Ferromagnetism in the two dimensional $t-t'$ Hubbard model at the Van Hove density

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Abstract

Using an improved version of the projection quantum Monte Carlo technique, we study the square-lattice Hubbard model with nearest-neighbor hopping $t$ and next-nearest-neighbor hopping $t'$, by simulation of lattices with up to $20 \times 20$ sites. For a given $R = 2t'/t$, we consider that filling which leads to a singular density of states of the noninteracting problem. For repulsive interactions, we find an itinerant ferromagnet (antiferromagnet) for $R = 0.94$ ($R = 0.2$). This is consistent with the prediction of the $T$-matrix approximation, which sums the most singular set of diagrams.

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The understanding of itinerant ferromagnetism (FM) is a long-standing problem of solid-state physics [1]. In search for a generic model of FM, the Hubbard model, describing electrons from a single band subject to a local electron-electron repulsion $U$, has been investigated extensively. Motivated by an exact result of Nagaoka [2], most papers studied the stability of a fully polarized state (believed to occur in the phase diagram of the Hubbard model at large interaction strength and close to half filling) against single spin flips. The results turned out to be strongly dependent on the quasiparticle spectrum [3], and, generically, unrealistically large $U$ were required to stabilize a fully polarized state. Motivated by the recent proofs of FM in certain models with flat bands [4], in this Letter we take a complementary route, investigating the stability of the paramagnetic phase of a model with a high density of states against FM at weak coupling.

We consider electrons on a square lattice with $L = l \times l$ (even $l$) sites, described by the Hamiltonian

$$H = -t \sum c_{i,\sigma}^\dagger c_{j,\sigma} + t' \sum c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum n_{i,\uparrow} n_{i,\downarrow},$$

where $t$ and $t'$ are nearest and next-nearest neighbor hoppings, respectively. The bare dispersion is $\varepsilon_k = -2t(\cos k_x + \cos k_y) + 4t'\cos k_x \cos k_y$ and its saddle points are, for $0 < R = 2t'/t < 1$ studied here, at $(\pi,0)$ and $(0,\pi)$. In what follows, we always consider the case when the chemical potential is $-4t'$, so that the noninteracting Fermi surface crosses the saddle points and the noninteracting density of states at the Fermi level diverges. At this so-called Van Hove (VH) density, both the particle-hole and particle-particle susceptibilities $\chi_{ph}, \chi_{pp}$ diverge at $\mathbf{q} = 0$ and $\mathbf{Q} = (\pi, \pi)$ and their singular parts are

$$\chi_{ph}(0) = (1/2\pi^2t)(1/\sqrt{1-R^2}) \ln(t/\omega),$$

$$\chi_{ph}(\mathbf{Q}) = (1/2\pi^2t) \ln[(1 + \sqrt{1-R^2})/R] \ln(t/\omega),$$

$$\chi_{pp}(0) = (1/4\pi^2t)(1/\sqrt{1-R^2}) \ln^2(t/\omega),$$

$$\chi_{pp}(\mathbf{Q}) = (1/2\pi^2t)[\arctan(R/\sqrt{1-R^2})/R] \ln(t/\omega),$$

where $\omega$ is an infrared energy cutoff. It follows that, in the mean field approximation,
infinitesimal interactions cause symmetry breaking: $U > 0$ implies FM for $R > 0.55$ and antiferromagnetism (AFM) for $R < 0.55$ \cite{3}, and $U < 0$ leads to superconductivity \cite{4}. The magnetic states are interesting because of their metallic character. However, particularly in the case of FM, it is known that the use of a bare susceptibility in the Stoner criterion leads to incorrect predictions. In order to go beyond mean field theory, let us calculate the $U^2$ correction to the energy of a FM state with magnetization $m = (N_\uparrow - N_\downarrow)/L$ where $N_\sigma$ is the total number of electrons with spin $\sigma = \uparrow, \downarrow$,

$$E^{(2)} = -\frac{U^2}{2} \sum_q \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} |\chi_{pp}(q, i\omega)|^2 .$$

$m \neq 0$ reduces the always negative $E^{(2)}$, because the anomalous contributions of processes with momentum (energy) transfers $q \sim 0, Q (\omega \sim 0)$ are cut off in the FM state. We have calculated the energy to order $U^2$ for $R = 0.94$ on a $64 \times 64$ lattice with 1612 electrons \cite{7} for 10 closed-shell configurations with magnetizations $m < 186/64^2$ and found that the lowest possible $m = 2/64^2$ was stable for all $U$. Fig. 1 shows a similar result for a $16 \times 16$ lattice. Thus a resummation of an infinite set of diagrams is necessary.

In the following, we use the $T$-matrix approximation (TMA) in order to go beyond perturbation theory. TMA is, in general, justified if the interaction range is much shorter than interparticle spacing. This situation is realized in the limit $R \to 1$. Moreover, scattering in the particle-particle channel is the most singular process for all $R > 0$. TMA has been shown previously to restrict severely the possibility of low-density FM \cite{8}. Following Ref. \cite{9} we find that, in TMA, the spin-antisymmetric Landau interaction function

$$f^a_{k,k'} = -U/[1 + U \chi_{pp}(k + k', \omega = 0)].$$

This means that the interaction between those points of the Fermi surface which are in the neighborhood of the VH points vanishes. Assuming that the shape of the noninteracting Fermi surface is not changed, let us consider now, within Landau’s Fermi liquid theory, the stability of the paramagnetic state against Pomeranchuk instabilities. The change of the energy under a local shift $\Delta_{k,\sigma}$ of the chemical potential for spin-$\sigma$ electrons close to the point $k$ on the Fermi surface is

$$\delta E = \frac{1}{2} \sum_\sigma \int dk N_k \Delta_{k,\sigma}^2$$
\[ + \frac{1}{2} \sum_{\sigma,\sigma'} \oint dk'N_{k'}k'f_{k,k'}^{\sigma,\sigma'} \Delta_{k,\sigma} \Delta_{k',\sigma'}, \]  

(2)

where \( N_k \propto 1/v_k \) is the angle-resolved density of states, \( v_k \) is the Fermi velocity, and \( \oint dk \) denotes an integral along the Fermi surface. For a ferromagnet \( \Delta_{k,\sigma} = \sigma \Delta \) and, consequently, \( \delta E \propto \Delta^2 [1 + F_{a0}] \), where \( F_{a0} = \oint dkN_k \oint dk'N_{k'}f_{k,k'}^f/\oint dkN_k \). Let us assume further that \( v_k \propto \delta k \), where \( \delta k \) is the distance between \( k \) and the closest VH point. For \( k, k' \) both in the neighborhood of the same VH point, we expect \( \chi_{pp}(k+k') \propto \ln [1/\max(\delta k, \delta k')] \). The contribution of such \( k, k' \) to the integral for \( F_{a0} \) is \( F_{a0} \propto -\sqrt{U/t} \). Thus, intrasaddle point processes do not lead to FM at weak coupling. However, if \( k, k' \) lie close to different VH points, we expect \( \chi_{pp}(k+k') \propto \ln [1/\max(\delta k, \delta k')] \). This contributes \( F_{a0} \propto -(U/t) \int_1^l dk/[k(1 + A \ln (1/k))] \propto -\ln [A \ln l] \) where \( A \propto U/t \) and \( l \) is the system size. Thus the FM instability criterion \( F_{a0} < -1 \) is satisfied for arbitrarily small \( U \) if \( l \to \infty \). Note that TMA predicts a much weaker divergence of \( F_{a0} \) with \( l \), as compared to the mean field prediction \( F_{a0} \propto -A \ln l \). This is shown explicitly for a 16×16 lattice in Fig. 1.

The above assumptions that the shape of the Fermi surface does not change and that \( v_k \propto \delta k \) close to a VH point, are supported by the Quantum Monte Carlo (QMC) data for \( R = 0.94 \) and \( U/t = 2 \) on a 16×16 lattice, which shows no appreciable change of the Fermi surface. Moreover, our QMC results suggest that the smearing of the momentum distribution function \( n(k) \) does not increase close to the VH points. This is in contrast to the predictions of the second-order perturbation theory in \( U \) that the quasiparticle residue \( Z \) vanishes logarithmically at the VH points, while being finite away from them.

Remarkably, for electrons described by \( \varepsilon_k = k_x k_y \) with the Fermi level \( \varepsilon = 0 \), \( Z \) is finite even at the VH point in TMA. Due to particle-hole symmetry, there is no change of the Fermi surface for this model and the imaginary part of the electron self-energy at \( k = 0 \) is \( \Sigma''(\varepsilon) \propto -|\varepsilon|/\ln^2 |\varepsilon| \) for \( \varepsilon \to 0 \). Thus the wavefunction renormalization \( Z^{-1} = 1 - \partial \Sigma'/\partial \omega|_{\omega=0} = 1 - (2/\pi) \int_0^\infty d\varepsilon \Sigma''(\varepsilon)/\varepsilon^2 \) does not vanish, although the inverse lifetime differs only marginally from the golden-rule result. Anyway, this anomalous lifetime is not likely to appear in the transport properties of the VH system. [10]
The projection QMC method is obtained by filtering out the ground-state component from a given trial state $|\psi_0\rangle = \lim_{\tau \to \infty} e^{-H\tau} |\psi_T\rangle$. Since the imaginary time propagation conserves the symmetries of the trial function $|\psi_T\rangle$, it is also possible to study, e.g., different spin subspaces of $H$ by choosing a definite spin for $|\psi_T\rangle$. The many-body propagator $e^{-H\tau}$ is implemented by use of the one-body time-dependent propagator $U_\sigma(\tau, 0)$ defined by the discrete Hubbard-Stratonovich fields $\sigma(r, \tau)$ defined on each site $r$. We use the usual Trotter discretization of the total imaginary time $\beta$ for $0 < \tau < \beta$, namely $e^{-H\tau} = \sum_\sigma U_\sigma(\tau, 0)$. \[11\] The ground state energy is obtained by $E_G = \lim_{\beta \to \infty} E_\beta$ where

$$E_\beta = \frac{\sum_\sigma \langle \psi_T | H U_\sigma(\beta, 0) | \psi_T \rangle}{\sum_\sigma \langle \psi_T | U_\sigma(\beta, 0) | \psi_T \rangle}.$$ 

Analogously, all relevant correlation functions are obtained by Monte Carlo sampling over the fields $\sigma(r, \tau)$, which become computable provided the trial function $|\psi_T\rangle$ is chosen to be a Slater determinant $|S\rangle$, as $U_\sigma(\tau, 0) |\psi_T\rangle$ remains a Slater determinant too. \[11\]

The main improvements of the present scheme are:

1) Optimization of the trial function $|\psi_T\rangle$, which has been extended to include not only simple Slater determinants $|S\rangle$ but also the more appropriate Gutzwiller wavefunction $|\psi_g\rangle = e^{-gD} |S\rangle$, with a variational parameter $g$ controlling the total number of doubly occupied sites $D$. This is obtained upon a slight change of the one-body propagator $U_\sigma(\tau, 0) \rightarrow U_{\sigma,\sigma_g}(\tau, 0)$, with extra discrete fields $\sigma_g(r)$ needed to decouple the correlated part of the wavefunction $e^{-gD}$ at the initial and final imaginary time $\tau = 0$ and $\tau = \beta$.

2) Use of the Gutzwiller wavefunction to implement an importance sampling strategy to reduce statistical fluctuation of the ground state energy, similar to what is already known for the Green function QMC. \[12\] We define an estimator that satisfies the “zero variance principle”, namely that the variance of the energy is zero if the trial wavefunction $|\psi_T\rangle$ approaches the ground state $|\psi_0\rangle$. In order to satisfy this principle the energy has to be computed at the initial and final imaginary times ($\tau = 0, \beta$) since only at those points the value of the estimator is independent from the random fields $\sigma$ in the limit when $|\psi_T\rangle \to |\psi_0\rangle$. 

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We define therefore

\[ E_\beta = \frac{\sum_{\sigma,\sigma_g} E_{\sigma,\sigma_g} w_{\sigma,\sigma_g}}{\sum_{\sigma,\sigma_g} s_{\sigma,\sigma_g} w_{\sigma,\sigma_g}}, \]

where \( w_{\sigma,\sigma_g} = |\langle S | U_{\sigma,\sigma_g}(\tau, 0) | S \rangle| \) is the conventional weight (the sign being \( s_{\sigma,\sigma_g} \)). The estimator is

\[ E_{\sigma,\sigma_g} = \frac{\langle S | H g U_{\sigma,\sigma_g}(\beta, 0) + U_{\sigma,\sigma_g}(\beta, 0) H_{-g} | S \rangle}{2w_{\sigma,\sigma_g}}, \]

(3)

and \( H_g = e^{gD} H e^{-gD} \) is a nonunitary transformation of the Hamiltonian, which can be computed by standard algebra. Suppose now that the ground state is well approximated by a Gutzwiller wavefunction (the method can be clearly generalized to any Jastrow wavefunction, \( |\psi_g\rangle = e^{-gJ} |S\rangle \), with \( J \) any two-body interaction term), then it is easy to show that the above estimator will acquire a small variance, because the left eigenvector of \( H_g \) and the right one of \( H_{-g} \) are well approximated by a single Slater determinant \( |S\rangle \).

In order to minimize the finite-size effects and also to stabilize the simulation we restrict the Slater determinant to a product of plane-wave Slater determinants in each spin sector \( |S\rangle = |S_\uparrow\rangle \otimes |S_\downarrow\rangle \), with the condition to fill all degenerate single-particle levels in both spin sectors (the closed-shell condition). In this case the total spin is \( S = |N_\uparrow - N_\downarrow|/2 \). Fig. 2a shows that the improvement \[ E \] in the energy estimator allows to obtain accurate values of energy in each spin sector even for small imaginary time \( \beta \), before the sign problem becomes serious. Among the states obtained with a trial state \( |\psi_T\rangle \) consistent with the closed-shell condition, on a 16×16 lattice the highest spin sector has the lowest energy, as shown explicitly by comparing to the lowest spin state (singlet in the thermodynamic sense).

We emphasize that, for a finite lattice, the instability occurs at a finite coupling \( U > U_c \), since the divergence of \( F_0^a \) is cut-off in this case. In fact, Fig. 2b shows that, for \( U/t = 4 \) and \( R = 0.94 \), the singlet ground state is stable on the 10×10 lattice, contrary to the 16×16 cluster. The tendency towards FM grows with increasing cluster size also in the mean-field approximation, TMA, and at the Gutzwiller variational level. The lattice-size dependence of the difference between the energies of a fully polarized state, and of a closed-shell state with minimal spin is shown in Fig. 2c. Our QMC data strongly support the FM state.
for \( l \to \infty \). The qualitative agreement of TMA with the QMC data is striking. TMA tends to slightly overestimate the FM correlations, but the improvement with respect to the mean-field approximation and the Gutzwiller wavefunction (see Fig. 1) is evident.

In order to confirm the prediction of AFM and superconductivity in the remaining part of the phase diagram, we have studied the imaginary time dependence of correlation functions in the following form:

\[
O(\tau) = \frac{\langle \psi_T | e^{-\tau H} \hat{O} e^{-(\beta-\tau)H} | \psi_T \rangle}{\langle \psi_T | e^{-\beta H} | \psi_T \rangle}. \tag{4}
\]

For \( \beta \to \infty \), \( O(0) \) tends to the so called mixed average \( O(0) = \frac{\langle \psi_T | \hat{O} | \psi_0 \rangle}{\langle \psi_T | \psi_0 \rangle} \), which is a property of both the ground state and the trial wavefunction itself. Instead, for \( \tau \sim \beta/2 \), one obtains the desired ground-state expectation value of \( \hat{O} \). Thus, if we choose as a trial wavefunction the singlet paramagnetic Gutzwiller wavefunction, i.e. a state without BCS or AFM order, an increase of the corresponding correlations is expected by varying \( \tau \) from 0 to \( \beta/2 \), whenever the electron system truly supports some kind of order. The time-dependent functions \( O(\tau) \) defined in (4), directly indicate enhanced or depressed correlations with respect to a reference finite-size Gutzwiller state \( |\psi_T\rangle \). They represent therefore clear fingerprints of the nature of the ground state \( |\psi_0\rangle \) even with a short imaginary-time propagation \( \beta \), provided the reference state \( |\psi_T\rangle \) is sufficiently close to \( |\psi_0\rangle \). A similar idea was used also in Ref. [14].

In Fig. 3a we plot the spin-isotropic magnetic structure factor for the AFM wavevector \( Q = (\pi, \pi) \) as a function of the lattice size \( l \). Only for \( l > 12 \) the AFM correlations are clearly enhanced, supporting the existence of a true AFM long range order. Unfortunately, the need for \( \beta t > 2 \) at large \( l \) precludes the possibility of a detailed finite-size scaling of AFM order. For negative \( U \) (Fig. 3b) \( s \)-wave superconductivity with an order parameter \( s = \frac{1}{2} \sum_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \) should take place. The plot of \( O(\tau) \) where \( \hat{O} = s^i s \) clearly shows this tendency even for a short imaginary-time propagation, in agreement with Ref. [6].

Based on the results of QMC simulations and on the analysis of TMA we conclude that, in the \( t-t' \) Hubbard model at the VH density, interactions tend to remove the singular density of states, via a splitting of the Fermi surface (FM) or the opening of a gap at the
VH points (AFM and superconductivity). This has been shown numerically at realistic coupling strengths $U$ and is expected analytically for all $U$, if we neglect the change of the quasiparticle dispersion. Since we find magnetism at $U > 0$ despite the finite-size cut-offs, we expect that it appears, for $U$ large enough, in a finite window of densities around the VH filling. Our results for repulsive interactions reduce in the limits $R \to 0$ and $R \to 1$ to AFM of the half-filled $t' = 0$ Hubbard model and to an analogue of the flat-band FM [4], respectively. An interesting question arises about the transition from AFM to FM as $R$ increases. Since already on the mean field level both FM and AFM susceptibilities are suppressed for $R \approx 0.55$ as compared to their values at $R = 0.94$ and $R = 0.2$, respectively, a numerical solution of this question will require even bigger lattices than those used here. We cannot exclude that close to $R \approx 0.55$, there is no magnetic ordering and a superconducting instability develops via the Kohn-Luttinger effect [15].

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FIGURES

FIG. 1. The energy per site (in units of $t$) as a function of $m$ for $N = N^\uparrow + N^\downarrow = 108$ electrons. Full lines: free electrons (bars), mean-field approximation (triangles), 2$^\text{nd}$ order perturbation theory (squares), and $T$-matrix approximation without self-consistency condition for the electron Green’s function (circles). Dashed lines: optimal Gutzwiller wavefunction (squares) and QMC data at $\beta t = 2$ (triangles).

FIG. 2. The energy per site (in units of $t$) (a) of a $L = 16 \times 16$ lattice with $N = 108$ electrons as a function of $\beta$, for $N^\uparrow = 55$ (total spin $S = 1$, continuous line) and the $\beta$ converged one for the FM state (total spin $S = 53$, dashed line); (b) as a function of $m$ at $\beta t = 2$ for $N = 108$, $L = 16 \times 16$ (upper curve) and $N = 44$, $L = 10 \times 10$ (lower curve). The optimal $g = \sim 0.65$ (see text) is used in all simulations. The error due to the imaginary time discretization ($\Delta \beta t = 0.2$) is negligible, as the new estimator considerably reduces both this ($\sim 10 \div 100$ times) and the statistical error ($3 \div 4$ times) at the optimal $g$. (c) Difference between the energy per site (in units of $t$) of the minimal-spin ($S = 1$) state and of the fully polarized state, both at the VH density, as a function of the lattice size.

FIG. 3. QMC simulation for $t'/t = 0.1$ at the VH density in the singlet sector. (a) Isotropic magnetic structure factor $S(\pi, \pi) = \frac{1}{L^2} \sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle e^{iQ(R_i - R_j)}$ at the AF wavevector $Q$ as a function of $\tau$ (see text) for $U/t = 4$. The curves (guides to the eye) correspond to square lattices $l \times l$ with $l = 6, 8, 10, 12, 16, 20$ ($N_{\sigma} = 15, 27, 43, 63, 115, 183$) from bottom to top. The optimal Gutzwiller parameter $g = 0.625$. (b) The same plot as in (a) for the s-wave BCS order parameter described in the text on a lattice $16 \times 16$ for $U/t = -2$. The optimal $g = -0.3$ and $\Delta \beta t = 0.1$. 

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Energy per site

16×16

U/t=4 t′/t=0.47

R. Hlubina et al. Fig. 1
(a) --- FERRO
     --- SINGLET

(b) $U/t=4$ $t'/t=0.47$

R. Hlubina et al. Fig. 2
R. Hlubina et al. Fig. 2
\[ S(\pi,\pi) \times 1000 \]

\[ \langle s^t_s \rangle \]

(b)

\[ U/t = -2 \quad t'/t = 0.1 \]

R. Hlubina et al. Fig.3