Magnetic susceptibility of the strongly correlated Hubbard model

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Using the linked-cluster expansion method, we have calculated the uniform and the staggered susceptibility of a single-band Hubbard model. We make correction of previous results of Kubo and Zhao *et al.*

The Hubbard model was introduced to study the effect of electron correlations.[1] It has long been used in describing the most essential part of itinerant magnetism and metal-insulator transition. The model has also been proposed[2] to investigate the physical mechanism of high-temperature superconductivity. The magnetism may play an important role in the superconductivity of such high-temperature superconductors. However, it is very complicated to solve this many-body problem. Even the simple single-band Hubbard model has the exact solution of the ground state for one-dimensional system only.[3] In the strong-correlation limit, Nagaoka[4] rigorously proved the existence of ferromagnetic ordering with the number of electrons one less than the total number of lattice sites for the simple-cubic and body-centered-cubic lattices. In the thermodynamic limit and in the region of strong correlation, the magnetic properties were studied by Beni *et al.*,[5,6] Kubo,[7] and Zhao *et al.*[8] using the perturbation expansion for the single-band Hubbard model. The behaviors of the three-dimensional simple-cubic and body-centered-cubic systems have been discussed from the qualitative analysis of the perturbation series up to fourth order. One of the major problems is that their calculated series are in conflict with each other. The qualitative behavior shown by Zhao *et al.*[8] is more reasonable. The question is still whether the calculated results are really correct. Actually, their methods of calculation are the same. The evaluations of the fourth-order terms are all lengthy. In this Brief Report we make a correction of their results and present a linked-cluster series expansion technique to obtain the perturbation series of the single-band Hubbard. This method has been extensively used on spin systems with crystalline potentials involved. Since the multiple-site Wick reduction theorem[9,10] automatically makes the integration procedures saved, it is more convenient to calculate all terms in the series expansion especially by using computer.

The Hamiltonian of the single-band Hubbard model being considered is given by

$$H=U\sum_i n_{i\uparrow}n_{i\downarrow}-\sum_{i,\sigma}\mu_{i\sigma}n_{i\sigma}+t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma}) , \tag{1}$$

where U is the on-site Coulomb repulsion potential, t is the nearest-neighbor hopping integral. The chemical potential $\mu_{i\sigma}$ includes a uniform magnetic field h and a staggered magnetic field g,

$$\mu_{i\sigma}=\mu+\alpha(\sigma)(h\pm g) , \tag{2}$$

where the sign ± 1 depends on whether the ith site belongs to the A or B sublattice and $\alpha(\sigma)$ is $+1$ and -1 for spin $\sigma=\uparrow$ and $\downarrow$, respectively. We consider only those lattices which can be seperated into two interpenetrating sublattices.

The Hamiltonian is split into an unperturbed Hamiltonian H_0 and a perturbation part H_1 as

$$H_0=U\sum_i n_{i\uparrow}n_{i\downarrow}-\sum_{i\sigma}\mu_{i\sigma}n_{i\sigma} \tag{3}$$

and

$$H_1=t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma}) . \tag{4}$$

The free energy F can be written as

$$F=F_0+\Delta F , \tag{5}$$

where F_0 is the free-energy term corresponding to the unperturbed Hamiltonian H_0 and ΔF is expressed as[11]

$$\Delta F=-\frac{1}{\beta}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\int_0^{\beta}d\tau_1\cdots\int_0^{\beta}d\tau_n\langle T_{\tau}[H_1(\tau_1)\cdots H_1(\tau_n)]\rangle_c , \tag{6}$$

where $\beta=(k_BT)^{-1}$ and T_{τ} is the τ-ordering operator which orders operators in the product with τ labels decreasing from left to right. The subscripts c denote the cumulant part of the τ-ordered product, or, in the diagram analysis, the contribution of the connected diagrams. To compute ΔF we need a technique to calculate the thermal average of the τ-ordered products of fermion operators. In this report we adopt the technique developed by Yang and Wang[12] and extend their consideration to the fermion operators of Hubbard model. We define four standard basis pseudofermion operators[1] as

$$L_{12}^i\equiv c_{i\uparrow}(1-n_{i\downarrow}),\quad L_{13}^i\equiv c_{i\downarrow}(1-n_{i\uparrow}) ,$$
$$L_{24}^i\equiv -n_{i\uparrow}c_{i\downarrow},\quad L_{34}^i\equiv n_{i\downarrow}c_{i\uparrow} , \tag{7}$$

and two standard basis pseudoboson operators as

$$L_{14}^i\equiv -c_{i\uparrow}c_{i\downarrow},\quad L_{23}^i\equiv c_{i\uparrow}^{\dagger}c_{i\downarrow} . \tag{8}$$

Adjoint operators are $(L^i_{\alpha\beta})^\dagger = L^i_{\beta\alpha}$.

These operators satisfy the multiplication rule and the commutation relation[1]

$$L^i_{\alpha\beta}L^i_{\gamma\eta} = \delta_{\beta\gamma}L^i_{\alpha\eta} \ , \tag{9}$$

$$[L^i_{\alpha\beta}, L^j_{\gamma\eta}]_\epsilon = \delta_{ij}(\delta_{\beta\gamma}L^i_{\alpha\eta} + \epsilon\delta_{\eta\alpha}L^i_{\gamma\beta}) \ , \tag{10}$$

where $\epsilon = -1$ if one of the two operators or both are pseudoboson operators and $\epsilon = +1$ if both are pseudofermion operators. So any single-site fermion operator can be expressed as a linear combination of the standard basis operators in Eq. (11):

$$\begin{aligned} c_{i\uparrow} &= L^i_{12} + L^i_{34}, \quad c_{i\downarrow} = L^i_{13} - L^i_{24} \ , \\ n_{i\uparrow} &= L^i_{22} + L^i_{44}, \quad n_{i\downarrow} = L^i_{33} + L^i_{44} \ . \end{aligned} \tag{11}$$

The standard basis operators in the interaction picture have the simple τ dependence required by the Wick reduction theorem

$$L_{\alpha\beta}(\tau) = e^{(E_\alpha - E_\beta)\tau}L_{\alpha\beta}(0) \ . \tag{12}$$

The multiple integrals using the multiple-site Wick reduction theorem[9,10] can be done by machine. A computer program has been developed to calculate free energy F, uniform susceptibility

$$-\frac{\partial^2}{\partial h^2}F|_{h=g=0}$$

and staggered susceptibility

$$-\frac{\partial^2}{\partial g^2}F|_{h=g=0}$$

with the general symbolic manipulation program SCHOONSCHIP.[13]

The free energy per site up to the fourth order at $h = g = 0$ is obtained as

$$F = F_0 + F_2 + F_{41} + F_{42} + F_{43} + F_{44} \tag{13}$$

with

$$F_0 = -k_B T \ln\zeta \ , \tag{14}$$

$$F_2 = -zt^2\left[\beta(\gamma - 2\gamma^2) + \frac{2}{U}(1 - e^{-\beta U})\gamma^2\right] \ , \tag{15}$$

$$F_{41} = -zt^4\left[\frac{1}{12}\beta^3(\gamma - 2\gamma^2) + 4\frac{\beta}{U^2}(1 + e^{-\beta U})\gamma^2 - \frac{8}{U^3}(1 - e^{-\beta U})\gamma^2\right] \ , \tag{16}$$

$$\begin{aligned} F_{42} = -z(z-1)t^4\Bigg[&\frac{1}{6}\beta^3(\gamma - 2\gamma^2) + 3\frac{\beta^2}{U}[\gamma^2 - 2(1 + e^{-\beta U})\gamma^3] \\ &- 2\frac{\beta}{U^2}[(2 - e^{-\beta U})\gamma^2 - 6(1 - e^{-\beta U})\gamma^3] + \frac{2}{U^3}(1 - e^{-\beta U})\gamma^2\Bigg] \ , \end{aligned} \tag{17}$$

$$\begin{aligned} F_{43} = -p_4 t^4\Bigg[&\frac{2}{3}\beta^3[\gamma - 10\gamma^2 + (29 - 3e^{-\beta U})\gamma^3 - (26 - 14e^{-\beta U})\gamma^4] + 8\frac{\beta^2}{U}[\gamma^2 - (5 - e^{-\beta U})\gamma^3 + 6(1 - e^{-\beta U})\gamma^4] \\ &+ 8\frac{\beta}{U^2}[-2\gamma^2 + (9 + e^{-\beta U})\gamma^3 - 10(1 - e^{-\beta U})\gamma^4] + \frac{16}{U^3}(1 - e^{-\beta U})[\gamma^2 - 5\gamma^3 + 5(1 - e^{-\beta U})\gamma^4]\Bigg] \ , \end{aligned} \tag{18}$$

and

$$F_{44} = z(2z-1)t^4\left[\beta^3(\gamma - 2\gamma^2)^2 + 4\frac{\beta^2}{U}(1 - e^{-\beta U})(\gamma^3 - 2\gamma^4) + 4\frac{\beta}{U^2}(1 - e^{-\beta U})^2\gamma^4\right] \ , \tag{19}$$

where $\zeta = (1 + 2e^{\beta\mu} + e^{2\beta\mu}e^{-\beta U})$ and $\gamma = e^{\beta\mu}/\zeta$. Comparing with Kubo's result,[7] only the F_{42} term contradicts with Kubo's Ω_{c+d} term. Since all previous results[5-8] of such perturbation expansion are inconsistent with each other and our calculated series is also shown a different result, in order to prove that some errors exist in the previous results, we can consider a special case with the on-site repulsion potential U equal to zero. The Hamiltonian becomes trivial, and the exact solution for the free energy per site is

$$F = -k_B T\frac{1}{N}\sum_{k,\sigma}\ln(1 + e^{\beta(\mu - \varepsilon_k)}) \ , \tag{20}$$

where $\varepsilon_k = t\sum_\delta e^{i\mathbf{k}\cdot\delta}$ with δ as nearest-neighbor vectors.

Through the Taylor series expansion in terms of βt, the fourth-order term is

$$\begin{aligned} F_4 = &-\tfrac{2}{3}p_4 t^4\beta^3(\gamma - 6\gamma^2) + \tfrac{1}{12}zt^4\beta^3(\gamma - 6\gamma^2) \\ &- \tfrac{1}{6}z^2t^4\beta^3(\gamma - 6\gamma^2) \ , \end{aligned} \tag{21}$$

where $\gamma = e^{\beta\mu}/(1 + e^{\beta\mu})^2$.

We find out that, in the $U = 0$ limit, our results are the same as the exact solution given above. The fourth-order Kubo result[7] becomes

$$\begin{aligned} F_4^{\text{Kubo}} = &-\tfrac{2}{3}p_4 t^4\beta^3(\gamma - 6\gamma^2) + \tfrac{1}{12}zt^4\beta^3(\gamma - 14\gamma^2) \\ &- \tfrac{1}{6}z^2t^4\beta^3(\gamma - 10\gamma^2) \ , \end{aligned} \tag{22}$$

which is incorrect. Excluding the "diagram f" of Kubo's calculation, as suggested by Zhao *et al.*,[8] does not make the result correct. As a matter of fact, the "diagram f" is obtained when the "semi-invariants" (the connected diagrams) are expressed in terms of thermal moment products.[14] The results of Beni *et al.*[6] are also incorrect, as

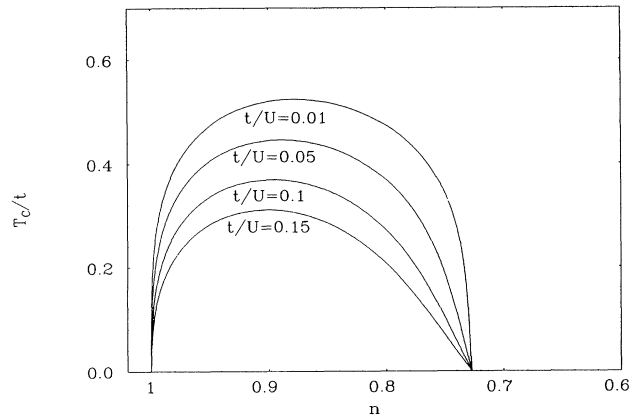

FIG. 1. The Curie temperature T_C/t as function of the electron density n for the simple-cubic system.

already mentioned by Kubo.[7]

There is another simple way to check up on part of the calculated series expansion. The finite-cluster method is a well-developed method for finding the high-temperature series for classical spin and certain quantum spin systems.[15] It can also be used to work on the Hubbard model. However, it is more complicated because the size of the matrices is much larger. A two point (connected) cluster in the finite-cluster method can still be calculated easily. This result can be compared with the series by taking $z=1$ and $p_n=0$ because no other finite cluster will contribute to the series under this condition. The free-energy series obtained by the two-point cluster calculation agrees fully with the series [Eqs. (14)–(19)] by taking $z=1$ and $p_4=0$. Only the two terms F_{42} and F_{43} cannot be checked by the two-point cluster calculation. In Kubo's calculation only the corresponding terms of F_{42} contain an error. It has been proved by comparing with the special case $U=0$, as shown above.

The *uniform susceptibility* as a function of the electron density n with $e^{-\beta U} \ll 1$, corrected up to fourth order of t, is obtained as follows:

$$\chi_{u0}=\beta n \ , \tag{23}$$

$$\chi_{u21}=-zt^2\frac{\beta^2}{U}n^2 \ , \tag{24}$$

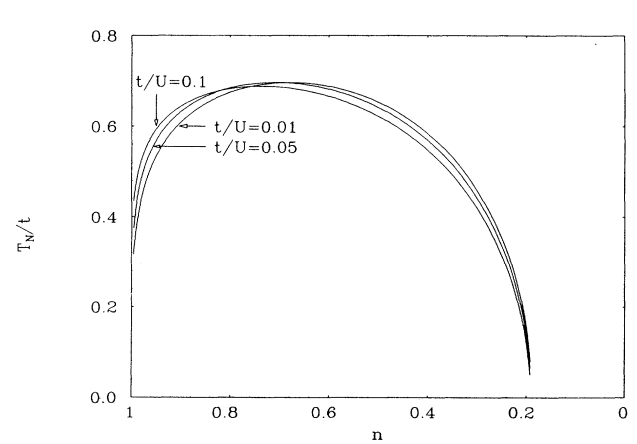

FIG. 2. The Néel temperature T_N/t as function of the electron density n for the simple-cubic system.

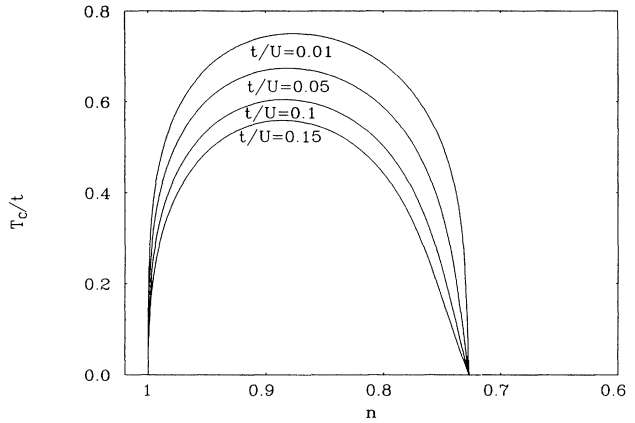

FIG. 3. The Curie temperature T_C/t as function of the electron density n for the body-centered-cubic system.

$$\chi_{u41}=-2zt^4\left[\frac{\beta^3}{U^2}-2\frac{\beta^2}{U^3}\right]n^2 \ , \tag{25}$$

$$\chi_{u42}=-\tfrac{1}{2}z(z-1)t^4\left[3\frac{\beta^4}{U}n^2(1-n)-2\frac{\beta^3}{U^2}n^2(2-3n)+2\frac{\beta^2}{U^3}n^2\right] , \tag{26}$$

$$\chi_{u43}=p_4t^4\left[-\tfrac{1}{6}\beta^5n^2(1-n)(8-11n)-2\frac{\beta^4}{U}n^2(1-n)(2-3n)+2\frac{\beta^3}{U^2}n^2(1-n)(4-5n)-4\frac{\beta^2}{U^3}n^2(2-5n)\right] , \tag{27}$$

$$\chi_{u44}=z(2z-1)t^4\left[\frac{\beta^4}{U}n^3(1-n)+\frac{\beta^3}{U^2}n^4\right] , \tag{28}$$

$$\chi_{u22}=z^2t^4\left[\frac{\beta^4}{U}n^2(1-n)(1-2n)+2\frac{\beta^3}{U^2}n^3(1-n)\right] . \tag{29}$$

The *staggered susceptibility is*

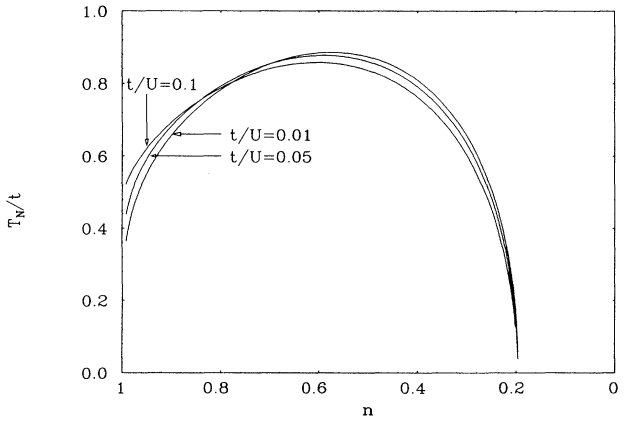

FIG. 4. The Néel temperature T_N/t as function of the electron density n for the body-centered-cubic system.

$$\chi_{s0}=\beta n \ , \tag{30}$$

$$\chi_{s21}=zt^2\left[-\tfrac{1}{3}\beta^3 n(1-n)+\frac{\beta^2}{U}n^2-4\frac{\beta}{U^2}n^2+\frac{4}{U^3}n^2\right], \tag{31}$$

$$\chi_{s41}=zt^4\left[-\tfrac{1}{30}\beta^5 n(1-n)+\frac{2}{3}\frac{\beta^3}{U^2}n^2-12\frac{\beta^2}{U^3}n^2+48\frac{\beta}{U^4}n^2-\frac{64}{U^5}n^2\right], \tag{32}$$

$$\chi_{s42}=z(z-1)t^4\left[-\tfrac{1}{30}\beta^5 n(1-n)(2+n)-\frac{1}{3}\frac{\beta^4}{U}n^2(1-n)\right.$$
$$\left.-\frac{1}{3}\frac{\beta^3}{U^2}n^2(4-13n)+\frac{\beta^2}{U^3}n^2(5-18n)-4\frac{\beta}{U^4}n^2-\frac{4}{U^5}n^2(1-14n)\right], \tag{33}$$

$$\chi_{s43}=p_4 t^4\left[-\tfrac{1}{30}\beta^5 n(1-n)(8-48n+47n^2)-\frac{2}{3}\frac{\beta^3}{U^2}n^2(1-n)(12-19n)\right.$$
$$\left.+4\frac{\beta^2}{U^3}n^2(5-4n)(2-3n)-16\frac{\beta}{U^4}n^2(6-14n+7n^2)+\frac{16}{U^5}n^2(6-14n+7n^2)\right], \tag{34}$$

$$\chi_{s44}=z(2z-1)t^4\left[\tfrac{1}{3}\beta^5 n^2(1-n)^2-\frac{2}{3}\frac{\beta^4}{U}n^3(1-n)+\frac{\beta^3}{U^2}n^3(4-5n)-4\frac{\beta^2}{U^3}n^3(1-2n)-4\frac{\beta}{U^4}n^4\right], \tag{35}$$

and

$$\chi_{s22}=z^2t^4\left[\tfrac{1}{6}\beta^5 n(1-n)(1-2n)^2-\frac{2}{3}\frac{\beta^4}{U}n^2(1-n)(1-2n)+2\frac{\beta^3}{U^2}n^2(1-n)(2-5n)-4\frac{\beta^2}{U^3}n^2(1-n)(1-4n)-8\frac{\beta}{U^4}n^3(1-n)\right]. \tag{36}$$

In all the previous works[5–8] qualitative analyses of their results have been performed. Even though the perturbation series up to fourth order is a low series and may not be convergent yet, it may still provide some qualitative behavior of the model. We follow the way of Kubo[7] and Zhao *et al.*[8] to estimate the critical temperature T_C and T_N from the vanishing of χ_u^{-1} and χ_s^{-1}, respectively, with given values of electron density n and the ratio t/U. In Fig. 1 the analysis of the uniform susceptibility shows T_C/t as a function of n for various values of t/U for the simple-cubic lattice. It indicates that the ferromagnetic ordering can only occur in the region $\frac{8}{11}<n<1$. The critical temperature also decreases as the ratio of t/U is increased for any fixed electron density. This behavior is physically reasonable as mentioned by Zhao *et al.*[8] The Néel temperature T_N of the simple-cubic lattice is shown in Fig. 2. At half-filling ($n=1$) $T_N/t=0.34$, 0.19, and 0.04 for $t/U=0.1$, 0.05, and 0.01, respectively. Our results for T_N/t versus U/t are qualitatively consistent with the previous approximate results of the half-filled Hubbard model.[16,17] For each value of electron density and t/U ratio, T_N is higher than T_C which demonstrates that no ferromagnetic phase is stable. The occurrence of finite T_N at low electron density is also difficult to understand. Figures 3 and 4 are for the body-centered-cubic lattice. Qualitatively the curves are similar to the simple-cubic ones shown in Figs. 1 and 2. In a certain region, T_C can be higher than T_N. We still presume that the higher-order terms in the perturbation series may alter the results analyzed here. It is very important to obtain even higher-order terms to describe more correctly the behavior of the single-band Hubbard model. The calculation of the higher-order terms is complicated. The linked-cluster expansion method with the multiple-site Wick reduction theorem applied may be the best approach. We are in the process of developing more efficient computer programs to evaluate the high-order terms of free energy of the Hubbard model.

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