Ferromagnetic Instability for single-band Hubbard model in the strong-coupling regime

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We study a ferromagnetic instability in a doped single-band Hubbard model by means of dynamical mean-field theory with the continuous-time quantum Monte Carlo simulations. Examining the effect of the strong correlations in the system on the hypercubic and Bethe lattice, we find that the ferromagnetically ordered state appears in the former, while it does not in the latter. We also reveal that the ferromagnetic order is more stable in the case that the noninteracting DOS exhibits a slower decay in the high-energy region. The present results suggest that, in the strong-coupling regime, the high-energy part of DOS plays an essential role for the emergence of the ferromagnetically ordered state, in contrast to the Stoner criterion justified in the weak interaction limit.

I. INTRODUCTION

Ferromagnetic (FM) metallic state in the strongly correlated electron systems is a long standing problem though iron is known to be a magnet from ancient times. In the multiorbital system, there exists the Hund coupling between electrons in degenerate orbitals, which tends to realize the FM ordered states at low temperatures [1–3]. In fact, the ordered state has been reported in the doped Hubbard model with degenerate states at low temperatures [1–4]. We then discuss the FM instability in the infinite dimensional systems since there are no closed loop in the Bethe lattice. However, in the framework of DMFT, the lattice structure is involved only via the noninteracting DOS, which should lead to a minor change in the system, e.g., the critical interactions for Mott transitions [51,52]. Therefore, key factors for stabilizing the strong-coupling FM ordered state remain unclear. Furthermore, quantitative treatments are still lacking even in the infinite dimensional systems since the conventional impurity solvers such as the noncrossing approximation [29,33–35] and numerical renormalization group [28,30,36–39] are hard to obtain the dynamical quantities in both low and extremely high energy regions precisely. To overcome this, in this study, we make use of the continuous-time quantum Monte Carlo (CTQMC) method [40,41] based on the segment algorithm. We then discuss the FM instability in the system more precisely to determine the finite temperature phase diagram.

The paper is organized as follows. In Sec. II we introduce the single-band Hubbard model and briefly explain the framework of DMFT. In Sec. III we consider the infinite dimensional Hubbard model on the hypercubic and Bethe lattices to discuss the FM instability at low temperatures. The effect of the noninteracting DOS is also addressed, by examining magnetic properties in the system with t-distribution DOS. A summary is given in the final section.
II. MODEL AND METHODS

We consider the single-band Hubbard model, which is described by the following Hamiltonian as,

$$H = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) annihilates (creates) an electron with spin $\sigma(=\uparrow, \downarrow)$ at the $i$th site and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. $t$ is the transfer integral, $U$ the on-site interaction, $\mu$ the chemical potential, and $h$ the external magnetic field.

To study magnetic properties in the single-band Hubbard model, we make use of the DMFT [24, 27]. In DMFT, the lattice model is mapped to the problem of a single impurity connected dynamically to a "heat bath". The electron Green’s function is obtained via the self-consistent solution of this impurity model, one can obtain the self-energy and Green function.

In our calculations, we consider the Hubbard model on the Bethe and hypercubic lattices to study their magnetic properties. The corresponding noninteracting DOS, which is important in the framework of DMFT [see Eq. (4)], is given as,

$$\rho_{0}(x) = \frac{2}{\pi D} \sqrt{1 - \left(\frac{x}{D}\right)^2},$$

and

$$\rho_{\text{hc}}(x) = \frac{1}{\sqrt{\pi D}} \exp \left[-\left(\frac{x}{D}\right)^2\right],$$

where $D$ is the characteristic energy scale. It has been clarified that the difference in the shape of DOS simply leads to the quantitative change in the critical interaction of the Mott transition [31,32]. On the other hand, away from commensurate fillings, the shape has been discussed to be crucial for the instability to the FM ordered state in strongly correlated metals [18, 28–30]. In particular, as for the above two forms of the DOS, their high-energy parts are obviously different; the DOS of the hypercubic lattice has a exponentially decaying rate fillings, the shape has been discussed to be crucial for the quantitative change in the critical interaction of the Mott transition [31,32]. On the other hand, away from commensurate fillings, the shape has been discussed to be crucial for the instability to the FM ordered state in strongly correlated metals [18, 28–30]. In particular, as for the above two forms of the DOS, their high-energy parts are obviously different; the DOS of the hypercubic lattice has an exponentially decaying tail, but that of the Bethe lattice is finite only in the limited region, as shown in Fig. 1. In the following, we discuss the role of the shape of the DOS for the FM instability through the systematic finite temperature calculations.

III. NUMERICAL RESULTS

We first consider the Hubbard model on the hypercubic lattice [29, 30] to clarify the presence of the FM ordered phase when the system is away from half filling ($n < 1$) in the case of large Coulomb interactions. Figure 2 shows the magnetic susceptibility little depends on the electron density and temperature in this scale ($\sim 0.5$). In the noninteracting system ($U = 0$), the susceptibility little depends on the electron density and temperature in this scale ($\sim 0.5$). When the interaction strength is much larger than the hopping (bandwidth) and temperature, nonmonotonic behavior appears in the susceptibility as a function of the filling $n$. The peak structure develops...
with increasing the Coulomb interaction and decreasing the temperature. At the low temperature \( T/D = 0.05 \), the susceptibility has a maximum around \( n \sim 0.95 \), where ferromagnetic fluctuations are enhanced. This suggests that the FM instability appears away from the half filling when the system has a larger interaction strength at lower temperatures.

To examine the presence of the FM ordered phase at finite interactions and temperatures, we calculate the uniform susceptibility and magnetization in the system with \( U/D = 100 \) at \( T/D = 0.01 \), as shown in Fig. [3]. In the small \( n \) case, the system is in the paramagnetic (PM) state with the finite susceptibility. Increasing the electron number, the susceptibility monotonically increases and at last diverges at the critical value \( n = n_c \). Beyond the critical value, the finite magnetization is induced, implying that the FM ordered state is realized in the single-band Hubbard model on the hypercubic lattice. The magnetization has a maximum around \( n \sim 0.95 \) and finally it vanishes at \( n = n_{c2} \), where the phase transition occurs again to the PM metallic state. By examining critical behavior, we obtain the critical densities \( n_{c1} = 0.90 \) and \( n_{c2} = 0.98 \).

To reveal how stable the FM ordered state is against thermal fluctuations, we show in Fig. [4] the temperature dependence of the magnetization and magnetic susceptibility in the system with \( U/D = 100 \) and \( n = 0.95 \). We find that decreasing temperatures, the magnetic susceptibility monotonically increases and at last, diverges at a finite temperature \( T_c \). Further decrease of temperatures drives the system to the FM ordered...
The critical temperature $T_c/D \sim 0.013$ is obtained, examining critical behavior in these quantities $m \sim (T_c - T)^\beta$ and $\chi \sim (T - T_c)^{-\gamma}$ with $\beta = 1/2$ and $\gamma = 1$, as shown in the inset of Fig. 4. These critical exponents are consistent with the mean-field theory. On the other hand, in the case with $U/D = 20$, the magnetic susceptibility approaches a certain value with decreasing temperatures, implying that the ground state is the PM metal.

By performing similar calculations for different values of $U$ and $n$, we obtain the phase diagram at the temperature $T/D = 0.0067$, as shown in Fig. 5(a). It is found that the FM ordered state is realized around $n \sim 0.95$ in the strong-coupling regime. In addition, increasing the interaction strength, the magnetization smoothly increases and approaches a certain value at the fixed temperature, as shown in Fig. 5(b). This suggests that the FM ordered state becomes stable even in the large $U$ region. This is in contrast to the AFM ordered state at half filling. In the state, the AFM order parameter decreases with increasing the interaction at a fixed temperature since intersite correlations scaled by $\sim T^2/U$ in the strong-coupling limit [42, 43]. By contrast, in the case away from the half filling, the uniform magnetization is saturated in the large $U$ limit, as shown in Fig. 5(b). This suggests that the stability of the FM ordered state is dominated by the kinetic energy. This is similar to the origin of the Nagaoka ferromagnetism, implying that the FM ordered state we find is adiabatically connected to the Nagaoka ferromagnetism, which is justified in the limits of $U \rightarrow \infty$ and $n \rightarrow 1$.

We also examine the ferromagnetism in the Hubbard model on the Bethe lattice with the semielliptical DOS. The results for the magnetic susceptibility at $T/D = 0.05$ and 0.1 are shown in Fig. 6. We find that the susceptibility monotonically increases with increasing $n$ when the temperature and interaction strength are fixed. This suggests that the magnetic instability should appear in the vicinity of the half filling, in contrast to the Hubbard model on the hypercubic lattice discussed above. To examine whether or not the FM ordered state is realized at low temperatures, we also calculate the temperature dependence of the susceptibility for the nearly half-filled system ($n = 0.99$), as shown in Fig. 7. It is found that, in the system with the strong interactions $U/D = 100$ and 200, the magnetic susceptibility monotonically increases with decreasing temperatures. However, we cannot find tendencies toward divergence (see the inset of Fig. 7). This suggests the absence of the FM ordered state in the single band Hubbard model on the Bethe lattice, which is consistent with the previ-
ous works [18, 28].

Up to now, we have treated the hypercubic and Bethe lattices to elucidate the origin of the magnetic instability to the FM ordered state in the single-band Hubbard model; the detailed finite temperature calculations clarified that the FM ordered phase appears in the hypercubic lattice, while this does not in the Bethe lattice. These facts might be understood by the Nagaoka mechanism [23]; in the \( U \to \infty \) limit, the FM ordered state is realized in the one-hole doped half-filled system with the closed-loop lattice structure. However, in the framework of DMFT, the lattice structure is indirectly treated only via the noninteracting DOS [Eq. (4)]. Therefore, it may be difficult to conclude that the loop structure plays an essential role in stabilizing the FM ordered state in the infinite dimensions. Now, we focus on the DOS in the noninteracting system. It is clear that the DOS around the Fermi level is similar to each other. This suggests that the FM ordered state found in the present system with large interactions is not attributed to the DOS at the Fermi energy, which is crucial for the FM ordered state caused by the Slater mechanism justified in the weak coupling limit.

On the other hand, in the high energy region, there exists a clear difference in DOS; \( \rho_b = 0 \) for the Bethe lattice, while \( \rho_{hc} \neq 0 \) for the hypercubic lattice. This expects that the asymptotic form of DOS away from the Fermi level plays an important role in stabilizing the FM ordered state in the strong-coupling limit. Here, we introduce another function form, so-called \( t \)-distribution [45],

\[
\rho_t(x, \nu) = \frac{\Gamma \left( \frac{\nu + 1}{2} \right)}{\sqrt{\pi \nu}} \left[ 1 + \frac{1}{\nu x^2} \right]^{-\nu/2},
\]

where \( \Gamma(x) \) is the Gamma function. This is reduced to the Cauchy-Lorentz distribution in the case \( \nu = 1 \) and the Gaussian distribution (hypercubic) in the case \( \nu \to \infty \). As an example, we consider the \( t \)-distribution with \( \nu = 3 \),

\[
\rho_t(x, 3) = \frac{1}{\sqrt{2\pi D}} \left[ \left( \frac{x}{D} \right)^2 + \frac{1}{2} \right]^{-2},
\]

where \( D \) is the unit of energy, which is determined such that its variance coincides with that of the DOS of the hypercubic lattice given in Eq. (9). The filling dependence of the magnetic susceptibility in the system with \( \rho_t(x, 3) \) is shown in Fig. 8. We find that nonmonotonic behavior appears in the magnetic susceptibility and the maximum of the curves is located around \( n \sim 0.95 \) at \( T/D = 0.1 \). The results are similar to those for the hypercubic lattice, which expects that the FM ordered state is realized in a finite parameter space unlike the case on the Bethe lattice. Figure 9 shows the magnetization and magnetic susceptibility as a function of the temperature in the system with \( t \)-distribution when \( U/D = 100 \) and \( n = 0.95 \). The inset shows critical behavior of the susceptibility and magnetization. Solid lines are guides to the eyes.

\[ T/U=0.05 \]

\[ T/U=0.1 \]

\[ \chi D \]

\[ \m^2 \]

\[ \frac{(\chi D)^{-1}}{T/D} \]

IV. SUMMARY

We have studied magnetic properties in the single-band Hubbard model in the infinite dimensions. Combining DMFT with the continuous-time quantum Monte Carlo simulations, we have calculated uniform magnetic susceptibility and magnetization systematically and have found that the FM ordered state is realized in the system on the hypercubic lattice, while no ordered state appears on the Bethe lattice. We have also examined the system with \( t \)-distribution DOS which

\[ \chi D \sim 0.3 \] is the results for the noninteracting system at \( T/D = 0.05 \) and 0.1.

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has a power-law tail unlike the Gaussian distribution. We have found that the FM ordered state in the system with t-distribution is more stable than with that in the system on the hypercubic lattice.

The present results suggest that the noninteracting DOS in the high energy region contributes to the stability of the FM ordered state in the strong-coupling regime while the DOS around the Fermi level is not relevant to the emergence of the ferromagnetism. It is then expected that, in the finite dimensional systems on a simple lattice such as square and cubic lattices, no FM instability appears due to the absence of DOS in the high energy region. It is an interesting problem to discuss the the FM stability, by taking into account non-local electron correlations, which is now under consideration.

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