the three-site terms) shows the absence of the intermediate partial polarization in the ground state, (Fig. [2]) where the range of \( J \) for the partially polarized region decreases systematically to zero (Fig. [3]). This suggests that an abrupt crossover from
the fully spin-polarized state to an unpolarized state occurs for larger systems.

We can relate this feature with the spectrum in the strong-coupling limit via the scaling property of the level crossings. We have previously reported from the value of $U_c$ for the level crossings that a 2SF mode takes over Nagaoka’s state before a 1SF mode does so. If we plot here the crossing point, $U_c^{AF}$, between Nagaoka’s state and the AF state as well, we see that this is the crossing that comes downwards most rapidly for increasing $J$ (inset of Fig. 2). Thus we obtain a lower bound for $U_c^{AF}$ as $U_c^{AF} > \frac{4t}{\pi} N \ln N$. The asymptotic form for the energy of the AF state is expected to be

\[ E_{AF} = -4t + \Delta_{AF} - aN \frac{4t^2}{U} , \]  

(0.3)

where $\Delta_{AF}$ is the energy gap between the AF state above Nagaoka’s state at $U = \infty$ and the last term with $a \sim O(1)$ is the AF exchange interaction. Hence we end up with an upper bound for $\Delta_{AF}$, via $E_{AF}(U_c^{AF}) = E_{Nagaoka} = -4t$, as

\[ \Delta_{AF} < a\pi t / \ln N , \]  

(0.4)

which vanishes in the thermodynamic limit. Therefore the huge degeneracy of the ground state in Nagaoka’s limit is seen to include even the AF state.

Although it is premature to discuss whether a spin-polaron picture or string picture applies here, we have confirmed that the lowest $S = 1/2$ state has the energy that varies approximately linearly with $J$ for $J_c^{AF} \leq J \lesssim 0.1t$ and $S(Q)$ that remains to be peaked at $(\pi, \pi)$, which implies that the AF state experiences no level crossing prior to the crossing with Nagaoka’s for systems up to 26-sites. (See also \[26\].)

As far as finite systems are concerned, we find that the number of holes is crucial while the concentration of holes is ill-defined in the Hubbard model at $U \sim \infty$. As already noted by Riera and Young, \[13\] there are similarities among the systems having the same number of holes. Thus we can look for a scaling property in the series of finite samples with the same number of holes. For two holes, we can look at the level crossing between the spiral-spin ground state for large $U$ characterized by $S(Q)$ having four peaks around the $\Gamma$-point and
the AF state. If we fit the crossover point from Nagaoka’s state, $J_{c}^{AF} (= 4t^2/U_{c}^{AF})$ against $\delta$ with a power-low, we have $J_{c}^{1\text{hole}} \propto \delta^{1.73}, J_{c}^{2\text{hole}} \propto \delta^{1.74}$. Thus for $J \rightarrow 0$ Nagaoka’s (or spiral) state is only realized for an infinitesimal doping, if this scaling persists to $\delta \rightarrow 0$. We notice in Fig. 3 that two scaling curves, although having similar exponents, differ considerably, which endorses the difficulty in defining the hole concentration. Since both $J_{c}^{1\text{hole}}$ and $J_{c}^{2\text{hole}}$ are tangent to the $\delta$ axis, a convex functional form for other number of holes would be required to have a finite region for magnetism. If we compare our scaling relation with the result (dashed line in Fig. 3) from the high-temperature expansion by Putikka et al, the width for the partial polarization for one- and two-holes vanishes in what they call is the ferrimagnetic region. As far as finite systems with $N \sim 20$ are concerned, our result thus indicates the absence of magnetism in this region.

However, since a finite number of holes only correspond to an infinitesimal hole doping for $N \rightarrow \infty$, the true problem of the ground state for finite concentrations of holes in the thermodynamic limit remains an open question.

We wish to thank Prof. M. Ogata for illuminating discussions. We are also grateful for Prof. Y. Nagaoka in the early stage of the present work.
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FIGURES

FIG. 1. Spin-wave excitations from Nagaoka’s state (solid circle) in a 290-site 2D square lattice with $U = \infty$. Open circles represent one-spin-flip (1SF) excitations, while hatched regions represent continuum of two-spin-flip excitations. The arrow denotes the first single-particle excitation energy, $\Delta_{\text{single}}$. The inset shows the size dependence of the band width, $\Delta_{\text{1SF}}$, of the lowest 1SF mode (solid line), the width, $\Delta_{\text{2SF}}$, of the lowest 2SF continuum (broken line), and the bottom-to-bottom spacing of the first two 2SF continua, $W_{\text{2SF}}$ (chain line). We also indicate the dependence, $4\pi t/N \ln N$ (lower dotted line), and the single-particle energy $\Delta_{\text{single}}(\sim 1/N)$ (upper dotted line).

FIG. 2. Level crossings in a 20-site $t$-$J$ model in the small $J$ regime. The ground state changes from Nagaoka’s state to a singlet state at $J_{c}^{\text{AF}} = 0.0413t$. The inset shows the scaling of various $U_c$’s for $t$-$J$ models with 3-site terms defined in the text. The dotted line represents the analytic evaluation, $U_{c}^{\text{1SF}} = (4t/\pi)N \ln N$, while the dashed, chain and solid lines are a guide to the eye.

FIG. 3. Scaling for the crossover point, $J_c$, for the one-hole doped case between Nagaoka’s state and the antiferromagnetic (AF) state, and for the two-hole doped case between the spiral-spin state and the AF one. Bars represent not the error bar but the range over which partially polarized states are realized. A broken line is the boundary for the ‘ferrimagnetic’ region obtained by Putikka et al. (Ref. [10],[11]).