

## Itinerant ferromagnetic phase of the Hubbard model

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Using a quantum Monte Carlo technique, we provide strong evidence for the stability of a saturated ferromagnetic phase in the high-density regime of the two-dimensional infinite- $U$  Hubbard model. By decreasing the electron density, we observe a discontinuous transition to a paramagnetic phase, accompanied by a divergence of the susceptibility on the paramagnetic side. This behavior, resulting from a high degeneracy among different spin sectors, is consistent with an infinite-order phase transition. The remarkable stability of itinerant ferromagnetism renews the hope of describing this phenomenon within a purely kinetic mechanism and will facilitate the validation of experimental quantum simulators with cold atoms loaded in optical lattices.

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Ever since classical antiquity, ferromagnetism has attracted the attention of natural philosophers.<sup>1</sup> A proper understanding of this phenomenon was only made possible by the advent of quantum mechanics, from the early interpretations<sup>2,3</sup> to its modern realizations in *quantum simulators* engineered by means of cold atomic gases.<sup>4</sup> In some solids, such as transition metals, the spin-independent nature of interactions has led to the conjecture that long-range magnetic order is due to an itinerant mechanism in which the Coulomb interaction and the Pauli exclusion principle play fundamental roles. The single-band Hubbard model, possibly the simplest and most studied lattice model of correlated electrons, was first thought to encompass a minimal description of itinerant ferromagnetism.<sup>5</sup> Recent experiments on ultracold atoms hinted at the formation of ferromagnetic domains in a gas of repulsively interacting fermions.<sup>4</sup> This important result and subsequent numerical calculations in the continuum<sup>6</sup> suggested that this phenomenon has some general features independent of the details of the repulsive interaction, thus renewing the interest in the understanding of a minimal model for itinerant ferromagnetism. In spite of its simplicity, exact solutions of the Hubbard model are not available in more than one spatial dimension, leaving the question of the stability of a ferromagnetic phase unsolved. One of the very few exact results that is known is due to Nagaoka,<sup>7</sup> who proved a theorem stating that, in the infinite- $U$  limit, a single hole stabilizes a fully polarized ground state. Following this pioneering work, much effort has been devoted to studying the fully polarized state for finite hole densities.<sup>8-14</sup> However, the possible stability of ferromagnetic phases and the nature of the involved quantum phase transitions are still matters of debate.<sup>15</sup>

In this Rapid Communication we present results for the infinite- $U$  Hubbard model, based on accurate fermionic quantum Monte Carlo (QMC) simulations, which indicate that at high electron density the Nagaoka state is stable not only with respect to the paramagnetic phase, but also with respect to other previously proposed partially polarized states.<sup>12</sup> A nontrivial transition to a paramagnetic phase is observed upon decreasing the electron density. Near the transition this phase is characterized by highly degenerate states with different values of the total spin, thus indicating a divergence of the

magnetic susceptibility, consistent with an infinite-order phase transition.<sup>16</sup>

The QMC simulation of systems of interacting electrons, at variance with that of bosons, is beset by the antisymmetry of the ground-state wave function which cannot be treated as the stationary distribution of a diffusion process. The main attempt to cope with the ensuing difficulties is the *fixed-node* (FN) approximation, which, for lattice models, amounts to defining an effective Hamiltonian whose ground-state energy is a variational upper bound to the exact energy.<sup>17</sup> If complemented by an accurate variational ansatz for the wave function, the FN method provides a method to study the properties of large fermionic systems, making it possible reliable extrapolations to the thermodynamic limit. Unfortunately, the nature of the approximation does not allow for an estimate of the residual error, which not rarely can lead to biased results. However, the infinite- $U$  Hubbard model belongs to an interesting class of Hamiltonians whose eigenstates of fermionic symmetry are sufficiently close in energy to the bosonic ground state to allow them to be treated on an equal footing; for this class of Hamiltonians we propose a strategy to overcome the sign problem via the dissection of the excitation spectrum of the corresponding bosonic auxiliary problem, providing an essentially *unbiased* scheme for medium-size fermionic systems.

*Fermionic-correlation method.* The spectrum of a Hamiltonian of identical particles,  $\mathcal{H}$ , can be classified according to the irreducible representations of the symmetric (permutation) group. The Pauli principle asserts that only totally antisymmetric states are physically allowed for fermions, but mathematical states of any symmetry can also be considered. In particular, the (unphysical) state of lowest energy is in general totally symmetric, so that the fermionic ground state can be formally considered as an excited state of a bosonic system. As such, it can be studied via excited-state techniques, provided the Bose-Fermi gap is not too large with respect to the physical gap in the fermionic sector of the spectrum. Let  $|\Psi_b^0\rangle$  be the bosonic ground state of the system and  $\mathcal{A}$  an arbitrary observable. A recent extension of the reptation QMC method<sup>18</sup> to lattice models<sup>19</sup> allows for an efficient and unbiased evaluation of imaginary-time  $\tau = it$  correlation functions  $\mathcal{C}_{\mathcal{A}}(\tau) = \langle \Psi_b^0 | \mathcal{A}^\dagger(\tau) \mathcal{A} | \Psi_b^0 \rangle / \langle \Psi_b^0 | \Psi_b^0 \rangle$ , where  $\mathcal{A}(\tau) = e^{\mathcal{H}\tau} \mathcal{A} e^{-\mathcal{H}\tau}$  is the Heisenberg representation of  $\mathcal{A}$ .

The connection of such correlation functions with the excited states  $|\Psi^k\rangle$  of  $\mathcal{H}$  is obtained by considering the Lehman spectral representation,

$$\mathcal{C}_{\mathcal{A}}(\tau) = \frac{\sum_k |\langle \Psi_b^0 | \mathcal{A} | \Psi^k \rangle|^2 e^{-\Delta_k \tau}}{\langle \Psi_b^0 | \Psi_b^0 \rangle}, \quad (1)$$

where  $\Delta_k = E^k - E_b^0$  are excitation energies with respect to the bosonic ground state. Selection rules act in such a way as to exclude from Eq. (1) those excited states whose symmetry is different from that of the state  $\mathcal{A}|\Psi_b^0\rangle$ . In particular, if  $\mathcal{A}$  is chosen to be totally antisymmetric with respect to permutations, only fermionic (ground and excited) states will contribute to  $\mathcal{C}_{\mathcal{A}}(\tau)$ . For example, if  $\mathcal{A}$  is the local operator whose coordinate representation is the ratio between the fermionic and bosonic ground-state wave functions [ $\mathcal{A}_f(n) = \langle n | \Psi_f^0 \rangle / \langle n | \Phi_b^0 \rangle$ , where  $|n\rangle$  denotes the many-body lattice configuration], the correlation function  $\mathcal{C}_{\mathcal{A}}(\tau)$  will be proportional to the single exponential  $e^{-\Delta_0 \tau}$ .

In practice, neither the bosonic nor the fermionic ground state is known exactly and only variational approximations to them are available, which we denote here by  $|\Phi_b\rangle$  and  $|\Phi_f\rangle$ , respectively. Correspondingly, the antisymmetric observable is defined as  $\mathcal{A}_f(n) = \langle n | \Phi_f \rangle / \langle n | \Phi_b \rangle$ . In this way, the leading coefficient of the expansion is given by  $\langle \Psi_b^0 | \mathcal{A}_f | \Psi_f^0 \rangle \simeq \langle \Phi_f | \Psi_f^0 \rangle$  and can be systematically maximized by improving the quality of the variational states. The energy of the fermionic ground state can be then extracted either directly by noticing that  $E_f^0 = E_b^0 - \lim_{\tau \rightarrow \infty} [\partial_\tau \log \mathcal{C}_{\mathcal{A}}(\tau)]$  or, indirectly, by fitting the exponential decay of the correlation function of Eq. (1) and extracting the smallest energy gap. In order for this procedure to make any sense, it is necessary that the (unphysical) Bose-Fermi gap is not too large with respect to the physical excitation energies in the fermionic sector of the spectrum. If this condition is not met, the antisymmetric correlation function gets effectively extinguished before the selection of the fermionic ground state from its excitation background is attained by imaginary-time evolution. This condition is actually verified for infinite- $U$  fermionic Hubbard models of moderate size, whose properties are not too dissimilar from those of a system of hard-core bosons. The condition of a small fermion-boson gap is also met in other interesting systems, where the effects of statistics on the total energy are overwhelmed by the effects of correlations, such as the low-density electron gas, liquid  $^3\text{He}$ , quasiunidimensional systems, and mixtures of bosons and fermions. It should nonetheless be noticed that the Fermi-Bose gap is, in general, an extensive property, thus providing restrictions on the affordable system size.

We further notice that this fermionic-correlation method is related to the *transient estimate* (TE) method for the fermionic ground state,<sup>20</sup> or its generalization for a few excitations.<sup>21</sup> However, the TE method works with *ratios* of decaying correlation functions, thereby reducing the signal-to-noise ratio, and typically uses suboptimal bosonic guiding functions, with increased fluctuations in the weights of the random walks. A crucial point for our method to succeed is instead the calculation of spectra directly from imaginary-time correlation functions. Although, in general, this is an ill-posed problem, in practice sharp peaks with strong spectral weight can be

reliably extracted if the correlation function is known with good statistical precision for sufficiently long times.<sup>18,22</sup> In the present work this condition is met even for systems of several tens of particles, due to the relatively small Bose-Fermi gap, as well as to the good quality of the variational states.

*The model.* The Hamiltonian of the infinite- $U$  Hubbard model reads

$$\mathcal{H}_f = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P}_G c_{i,\sigma}^\dagger c_{j,\sigma} \mathcal{P}_G + \text{H.c.}, \quad (2)$$

where  $c_{i,\sigma}^\dagger$  ( $c_{i,\sigma}$ ) creates (destroys) an electron on site  $i$  with spin  $\sigma$ ,  $\langle i,j \rangle$  denotes nearest-neighbor site pairs, and the Gutzwiller projector  $\mathcal{P}_G$  forbids double occupancy. In the following, we will consider a square lattice and take  $t = 1$  as the energy scale. The total number of sites will be denoted by  $L$ , the number of electrons by  $N$  and we will present the results for different magnetizations  $m = (n_\uparrow - n_\downarrow) / (n_\uparrow + n_\downarrow)$  and densities  $n = n_\uparrow + n_\downarrow$ .

Relatively simple variational wave functions have been constructed,<sup>9,10</sup> by flipping one (say up) spin with respect to the saturated ferromagnetic state. The flip of the spin leads to a gain of kinetic energy for the down spin, but also a loss in the spin-up kinetic energy (since the motion of spin-up electrons is restricted by the necessity of avoiding double occupancy). Here, we consider

$$\langle n | \Phi_f \rangle = \mathcal{J}^f(n) \text{Det}\{\phi_k(R_j^\uparrow)\} \text{Det}\{\phi_k(R_j^\downarrow)\}, \quad (3)$$

where the Jastrow factor  $\mathcal{J}^f(n) = \exp[\sum_{i,j} V_{ij}^f n_i n_j]$  multiplies two Slater determinants that are constructed by applying backflow correlations to single-particle orbitals for up and down spins.<sup>23</sup> The correlated orbitals are defined by  $\phi_k(R_j^\sigma) = \phi_k^0(R_j^\sigma) + b_k \sum_{R_l, \sigma'} \phi_k^0(R_l^{\sigma'})$ , where  $b_k$  are orbital-dependent backflow parameters,  $\phi_k^0(R_j^\sigma)$  are plane waves, and the sum includes all nearest neighbors of the  $j$ th particle, thus preserving the spin rotational invariance. The proposed backflow wave function (3) encodes the effect of correlation on the deformation of the free-orbital nodal structure and consistently catches much of the physics of previous treatments,<sup>9-11</sup> while leaving room for a systematic improvement with the QMC methods.

The bosonic counterpart of the model studied is a purely kinetic hard-core-boson Hamiltonian, where the fermionic operators are substituted by bosonic ones. Our QMC method is particularly suitable to study the high-density region, namely, few holes and close to full filling ( $N = L$ ), where the boson-fermion gap is very small and increases upon decreasing the density.<sup>24</sup> The bosonic trial state is given by a Jastrow wave function  $\langle n | \Phi_b \rangle = \mathcal{J}^b(n)$ , which is similar to the fermionic one (but with different parameters  $V_{i,j}^b$ ) and represents an excellent ansatz for the bosonic ground state.<sup>25</sup> In all cases, the variational parameters are fully optimized, by minimizing the variational energy with the method of Ref. 26.

*Results.* The fermionic correlation technique remains efficient up to relatively large system sizes (i.e.,  $L = 50-100$ ) and allows us to reach numerical results, which are exact within statistical accuracy. In Fig. 1, we report our results for  $L = 50$  and  $N = 42$  electrons, for different values of the magnetization  $m$ . In addition, we also report the results based upon the FN

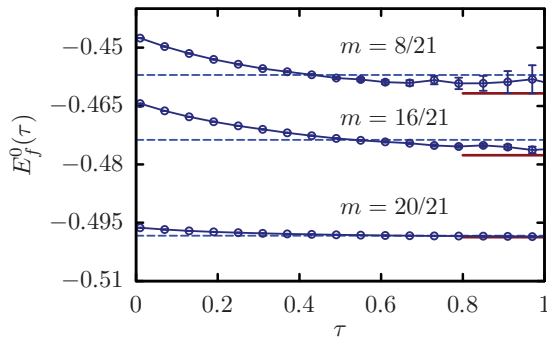


FIG. 1. (Color online) Energy  $E_f^0(\tau) = E_b^0 - \partial_\tau \log C_A(\tau)$  as a function of the imaginary time  $\tau$  for  $L = 50$  and  $N = 42$  electrons and different magnetizations. The dashed horizontal lines are FN energies, while the solid lines are the energies as obtained by fitting the imaginary-time correlations.

approach. The possibility of obtaining numerically exact results on rather large systems allows us to assess the accuracy of the FN method, which can be extended to much larger sizes (i.e.,  $L \lesssim 1000$ ), without any numerical instability. Thanks to backflow correlations, we get a considerable improvement upon the standard plane waves that were used in Ref. 12. There is a small difference between the FN results and the energies obtained by the imaginary-time correlations, indicating a very small residual FN error, namely,  $\Delta E/t \lesssim 0.01$ .

In Fig. 2, we report the overall phase diagram obtained by considering large-scale FN calculations. A saturated ferromagnetic phase is stable for  $n \gtrsim 0.75$ , while for smaller densities a paramagnetic ground state is found. The narrow shaded region denotes the uncertainty due to the residual numerical error, which can be estimated by comparing the FN energies with the *exact ones* (obtained from the fermionic correlations) on smaller clusters (see Fig. 1). This direct comparison puts us on secure grounds as concerns the robustness of the dependence of the ground-state magnetization on the electron density.

In Fig. 3 we display the dependence of the ground-state energy upon magnetization, for different values of the electron density. The remarkable feature emerging from this figure is the strong flattening of the energy as a function of the magnetization (i.e., the spin) close to the transition between the fully polarized ferromagnet and the paramagnetic state.

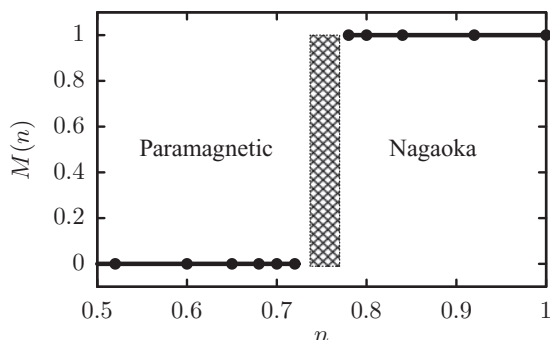


FIG. 2. Ground-state magnetization of the infinite- $U$  Hubbard model on the square lattice. The shaded area represents a small region of uncertain attribution due to the effect of the residual Monte Carlo error.

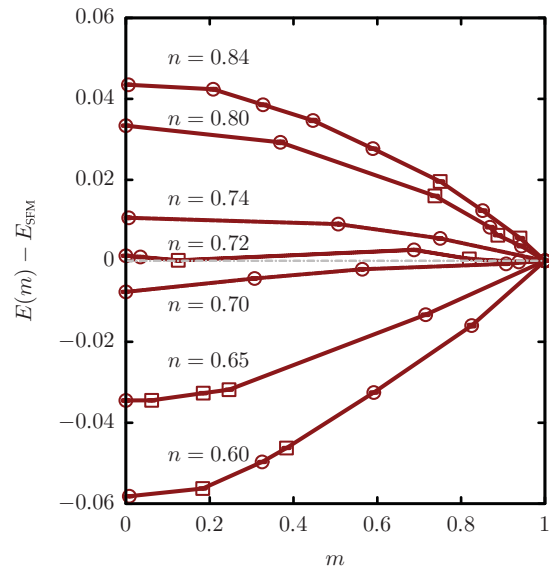


FIG. 3. (Color online) Difference between the energy per site of different magnetizations and that of the saturated ferromagnet as a function of the density  $n$ . The cases with  $L = 200$  (squares) and  $400$  (circles) are reported; lines connecting points are a guide for the eye.

Indeed, at low and high densities the energy has a monotonic behavior as a function of the magnetization  $m$ . At low density a clear minimum exists at  $m = 0$ , typical of a paramagnetic phase, where the curvature of the energy-versus-magnetization curve indicates a finite spin susceptibility. On the other hand, in the high-density ferromagnetic phase,  $E(m)$  displays a well-defined minimum for  $m = 1$ . On approaching the transition,  $E(m)$  becomes flatter and flatter, suggesting that the susceptibility may diverge at the critical point. Although we cannot exclude a tiny region with a finite but nonsaturated magnetization, these results would suggest that the paramagnetic-to-ferromagnetic transition is not due to a simple level crossing, namely, to the creation of a local minimum in  $E(m)$  at  $m = 1$  that eventually prevails over the paramagnetic one, but rather to the progressive flattening of the *whole*  $E(m)$  curve.

Our scenario is compatible with an infinite-order phase transition, which, in general, is described by  $E(m) = (g - g_c)m^2 + bm^{2r}$ , where  $r \rightarrow \infty$ ; a phase transition is obtained by varying the order parameter  $g$  (in our case the electron density) across its critical value  $g_c$ . The critical exponent of the order parameter is  $\beta = 1/(2r - 2)$ , generating a jump from zero to the saturation value for  $r \rightarrow \infty$ . Moreover, the susceptibility  $\chi \sim A_\pm/|g - g_c|^\gamma$  has an exponent  $\gamma = 1$  independent of  $r$ , with an amplitude ratio  $A_-/A_+$  that vanishes for  $r \rightarrow \infty$ .<sup>16</sup> Even though the order parameter shows a finite jump, as in ordinary first-order phase transitions, there is no hysteresis. We have indeed verified that the ground-state energy is a convex function of the electron density, implying a finite compressibility in the neighborhood of the ferromagnetic-paramagnetic transition. This picture implies that spin-flip excitations over the fully polarized state are noninteracting at the transition point. In fact, we find that, at small distances, the minority spins repel each other, whereas at large distances they do not interact. In the variational wave function, this fact

generates a sizable repulsive short-range Jastrow factor, while at long range the  $V_{i,j}^f$  pseudopotential vanishes.

*Conclusions.* In this Rapid Communication we have analyzed with high accuracy the magnetic phase diagram of the fermionic Hubbard model on the square lattice in the limit of infinite on-site repulsion  $U$ . By the combination of different QMC methods, we are able to give a very precise determination of the transition between the ferromagnetic and the paramagnetic states. Interestingly, all spin excitations become essentially gapless at the transition, possibly indicating that the transition is of infinite order. Such a behavior emerges from the study of intermediate polarizations, not considered in previous calculations. Indeed, given the extreme difficulty of treating this highly correlated system, most of the theoretical efforts have been limited to the study of very high densities or a single spin flip.<sup>8-11</sup> Our results pave

the way to a better understanding of itinerant ferromagnetic phenomena in both traditional condensed matter systems and recent and forthcoming realizations of such phases in cold atomic gases. Indeed, the recent achievements in the realization of interacting fermionic systems trapped in optical lattices<sup>27</sup> will most likely lead to experimental probes of the strongly correlated regime of the Hubbard model at sufficiently low temperatures. Lastly, the generality of the numerical methods used in this paper will also offer insights into other strongly correlated fermionic systems where currently available analytical and numerical treatments may fail to offer a quantitative or even qualitative account of the relevant physical properties.

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