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# Magnetic phase diagram of the half-filled Hubbard model for a simple cubic lattice

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We have calculated the $U$-$T$ phase diagram of the half-filled simple-cubic Hubbard model ($U$: interaction, $T$: temperature) by making use of the two interpolation theories, the single-site spin-fluctuation (SSF) theory proposed by Hubbard and Hasegawa and the Gutzwiller-type variational approach (VA) by Kakehashi and Fulde. The results are compared with those of the recent Monte Carlo (MC) calculations made by Hirsch for a three-dimensional 4×4×4 lattice. The Néel temperatures $T_N$ calculated with the MC method are about 70% *higher* than those calculated with the mean-field–type theories of the SSF and VA though the $U$ dependence of the amplitudes of the local moments and charge fluctuations agrees well with our results. This suggests an overestimation of $T_N$ up to 100% in Hirsch's calculations, whose conceivable origins are discussed. We present also the result of the internal energy as a function of $T$ and $U$ calculated using the SSF and VA.

Quite recently Hirsch[1] has reported the results of Monte Carlo (MC) simulations of the three-dimensional half-filled Hubbard model with a cluster of 4×4×4 or 6×6×6. He has obtained various quantities such as the energy and susceptibility as a function of the temperature $T$ and the electron-electron interaction $U$. This type of "exact" calculation has been expected for a long time for a deeper understanding of magnetism of three-dimensional systems.

On the other hand, several approximation theories[2–7] for three-dimensional finite-temperature magnetism, which interpolate between the weak- and strong-interaction limits, have been proposed in the last several years. All of them[2–7] employ the functional-integral method within the adiabatic approximation. They have been applied to the semielliptic-band model[3,5] and to various problems of transition metals and their alloys.[8–14]

We discuss in this Rapid Communication the $U$-$T$ phase diagram of the half-filled simple-cubic Hubbard model. Stimulated by Hirsch's MC simulations for this model, we have applied to it the two typical interpolation theories: the single-site spin-fluctuation (SSF) theory developed by Hubbard[2] and Hasegawa[3] and the variational approach (VA) proposed by Kakehashi and Fulde.[4] Then we compare the calculated results with those in the MC simulations.[1] This is certainly meaningful because the validity of the existing theories[2–7] and of the MC calculations for the three-dimensional systems has not been established yet.

The SSF and VA interpolate between the delocalized and localized limits within the two-field functional integral method. They are mean-field theories in which the short-range magnetic order is neglected, so that the system under consideration is regarded as a collection of local moments[15] which is treated within the coherent potential approximation (CPA). The VA theory employs the Gutzwiller-type approximation[16] to take account of the effect of the local electron correlation, which is neglected in the SSF. The SSF and VA in the weak-interaction limit are nothing but the Hartree-Fock approximation. In the opposite strong-interaction limit, both SSF and VA reduce to the molecular-field approximation to the Heisenberg model with Anderson's superexchange interaction. The free energy at $T=0$ K in the VA agrees with the Gutzwiller-type variational energy.[16,17]

The input parameters for numerical calculations in the SSF and VA are the density of states of noninteracting system, the electron-electron interaction $U$, and the electron number $n$. We adopt $n=1.0$ and the density of states for the simple-cubic lattice with the nearest-neighbor hopping $t$, which yields the total bandwidth of $W=12|t|$. The Fermi-distribution function has been correctly included in this work.

The $U$-$T$ phase diagrams[18] in the SSF and VA are shown in Fig. 1. The calculated Néel temperatures in the weak- and strong-interaction regions asymptotically reduce to those in the Hartree-Fock approximation and the molecular-field approximation to the Heisenberg model, respectively, as mentioned before. In the intermediate $U$ region, the $T_N$ curve has a maximum at $2U/W \cong 1.35$ (1.5) in the SSF (VA). The Néel temperature in the VA is lower than that in the SSF due to the effect of the electron correlation.

We show, by the dot-dashed curve in Fig. 1, the result of Moriya and Hasegawa[7] who made calculations along the interpolation theory of Moriya and Takahashi (MT).[6] Among various representations for the functional integral method, they employed the vectorial scheme, which completely neglects the quantum effect. We note that the calculated $T_N$ is only about $\frac{1}{5} \sim \frac{1}{6}$ of those in the SSF and VA. An underestimate of $T_N$ by a factor of 3 is expected in the strong-interaction region because of a classical

 

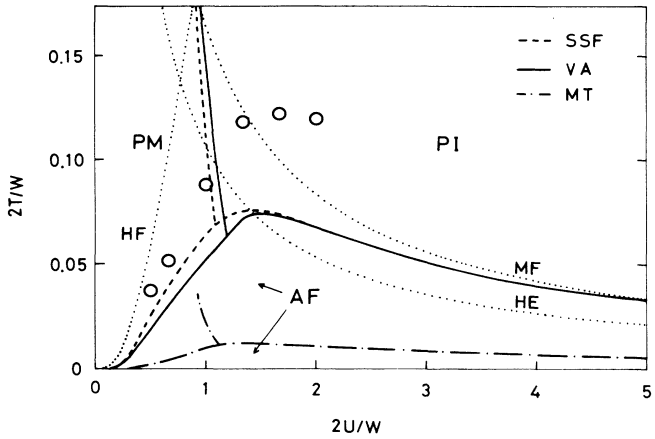


FIG. 1. The $U$-$T$ phase diagram (Ref. 18) of the half-filled simple-cubic Hubbard model, showing the antiferromagnetic state (AF), the paramagnetic metal (PM), and the paramagnetic insulator (PI). They are calculated by SSF (dashed curves, Refs. 2 and 3), VA (solid curves, Refs. 4 and 5), MT (dot-dashed curves, Refs. 6 and 7), and MC methods (open circles, Ref. 1). $W$ denotes the total bandwidth ($12|t|$). Dotted curves show the Néel temperatures in the Hartree-Fock (HF) approximation, and the molecular-field (MF) and high-temperature expansion (HE) approximations for the Heisenberg model.

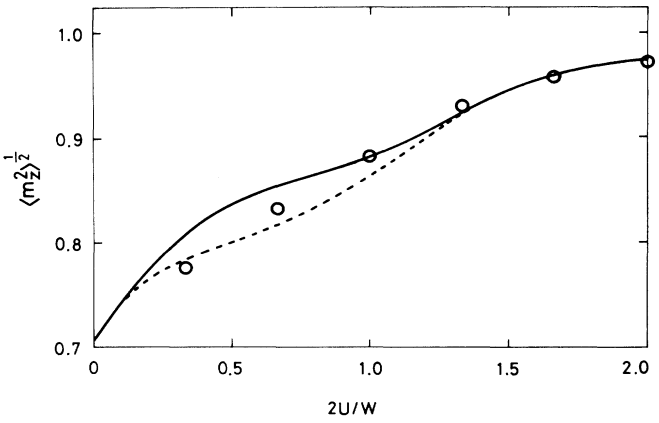


FIG. 2. The amplitude of local moments, $\langle m_z^2 \rangle^{1/2}$, at $2T/W=0.083$ as a function of the electron interaction $U$ in the VA (solid curve, Refs. 4 and 5), SSF (dashed curve, Refs. 2 and 3), and MC (open circles, Ref. 1).

treatment of spin in the MT theory [i.e. $S/(S+1)=\frac{1}{3}$ for $S=\frac{1}{2}$]. It should be noted that the quantum effect is included in the two-field theories of the SSF and VA, which reproduce, for example, the correct Curie constant of the susceptibility in the strong $U$ limit. A further lowering of $T_N$ in the MT theory is due to the effect of the short-range magnetic order, which is neglected in the SSF and VA.

The Néel temperatures of the Monte Carlo calculations by Hirsch[1] are shown by open circles in Fig. 1. The results are about 70% *higher* than those in the SSA and VA, and about twice as large as the Heisenberg result in the local-moment regime ($2U/W \gtrsim 2$). Hirsch attributed his large $T_N$ to a lack of charge fluctuations $\langle (\delta n)^2 \rangle$ in the Heisenberg model. His argument does not, however, explain the disagreement with the SSF and VA results. In order to clarify this point, we calculated the amplitude of local moments, $\langle m_z^2 \rangle^{1/2}$, at $T \sim T_N$ as a function of $U$. Figure 2 shows that the results calculated by the SSF and VA are in good agreement with those in the MC simulation. This implies that SSF and VA correctly takes the effect of charge fluctuations into account since $\langle (\delta n)^2 \rangle = 1 - \langle m_z^2 \rangle$ for the half-filled case.

We expect that the SSF and VA overestimate $T_N$ by about 50% for simple-cubic lattice since they are of single-site molecular-field theories; note that $T_N$(VA or SSF)/$T_N$(exact)=6/3.83 in the insulator limit.[19] Therefore we speculate that Hirsch's MC method overestimates $T_N$ by more than 50% or probably up to 100%.

One of the conceivable origins of this overestimate in $T_N$ is the finite-size effect. Simple calculations show that because of the finite-size effect both uniform and staggered susceptibilities of noninteracting system are overestimated at $2T/W \lesssim 0.15$ in Hirsch's calculations for $4\times4\times4$ lattice [see Figs. 8 and 9(a) in Ref. 1]. This is also seen in his two-dimensional lattice calculations (see Fig. 7 in Ref. 20). Since the Néel temperatures calculated in the MC are $2T_N/W \lesssim 0.13$ one expects that the finite-size effect might overestimate the staggered susceptibility for interacting case.

The other possible origin of the enhanced $T_N$ is expected to be the self-consistent boundary approximation[21] which Hirsch introduced for a calculation of the Néel temperature. In this approximation the interaction $m_z^2$ is replaced by $\langle m_z \rangle m_z$ outside the cluster, just as in the mean-field or Bethe-Peierls approximation. This certainly underestimates the short-range magnetic order and leads to 15% overestimate for the Ising model.[1] Since there exists further reduction due to the transversal quantum fluctuations, Hirsch's MC calculations of $T_N$ with the additionally introduced boundary approximation might overestimate the Néel temperature more than 100%. This shows that although the self-consistent boundary condition was reported to be useful for the classical systems,[21] it might not be so for the quantum systems, like the Hubbard model, for some reason, although we cannot draw any definite conclusions until the Binder's boundary approximation[21] is examined by further MC calculations by increasing systematically the cluster size.

Figure 3 shows the internal energy $E$ as a function of the temperature for various interaction strengths calculated by the SSF and VA. The curves have cusps at the Néel temperatures. We can obtain the specific heat from the derivative of $E$ with respect to the temperature. The specific heat in the SSF and VA has a large peak just below the Néel temperature and a small tail above it. This is a characteristic of the mean-field-type theories. We show in Fig. 4 the $U$ dependence of the internal energies at $2T/W=0.0$ and 0.0833 in the SSF and VA. For a comparison, the results of $E$ of the MC calculations are plotted in Figs. 3 and 4. The ground-state energies of the

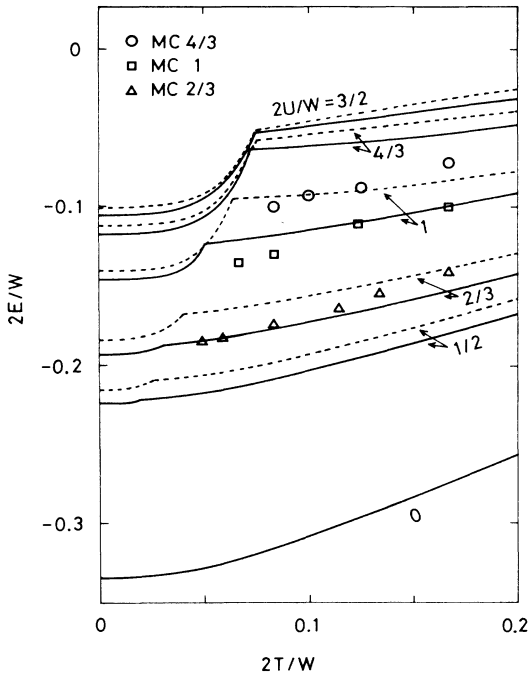


FIG. 3. The internal energy $E$ as a function of the temperature for various $U$ values; SSF (dashed curves, Refs. 2 and 3), VA (solid curves, Refs. 4 and 5), and MC (open squares, circles, and triangles, Ref. 1).

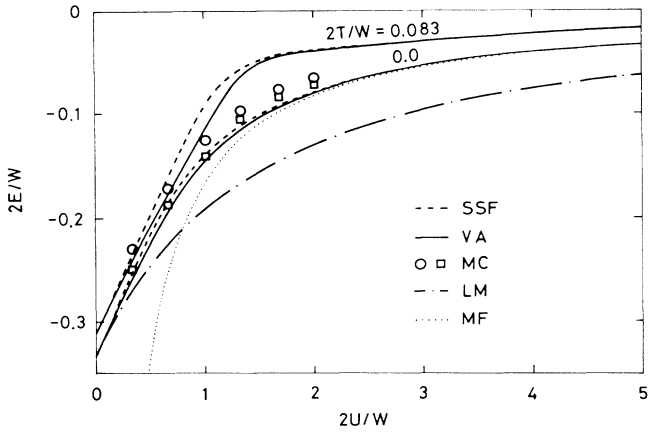


FIG. 4. The internal energy vs interaction curves for $2T/W$=0.0 and 0.083 in SSF (dashed curves), VA (solid curves), and MC (open squares and circles). The dotted curve shows the energy of the Heisenberg model in the molecular-field (MF) approximation at $T$=0 K. The dot-dashed curve shows Langer-Mattis's (LM) lower bound (Ref. 22).

MC in Fig. 4 are estimated by an extrapolation of its finite-temperature result. We note that at $T$=0 K, the result of the SSF and VA are in good agreement with those in the MC simulations. However, the agreement between the two approaches becomes worse at elevated temperatures where the paramagnetic states are realized in the interpolating theories, while a strong antiferromagnetic correlation seems to persist in the MC in the intermediate $U$ region. For example, the internal energy for $2U/W=\frac{4}{3}$ in the MC is much lower than those in the SSF and VA, as clearly seen in Fig. 3, where it stays near the dashed line for $2U/W$=1 in the SSF (see also Fig. 4). These again suggest an overestimate of the antiferromagnetic order in the MC for 4×4×4 lattice.

To summarize, we have presented the $U$-$T$ phase diagram and the internal energy of the half-filled simple-cubic Hubbard model calculated by the SSF and VA. Our results suggest that the Néel temperatures in Hirsch's simulations are much overestimated. Although our calculations cannot be definitely considered as superior to the MC because of their approximate nature, it is expected to be as the plausible guideline for future MC simulations. Such MC calculations with larger clusters will clarify the range of validity of the interpolation theories which have been successfully applied to various problems of magnetism of transition metals and alloys.

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