Ferromagnetism in the Two-Dimensional t-J Model

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The occurrence of ferromagnetism for the t-J model on a square lattice is investigated using high-temperature series for the Helmholtz free energy F and the uniform magnetic susceptibility χ_0. For $J=0$ fourteenth-order series have been calculated for F and χ_0 and we estimate $F(T=0)$ to find the ground-state energy. A region of fully polarized ferromagnetism is found for $J<0$. A ferrimagnetic region is observed for larger J/t where χ_0 is divergent, but $F(T=0)$ is below that of spinless fermions. Our results do not support Nagaoka's theorem at a thermodynamic density of holes.

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Nagaoka's theorem [1] is one of the few known exact results for strongly correlated fermions on a square lattice. The theorem states that for the $U=\infty$ Hubbard model, or equivalently the $J=0$ t-J model, on a bipartite lattice with exactly one hole in an otherwise half-filled band, the ground state is a fully polarized ferromagnet (FPFM). However, the theorem does not address a finite density of holes. To investigate Nagaoka's theorem in the two-dimensional (2D) t-J model on a square lattice, Putikka, Luchini, and Rice [2] studied the low-temperature behavior of the uniform magnetic susceptibility χ_0. They found a region in the phase diagram where χ_0 is divergent at $T=0$, but it was not possible to determine whether or not the ground state is a FPFM. In this paper we present results from fourteenth-order high-temperature series for the Helmholtz free energy F and χ_0 for $J=0$. Using the series for F we estimate the ground-state energy $E_0(n)$ as a function of electron density n. Comparison to the known FPFM (spinless fermions) ground-state energy $E_{\rm FM}(n)$ shows that FPFM is realized only for $n=1$. Furthermore, by studying the ferromagnetic t-J model ($J<0$) we are able to determine where FPFM occurs in the phase diagram. These results show that between the FPFM phase and the singlet region there is a ferrimagnetic region, including the region of diverging χ_0 previously observed. The literature on ferromagnetism in strongly correlated systems is vast, and we do not attempt a complete review. The interested reader is referred to the references and papers listed therein.

$E_0(n)$ for $J=0$ is the minimum energy for the kinetic part of the t-J Hamiltonian. In 1D this is independent of the spin configuration [3] and is thus equal to $E_0(n)$ for FPFM. For $J<0$ the FPFM state also minimizes the exchange energy; therefore in 1D for $J<0$ the ground state for all n is FPFM. For $J\gtrsim 0$ the exact ground state of the 1D t-J model is not rigorously known, but numerical diagonalization results [4] give a Tomonaga-Luttinger liquid ground state, not FPFM. In 2D, where no rigorous results are known for $E_0(n)$, we find for $J=0$ that $E_0(n)$ is below that of FPFM for $0<n<1$, implying that Nagaoka's theorem does not hold for a thermodynamic density of holes. It follows that for $J>0$ FPFM is not the ground state of the t-J model for any n. For $J<0$ FPFM is more favored and we plot a curve for stability of the FPFM state in the $(J/t,n)$ phase diagram. Our main conclusion is that FPFM is more difficult to obtain in the 2D t-J model than previous calculations have indicated.

Nagaoka's theorem has been extended to larger numbers of holes [5,6], but not to a thermodynamic density of holes. Douçot and Wen [7] have shown for $J=0$ and two holes on a bipartite lattice that the FPFM state is not the ground state for any dimension, in agreement with numerical calculations [8] in 2D. Kanamori [9] showed that for $n\ll 1$ the ground state for $J=0$ is paramagnetic and recent variational calculations [10] have established a rigorous critical density $n_c=0.71$ below which FPFM is unstable for the square lattice at $J=0$. Ferromagnetism in the large-U Hubbard model has also been investigated by using a Gutzwiller variational wave function [11-13] and by spin-wave analysis [14]. Numerical calculations on finite-size lattices [15] find for $J\gtrsim 0$ and $1-n\ll 1$ numerous level crossings for states with different total spin and a marked sensitivity to boundary conditions. The magnetic properties of the t-J model have also recently been investigated by high-temperature series by Singh and Glenister [16].

We generate the high-temperature expansion of the thermodynamic potential $\Omega(\mu,h)$ as a function of the chemical potential μ and an applied uniform magnetic field h for the t-J model by the finite-cluster method [17]. The Hamiltonian of the t-J model in an applied uniform magnetic field is

$$H=-t\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_in_j}{4}\right)-g\mu_Bh\sum_i S_i^z-\mu\sum_i n_i\,, \tag{1}$$

with the constraint of no doubly occupied sites. After calculating $\Omega(\mu,h)$ we use the thermodynamic relations $\bar{N}=-\partial\Omega/\partial\mu$ and $M=-\partial\Omega/\partial h$ to find series for n and $m=M/\mu_B\bar{N}$ at fixed μ and h. Inverting these series allows us to substitute n and m for μ and h, obtaining $F(n,m,T)$ and $g^2\mu_B^2/\chi_0=(1/n^2)\partial^2F/\partial m^2|_{m=0}$. Independent checks on our series are given by the previous results

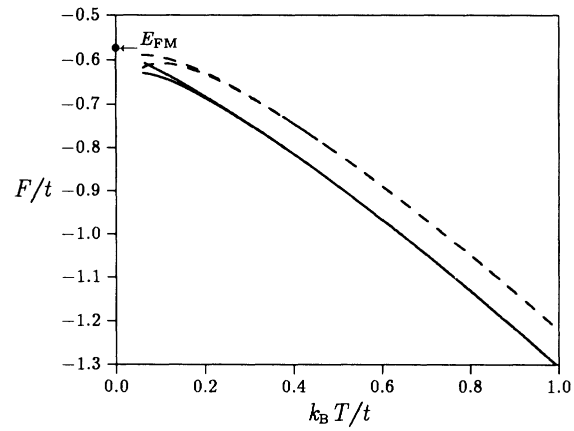

FIG. 1. Plot of two different integral approximants used in estimating F_0. Here $n=0.80$, and the solid curves are for $J/t=0$ and the dashed curves are for $J/t=-0.30$. To extrapolate F to $T=0$ we include the physically reasonable requirements that the entropy $S=-\partial F/\partial T$ be a monotonic function of T and $S=0$ at $T=0$. E_{FM} at $n=0.80$ is also indicated.

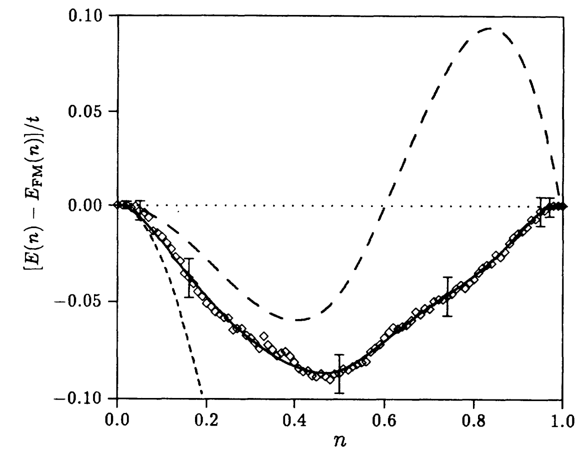

FIG. 2. Differences in ground-state energies from $E_{FM}(n)$ for $J=0$. Data points with representative error bars: estimates for $T=0$ free energy; solid curve: least-squares fit to the data points given by Eq. (2); short-dashed curve: free fermions; long-dashed curve: Gutzwiller wave function.

of Kubo and Tada [18] for the $U=\infty$ Hubbard model, the work of Baker, Eve, and Rushbrooke [19] on the Heisenberg model and the well-known correspondence of the FPFM state to noninteracting spinless fermions: Setting $m=1$ we recover the series expansion for the free energy of spinless fermions. We analyze our series by means of integral and Padé approximants [17,20]. Further details of the series calculation and our analysis will be given in Ref. [21].

For the case $J=0$ we have a fourteenth-order series which enables us to make better estimates for E_0. We extended our previous tenth-order calculation [2] by means of the clusters tabulated by Harris and Meir [22]. By using integral approximants we obtain a converged result for $F(n,m,T)$ to temperatures of order $\beta t \sim 5$, except for $n\approx 0$. An example showing the convergence of the integral approximants is given in Fig. 1. We compare our estimates $F(n,m=0,T=0)=F_0(n)$ for $E_0(n)$ to $E_{FM}(n)$ to determine the stability of the FPFM state for $0<n<1$. The data are plotted in Fig. 2. The data points are clearly below $E_{FM}(n)$ for most densities. For low densities the Gutzwiller wave function [12], which is also an upper bound for E_0, gives a better result than E_{FM} [see Eq. (3) below]. However, the estimated $F_0(n)$ is still lower, lying between the ground-state energy for the Gutzwiller wave function $E_{GW}(n)$ and the ground-state energy for free fermions. This indicates that a Jastrow factor is necessary to modify the Gutzwiller wave function [13,23]. It has been noted [24] that the Gutzwiller wave function should be a good trial wave function near $J/t=2$.

If there is long-range order we expect a discontinuity for some order of $d^kE_0(n)/dn^k$ at the critical density n_c where $E_0(n)$ would be nonanalytic. We see no kinks in $F_0(n)$ so there probably is not a first-order transition, but there may be higher-order transitions which we are unable to address due to uncertainty in the data points. We have calculated a least-squares fit of our data points by a polynomial of the form

$$\tilde{F}_0(n)=n(1-n)\left[-4+\sum_{i=1}^{6}a_i n^i\right]. \quad (2)$$

This fixes $\mu_0=\mu(T=0)$ at the end points, $\mu_0(n=0)=-4$ and $\mu_0(n=1)=4$, which we know from Nagaoka's theorem. The coefficients a_i are $a_1=-1.0463$, $a_2=14.1120$, $a_3=-40.0637$, $a_4=60.4847$, $a_5=-53.7067$, and $a_6=20.3059$. From the plot of $\tilde{F}_0(n)$ in Fig. 2 we see it is likely that E_0 for the $J=0$ t-J model is less than

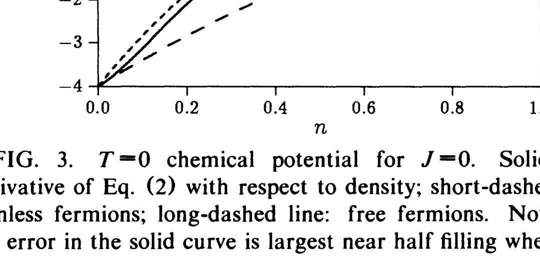

FIG. 3. $T=0$ chemical potential for $J=0$. Solid line: derivative of Eq. (2) with respect to density; short-dashed line: spinless fermions; long-dashed line: free fermions. Note that the error in the solid curve is largest near half filling where it is too low by 0.09. This provides an estimate of the error in our result for μ_0.

E_{FM} for all n. Our results are also consistent with known upper and lower bounds for E_0 [6,25]. From the least-squares fit we can estimate $\tilde{\mu}_0 = \partial\tilde{F}_0/\partial n$, plotted in Fig. 3. From $\tilde{\mu}_0$ and the original data points we see that $F_0(n)$ is asymmetric around $n=0.5$, with a minimum at $n \approx 0.48$. This slight canting of $F_0(n)$ favors FPFM for $1-n \ll 1$, but does not seem to be sufficient to stabilize the FPFM state away from half filling. In principle we could also examine F_0 as a function of m for fixed n to determine the average magnetic moment, but as can be seen from Fig. 2 the energy difference for $m=0$ and $m=1$ is small and our current accuracy prevents us from obtaining useful results.

For $J<0$ we have compared $F_0(n)$ to $E_{FM}(n)$ to determine where FPFM is stable in the phase diagram. Our data are plotted in Fig. 4. At half filling we have the ferromagnetic Heisenberg model, which is known to have a FPFM ground state. Nagaoka's theorem also remains valid for $J<0$ since with only one hole flipping any spin will increase the energy of the state. When $J<0$ we see that FPFM is more stable than for $J=0$, but for $n \lesssim 0.5$ a rather large value of $|J/t|$ is required. The curve for stability of the FPFM state we observe for $J<0$ is consistent with our result at $J=0$, where we believe a thermodynamic density of holes destabilizes the FPFM state.

We expect there is a critical J_c such that for $J<J_c$ we have FPFM for all n. For $J/t \lesssim -2$ the difference between $F_0(n)$ and $E_{FM}(n)$ is too small to be reliably determined with our current series. A simple estimate of J_c can be found by comparing low-density expansions through $O(n^2)$ of E_{FM} and E_{GW},

$$E_{FM} = -4nt + 2\pi n^2 t\,,$$
$$E_{GW} = -4nt + (\pi+2)n^2 t - n^2 J\,. \tag{3}$$

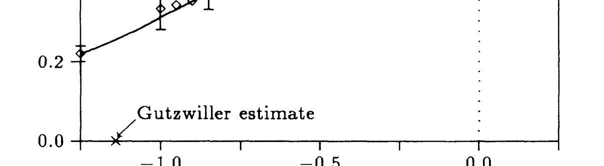

FIG. 4. Phase diagram for negative J/t. The data points with representative error bars give the curve for stability of FPFM while plain error bars denote the curve $\gamma=1$. The ferrimagnetic part of the phase diagram is the shaded region between these curves. The line is a guide for the eye.

A diagrammatic method [26] was used to calculate E_{GW}. Using this method the low-density expansion can be obtained analytically. Setting $E_{FM}=E_{GW}$ we find $J_c^{GW}/t = 2-\pi \approx -1.14$. This value is larger than indicated by our series results which give $n_c \approx 0.12$ at $J/t=-2$. However, we expect E_{GW} to give a larger result for J_c/t because E_{GW} is an upper bound for E_0. Thus E_{FM} will cross E_{GW} before E_0 and J_c^{GW}/t is an upper bound for the true J_c/t.

Long-range ferromagnetic order at $T=0$ should manifest itself in a diverging χ_0 as $T \to 0$. To investigate this possibility we extend our previous analysis for $J>0$ in Ref. [2] to $J<0$. We assume a power-law singularity of the form $\chi_0 = A(\beta t)^\gamma$ in the limit $T \to 0$ and form the biased logarithmic derivative,

$$(\beta t)\frac{d}{d(\beta t)}\ln\chi_0 = \gamma\,. \tag{4}$$

We estimate γ for $T=0$ by calculating diagonal Padé approximants for the resulting series. To estimate the range of ferromagnetic behavior in the phase diagram we use the criterion of Yedidia [27]. He chose the boundary of ferromagnetism to be where the susceptibility is like free spins, i.e., $\gamma=1$. The data points for $\gamma=1$ are plotted in Fig. 4.

The points for $\gamma=1$ lie outside the region of the phase diagram where FPFM is the ground state as determined by ground-state energy comparisons. For a 2D FPFM we expect χ_0 to diverge exponentially [28] as $T \to 0$. If this is the true behavior of χ_0, the logarithmic derivative calculated above would still give a divergent result instead of a constant. If we make J/t more negative at fixed n, γ does not become larger until the Padé approximants eventually have real poles at $T>0$, similar to the behavior of the series for the 2D Heisenberg ferromagnet. There is a large region between the $\gamma=1$ points and the FPFM phase indicated by the shading in Fig. 4. Since $F_0(n) < E_{FM}(n)$ in this region we must have $m<1$, but we have not determined the exact value of m. The value $\gamma=1$ is the same as for free spins and thus it is reasonable to expect that states of different total spin are degenerate on this line. It seems likely that this degeneracy is lifted when $\gamma>1$ and therefore $m \neq 0$. We interpret this region as ferrimagnetic. With our present series we cannot investigate the existence of more complicated spin orderings. A recent quantum Monte Carlo calculation [29] at $J=0$ has obtained an estimate of the moment in agreement with our results. As we go to more negative J/t the curves for $\gamma=1$ and FPFM come very close together. The error bars on the data points are currently too large to distinguish the two curves for $J/t \lesssim -0.5$.

For $J \geq 0$ and $1-n \ll 1$ we expect the t-J and Hubbard models to have similar behavior. However, $J<0$ does not correspond to $U<0$, since in the t-J case we still have the constraint of no double occupancy, while for $U<0$ in the Hubbard model double occupancy is favored. The parameter region expected to be most favorable for FPFM in the Hubbard model is $U/t \gg 1$ and $1-n \ll 1$. If this is true our results suggest FPFM in the 2D Hubbard model occurs only for $U=\infty$ and $n=1$, though there probably is a region of ferrimagnetism around this point.

We have investigated ferromagnetism in the 2D t-J model using high-temperature series for F and χ_0. By considering the parameter range $J/t<0$, we plot a curve for stability of FPFM. This, along with our ground-state energy estimates at $J/t=0$, suggests that the critical density for Nagaoka's theorem is $n_c=1$ instead of $n_c=0.71$ as given by variational calculations. For slightly larger J/t we expect ferrimagnetic behavior where E_0 of the t-J model is below that for a FPFM, but χ_0 is still divergent. The nature of the spin ordering (if any) in this region is not understood at present. Our results imply that the FPFM state is the ground state of the 2D Hubbard model only for $n=1$ and $U=\infty$.

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