High-temperature expansion for the single-band Hubbard model

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We study the single-band Hubbard model via high-temperature expansions to order $(\beta t)^9$ for the standard two- and three-dimensional lattices. Series are derived for the grand potential and for the ferromagnetic susceptibility, for general values of the Coulomb repulsion parameter U and electron density n. The series are difficult to analyze with any degree of precision, but estimates are obtained for the ferromagnetic critical temperature.

I. INTRODUCTION

The single-band Hubbard model[1] is probably the simplest model system for describing the essential physics of strongly correlated electrons on a lattice. As such, it has many areas of application, from its initial use to describe magnetism in transition metals,[2] through metal-insulator transitions, to, most recently, theories of high-temperature superconductivity.[3] While it seems likely that, for this latter phenomenon, more complex multiband models are needed, a necessary prerequisite is to understand the single-band case. Unfortunately, despite enormous effort, our understanding of even this simple case is meager. In one dimension some rigorous results are known,[4] but in higher dimensions only approximate results are available, notably from quantum Monte Carlo and finite lattice calculations.

An approach which has proven powerful in studying other strongly interacting lattice systems, both classical and quantum, is the method of high-temperature series expansions.[5] Variations of this approach have been used previously to study the Hubbard model, though with fairly limited success. Hone and co-workers[6] developed low-order expansions, which were subsequently extended by Brauneck[7] to fourth order for finite U and sixth order in the "strong-correlation" limit $U=\infty$. Kubo and Tada[8] extended the strong-correlation series to ninth order for close-packed lattices. Unfortunately, many of the early results contain errors, as summarized in a recent paper by Pan and Wang,[9] an indication of the difficulty of the calculation. At the present time, to the best of our knowledge, correct series exist to sixth order for general U (Ref. 9) and to ninth order for $U=\infty$.[8] In the present paper we report high-temperature series for general U to ninth order, a substantial extension of previous work. For completeness, we mention two other recent developments. Thompson *et al.*[10] have derived series to order 10 for $U=\infty$ and the special case of infinite spatial dimension. Metzner[11] has presented a general formulation of a linked-cluster expansion, but this approach has not yet been used to derive series expansions.

A brief outline of the paper is as follows. In Sec. II we present the method of derivation of the series, with some of the technical details given in an appendix, and give an outline of the results obtained. In Sec. III we present the result of an analysis of the susceptibility series and give the resulting phase diagrams showing the boundaries between ferromagnetic and paramagnetic regions. An investigation of antiferromagnetism is deferred to a future paper. Finally, in Sec. IV, we discuss our results, draw comparisons with previous work where appropriate, and present our conclusions.

II. DERIVATION OF THE SERIES

We start from the usual Hubbard Hamiltonian

$$\mathcal{H}=\mathcal{H}_0+V\ , \tag{1}$$

with

$$\mathcal{H}_0=U\sum_i n_{i\uparrow}n_{i\downarrow}-\mu\sum_i(n_{i\uparrow}+n_{i\downarrow})-h\sum_i(n_{i\uparrow}-n_{i\downarrow}) \tag{2}$$

and

$$V=t\sum_{\langle ij\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})\ . \tag{3}$$

Here μ is the chemical potential, h an external magnetic field, and the remaining notation is standard.

The grand canonical partition function Z can then be expanded in a perturbation series in the usual way:

$$Z=\mathrm{Tr}\{e^{-\beta\mathcal{H}}\}$$

$$=Z_0\left\{1+\sum_{n=1}^{\infty}(-1)^n\int_0^{\beta}d\tau_1\int_0^{\tau_1}d\tau_2\cdots\int_0^{\tau_{n-1}}d\tau_n\langle\tilde{V}(\tau_1)\tilde{V}(\tau_2)\cdots\tilde{V}(\tau_n)\rangle\right\}, \tag{4}$$

with

$$Z_0=\mathrm{Tr}\{e^{-\beta\mathcal{H}_0}\},\quad \beta=1/kT\ ,$$

$$\langle A\rangle=\mathrm{Tr}\{e^{-\beta\mathcal{H}_0}A\}/Z_0\ ,$$

and

$$\tilde{V}(\tau)=e^{\tau\mathcal{H}_0}Ve^{-\tau\mathcal{H}_0}\ .$$

The unperturbed partition function for N sites has the simple form

$$Z_0=z_0^N\ ,$$

with

$$z_0=1+2e^{\beta\mu}\cosh\beta h+e^{2\beta\mu}e^{-\beta U}\ . \tag{5}$$

From (4) we obtain the free energy (grand potential) as

$$-\beta F=N\ln z_0-\beta\Delta F\ , \tag{6}$$

with

$$-\beta\Delta F=\sum_{n=1}^{\infty}(-1)^n\int_0^{\beta}d\tau_1\cdots\int_0^{\tau_{n-1}}d\tau_n\langle\tilde{V}(\tau_1)\cdots\tilde{V}(\tau_n)\rangle_N\ . \tag{7}$$

In (7) the subscript N signifies that only the part proportional to N is to be included. There has been some confusion regarding this point. The contribution of any connected diagram (to be discussed below) is automatically proportional to N, while disconnected diagrams contain contributions linear in N, which must be retained in our method, as well as higher powers which cancel upon taking the logarithm.

Any nonvanishing contribution to (7) comes from a particular group of sites or a diagram. Each application of V results in the transfer of an electron between neighboring sites, and we represent this by a line in the diagram. In Fig. 1 we show the low-order diagrams through order 6. We have generated by computer all of the 305 diagrams which contribute to the expansion through tenth order. Many of these do not contribute for all lattices—in particular, for loose-packed lattices, all diagrams involving odd-order loops vanish. Thus, for example, only 104 diagrams contribute for the body-centered-cubic lattice to tenth order.

Any particular diagram contributes to some minimum order in the expansion, but also contributes to higher-order terms through multiple usage of one or more bonds. The contribution of a particular diagram G to order r in the expansion can be expressed as a sum of terms of the general form

$$X_r(G)=\frac{(\beta t)^r}{z_0^r}a_G\sum_k C_k x^{n_1}y^{n_2}(\beta U)^{-n_3}w^{n_4}\ , \tag{8}$$

where $x=e^{\beta\mu}$, $y=e^{\beta h}$, $w=e^{-\beta U}$, C_k is a numerical coefficient, and n_1,n_2,n_3,n_4 are integers. The quantity a_G is the usual "weak lattice constant" or embedding constant of diagram G in the lattice. Thus, for example, the contribution of the only second-order diagram is

$$X_2(\diagup)=\frac{(\beta t)^2}{z_0^2}(\tfrac{1}{2}Nq)[(x+x^3w)(y+y^{-1})+4(\beta U)^{-1}x^2(1-w)]\ ,$$

a result which has been given by many previous workers. Some of the technical details of the calculation are given in Appendix A. The expressions rapidly become too lengthy to include here, but our results agree with the previous results.[9]

The procedure then is to collect all of the contributions, weighted by the appropriate lattice constants, resulting in an expansion of the form

$$-\beta F/N=\ln z_0+\sum_{r=2}^{\infty}(\beta t)^r z_0^{-r}F_r(\beta U,x,y)\ , \tag{9}$$

with

$$F_r(\beta U,x,y)=\sum_{mlp}f_{rpml}(y)(\beta U)^{p-r}x^m w^l\ . \tag{10}$$

In Appendix B we display the values of f's for $h=0$ for the sc and fcc lattices to sixth order. Coefficients for nonzero h, to ninth order, for all lattices studied, are available on request.

The ferromagnetic susceptibility is then given by

$$\chi=\lim_{y\to 1}\left[y\frac{\partial}{\partial y}\right]^2(-\beta F/N)=\chi_0+\sum_{r=2}^{\infty}(\beta t)^r z_0^{-(r+1)}X_r(\beta U,x)\ , \tag{11}$$

where χ_0 is the susceptibility in the atomic limit $t=0$,

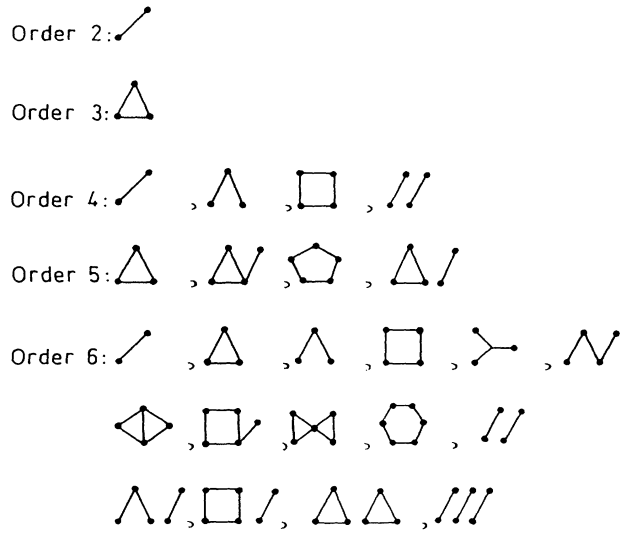

FIG. 1. Diagrams which contribute to the high-temperature free-energy expansion through order $(\beta t)^6$.

$$\chi_0 = 2x/(1+2x+x^2w)\ , \tag{12}$$

and X_r is a polynomial in the fugacity x.

Equation (11) is then the form of the high-temperature expansion for the susceptibility in the variable (βt) with the coefficients being closed expressions in (βU) and x. For most purposes it is more convenient to express the series in terms of the average number of electrons per site n, which can be obtained from the free energy (10) as

$$\begin{aligned} n &= x\frac{\partial}{\partial x}(-\beta F/N) \\ &= 2x(1+xw)/(1+2x+x^2w) \\ &\quad + \sum_{r=2}^{\infty} (\beta t)^r z_0^{-(r+1)} Y_r(\beta U; x)\ , \end{aligned} \tag{13}$$

with $Y_r(\beta U;x)$ being a polynomial in x whose coefficients are closed expressions in (βU). The task then is to eliminate the fugacity x from the expansion (11) in favor of the electron density n. While in the strong-correlation limit[8] or when $e^{-\beta U} \ll 1$ (Ref. 9) the reversion of the series can be done analytically, this is not possible for the general case, because the quantity z_0 is then a quadratic in x. Instead, we proceed as follows. We choose fixed values for n and βU and recursively solve Eq. (13) to obtain an expansion for x in powers of (βt). This is then substituted in (11) to obtain an expansion for χ,

$$\chi = \sum_{r=0}^{\infty} C_r(n,\beta U)(\beta t)^r\ , \tag{14}$$

in the single high-temperature variable (βt). The series for $1 \le n \le 2$ can be obtained from the one for $0 \le n \le 1$ by $n \to 2-n$ and $t \to -t$. Since the series for loose-packed lattices involve only even powers of t, there will be a symmetry in our results about the half-filling value $n=1$. We have computed series to eighth order for the standard loose-packed lattices—square, simple cubic, and body-centred cubic—and to ninth order for the triangular and face-centred-cubic lattices.

It is, of course, impossible to present all of the results here, but in Table I we quote a number of series to illustrate the way in which the coefficients change as n and (βU) are varied. We have checked that our series reduce to those of the Kubo and Tada[8] in the strong-correlation limit. In doing so we found a small discrepancy at ninth order for the fcc lattice, which we have identified as arising from minor errors in a few of the lattice constants used in Ref. 8.

Note that for the fcc series the coefficients appear to occur in pairs; i.e., C_{2m} and C_{2m-1} are nearly always of the same order of magnitude. This is true for other values of $(n,\beta U)$ and for the triangular lattice. For this reason we feel it would be premature to draw any conclusions from our ninth-order results without the tenth-order ones. In the next section we present an analysis of the series to eighth order.

III. ANALYSIS OF SERIES

The phase diagram of the Hubbard model in three dimensions is expected to contain thermodynamically

TABLE I. Coefficients $C_r(n,\beta U)$ for fixed values of $(n,\beta U)$ in the expansion of the magnetic susceptibility [see Eq. (14)]: (top) simple cubic lattice and (bottom) face-centred-cubic lattice.

r	$C_r(0.7,20)$	$C_r(0.85,20)$	$C_r(0.99,20)$	$C_r(0.7,40)$	$C_r(0.85,40)$	$C_r(0.99,40)$	$C_r(0.7,\infty)$	$C_r(0.85,\infty)$	$C_r(0.99,\infty)$
0	0.700 000 00	0.850 000 00	0.990 000 00	0.700 000 00	0.850 000 00	0.990 000 00	0.700 000 00	0.850 000 00	0.990 000 00
2	−0.147 000 00	−0.216 750 02	−0.294 030 47	−0.073 500 00	−0.108 375 00	−0.147 015 00	0.000 000 00	0.000 000 00	0.000 000 00
4	−0.073 059 00	0.067 355 05	0.072 694 26	−0.058 046 62	0.056 835 91	0.027 228 04	−0.022 050 00	0.073 153 12	0.014 162 44
6	0.283 069 31	−0.088 227 54	−0.034 617 00	0.196 156 94	−0.119 272 08	−0.025 794 73	0.107 105 43	−0.156 545 09	−0.024 675 60
8	−0.739 505 59	0.170 952 22	0.043 535 81	−0.557 283 21	0.234 395 83	0.040 809 12	−0.378 922 09	0.307 636 52	0.041 588 45
0	0.700 000 00	0.850 000 00	0.990 000 00	0.700 000 00	0.850 000 00	0.990 000 00	0.700 000 00	0.850 000 00	0.990 000 00
2	−0.294 000 00	−0.433 500 03	−0.588 060 95	−0.147 000 00	−0.216 750 00	−0.294 030 00	0.000 000 00	0.000 000 00	0.000 000 00
3	1.511 160 00	1.114 095 00	0.100 754 29	1.347 990 00	0.993 798 75	0.089 875 17	1.176 000 00	0.867 000 00	0.078 408 00
4	−0.439 383 00	0.920 293 36	0.488 013 74	−0.395 163 56	0.793 386 28	0.233 939 33	−0.242 550 00	0.804 684 38	0.155 786 90
5	−9.118 572 80	−5.675 964 10	−0.262 145 04	−7.972 761 34	−4.658 929 02	−0.160 515 32	−7.014 840 00	−3.788 248 12	−0.073 819 17
6	8.012 541 27	−5.022 814 34	−1.056 361 70	5.925 481 98	−5.238 612 83	−0.796 960 64	3.869 695 37	−5.564 032 90	−0.672 379 40
7	52.531 903 01	27.832 543 70	0.078 590 47	47.766 429 62	22.618 758 65	−0.218 345 13	44.207 854 57	18.384 085 12	−0.435 285 70
8	−75.514 916 43	31.312 881 70	3.528 904 08	−56.378 293 14	33.917 211 62	2.749 138 73	−39.313 694 14	36.488 125 93	2.174 960 06
9	−307.156 770 72	−144.162 640 25	2.996 186 52	−293.280 475 41	−115.898 343 32	3.529 358 51	−284.697 818 70	−92.667 847 09	3.914 311 70

stable regions of both ferromagnetic and antiferromagnetic order, as well as a high-temperature disordered phase. Nagaoka[12] has shown, in the strongly correlated limit, that for one electron more or less than the number of lattice sites, the ground state is ferromagnetically stable for sc and bcc lattices. This phase is also stable for the fcc lattice with one electron less than the number of sites ($t>0$). Kanamori[13] proposed that in the low-density limit even with infinitely strong correlations the electrons would not necessarily show ferromagnetism. For the two-dimensional case, a Mermin-Wagner[14] type theorem precludes the ferromagnetic phase from being stable at nonzero temperature, although not at $T=0$. More exotic phases have also been proposed.[15]

Our series for the ferromagnetic susceptibility should, in principle, indicate the existence of a paramagnetic-ferromagnetic transition and yield a quantitative estimate of the transition temperature. The standard method uses Padé approximants to the series for $(d/dK)\ln\chi(K)$, where K is an appropriate expansion variable; here, $K=\beta t$. If the susceptibility diverges at the transition with a simple power law

$$\chi(K)\sim(K_c-K)^{-\gamma},$$

then the logarithmic derivative will have a simple pole at K_c, which should be well represented by the Padé approximants. Unfortunately, the series for the loose-packed lattices are too short for this method to be usable. Previous workers have looked for zeros of the series for χ^{-1}, as indicative of a divergence in χ and hence a phase transition. This method is likely to be unreliable, but in the absence of any better method, we have used this approach also. For the fcc lattice, where more nonzero coefficients are available, we have used Padé approximants as well as the $\chi^{-1}=0$ method.

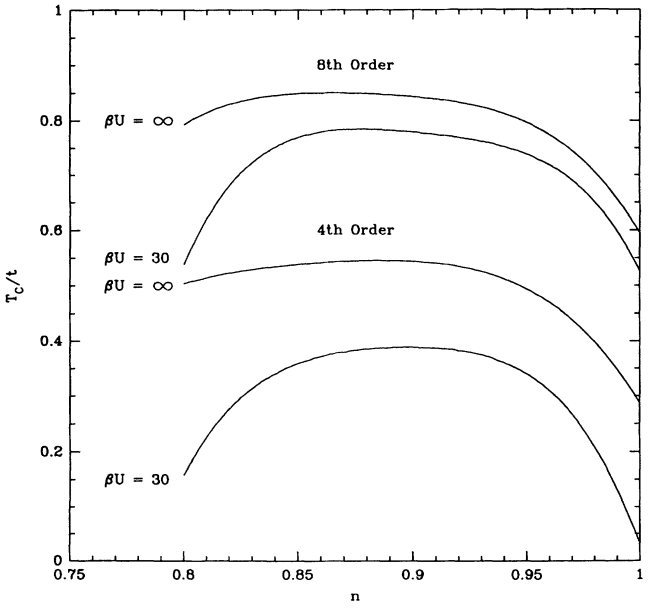

FIG. 2. Variation of T_c with n for fixed (βU) for the simple cubic lattice, obtained from $\chi^{-1}=0$.

TABLE II. Maximum critical temperature T_c and the corresponding density n for the standard lattices in the strong-correlation limit $U=\infty$. The values are approximate only.

Lattice	Fourth order $(T_c)_{max}$	Fourth order n	Eighth order $(T_c)_{max}$	Eighth order n
Square	0.4	0.85	0.6	0.90
Triangular ($n<1$)	0.7	0.77	1.0	0.80
($n>1$)	0.4	1.05	0.8	1.05
sc	0.5	0.85	0.8	0.85
bcc	0.8	0.85	1.1	0.85
fcc ($n<1$)	1.2	0.80	1.8	0.76
($n>1$)	0.8	1.10	1.5	1.10

Figure 2 shows the critical temperature kT_c/t (hereafter denoted simply by T_c) for the simple cubic lattice, as a function of electron density n, for fixed values of βU, as obtained from the equation $\chi^{-1}=0$. Both the eighth- and fourth-order results, which are shown for comparison, indicate an increase in T_c with increasing U. This is as expected since increasing electron correlations will increase the stability of the ferromagnetic phase. The higher-order results, which are presumably more indicative of the true picture, give a substantially higher T_c. The sixth-order series do not give a consistent real positive zero. The trend of T_c increasing on going from fourth to eighth order is also seen for the other lattices. Table II gives the maximum T_c and the value of n at which this occurs, for $U=\infty$, for the standard lattices. Two other points should be noted. The observed T_c values for the two-dimensional lattices are lower than for the three-dimensional ones, indicating a lower stability for ferromagnetic order in the former case. (Of course, in reality, T_c should be zero here.) Second, for the fcc lattice, where the phase diagram is not symmetric about $n=1$, the critical temperature is higher in the region $n<1$, indicating greater stability for ferromagnetism below half-filling than above.

The equation $\chi^{-1}=0$ has a real positive solution for only a range of electron densities and we take this to define, at least approximately, the range of n for which a ferromagnetic phase is stable. Table III gives the range of stability, for several values of βU, for the standard lattices, as obtained from the eighth-order series. Increasing U leads to a larger range of stability, as one would intuitively expect.

TABLE III. Range of electron densities defining the region of ferromagnetic stability, obtained from eighth order, for the standard lattices and for several values of βU. The values are approximate only.

Lattice	$\beta U=10$	$\beta U=30$	$\beta U=\infty$
Square	0.90–1.10	0.90–1.10	0.85–1.15
Triangular	0.65–1.20	0.65–1.20	0.65–1.25
sc	0.85–1.15	0.80–1.20	0.75–1.25
bcc	0.85–1.15	0.80–1.20	0.80–1.20
fcc	0.70–1.20	0.68–1.25	0.66–1.25

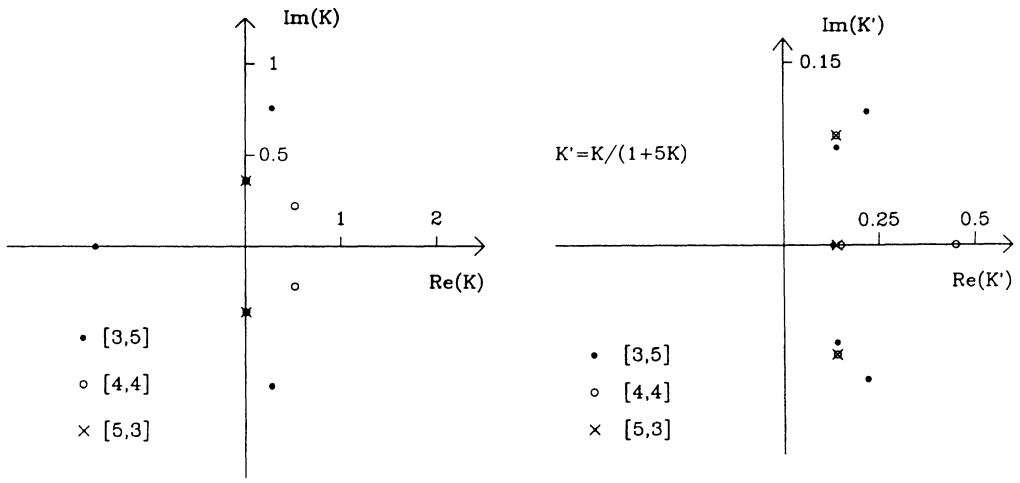

FIG. 3. Poles of Padé approximants to the series $(d/dK)\ln\chi(K)$ for the fcc lattice, for $n=0.8$ and $\beta U=30$: (a) direct series and (b) Euler-transformed series. The code indicates different Padé approximants.

For the fcc lattice we have also attempted to analyze the series using Padé approximants. In principle, this should provide a more reliable means of estimating the critical temperature. We discuss results for the case $n=0.8$, $\beta U=30$. In Fig. 3(a) we show the positions of poles for the [3,5], [4,4], and [5,3] Padé approximants to the logarithmic derivative $(d/dK)\ln\chi(K)$ $(K=\beta t)$. There is a very consistent pair of poles on the imaginary axis at $\pm 0.36i$, and these determine the radius of convergence of the series. There is no consistent pole on the positive real axis, which according to the χ^{-1} analysis might be expected to occur near $K\cong 1.5$. Presumably, this is completely masked by the closer complex singularities. In such situations transformations can sometimes be effectively used to move the physical singularity closer to the origin. In Fig. 3(b) we show the corresponding pole distribution for Padé approximants to the logarithmic derivative, after the Euler transformation $K'=K/(1+5K)$. There is now a consistent pole at $K'\cong 0.14$, which gives $K=0.47$. However, the nearby complex poles will have a marked effect on the accuracy of this estimate. In general, the Padé analysis supports the results obtained from the χ^{-1} analysis, but is not sufficiently precise to add substantially to that approach.

The χ^{-1} analysis, as shown in Fig. 2, yields estimates of T_c for fixed n and βU. These can be expressed in other ways, in particular as plots of T_c versus n for fixed t/U or as contours of fixed T_c in the plane $(n,t/U)$. We have chosen this latter representation to present the most complete overall picture of the results from eighth-order series for both the sc and fcc lattices. These are shown in Figs. 4 and 5.

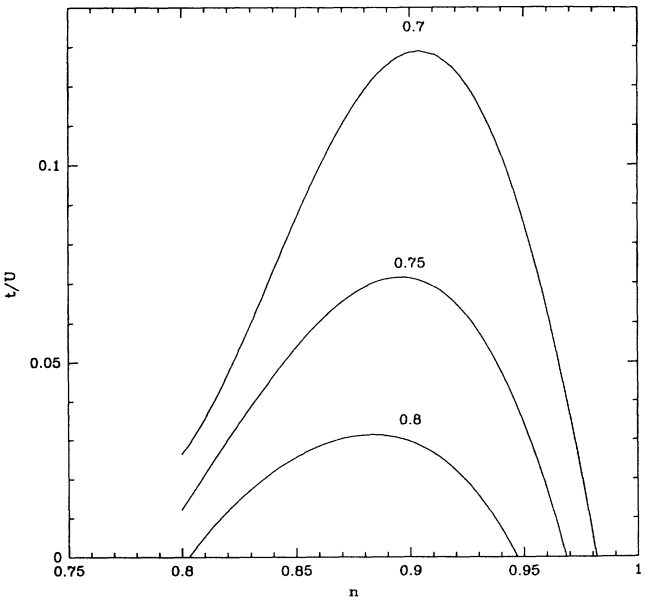

FIG. 4. Phase diagram for sc lattice from eighth-order χ^{-1} series. The curves are contour lines of constant T_c at the values shown.

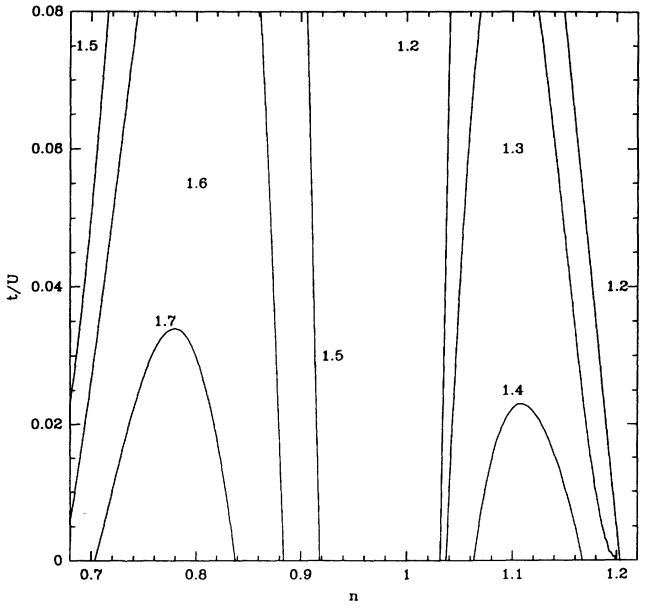

FIG. 5. Phase diagram for fcc lattice from eighth-order χ^{-1} series. The curves are contour lines of constant T_c at the values shown. Note the asymmetry about $n=1$.

IV. DISCUSSION AND CONCLUSIONS

We have developed high-temperature expansions for the free energy and ferromagnetic susceptibility of the single-band Hubbard model for general values of the electron density n and correlation energy U. Series have been obtained to ninth order in (βt) for all of the standard lattices. This extends previous work of many authors.

As has been remarked previously,[7,10] the series are quite erratic and difficult to analyze with any degree of precision. In common with previous workers, we have used the condition $\chi^{-1}=0$ to estimate the transition temperature, reflecting an instability to a ferromagnetic phase. We believe that this is qualitatively reasonable, although clearly not quantitatively accurate. The new higher-order series (eighth order) give in general higher estimates of T_c than previous (fourth order) analysis. This suggests that ferromagnetism at finite temperatures exists over a substantial region of the $(U/t,n)$ phase diagram of the three-dimensional Hubbard model.

We have made substantial progress toward obtaining the tenth-order term for loose-packed lattices, and it would certainly be feasible with our method to also extend the close-packed series to tenth order. For the strongly correlated case $(U=\infty)$, the computational effort is much less and these series could be carried to 12th order at least. The expansion for the antiferromagnetic susceptibility could also be extended beyond the known sixth-order result.[9] The same technique could also be used for more complex Hamiltonians, such as the extended Hubbard model. Some of these directions are being pursued.

When this paper had been essentially completed, we received a report which addresses, to a considerable degree, the same problem as we have studied. ten Haaf and van Leeuwen[16] have obtained series for the free energy to eighth order for the general case by a method very similar to ours. We have compared our results with their Table 4a and find complete agreement. They have considered only the square and simple cubic lattices and have not obtained the susceptibility series as such, and so in this sense our results are more extensive. Instead, they have looked at the nearest-neighbor spin-correlation function and have used the sign of this as an indicator of a tendency toward ferromagnetic or antiferromagnetic order. Our overall conclusions are consistent with theirs.

Note added in proof. We have completed the calculation of the tenth-order coefficients for the loose-packed lattices. Analysis of the extended series, together with that for close-packed lattices, which we hope to complete soon, will be reported elsewhere.

ACKNOWLEDGMENTS

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APPENDIX A

We describe here some of the technical details in obtaining the contribution of any particular diagram G to the free-energy expansion (7). To be specific consider the contribution of the diagram $\wedge$ to order 4:

$$X_4(\wedge)=\frac{1}{Z_0}\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2\int_0^{\tau_2}d\tau_3\int_0^{\tau_3}d\tau_4\,\mathrm{Tr}\{e^{-\beta\mathcal{H}_0}\tilde{V}(\tau_1)\tilde{V}(\tau_2)\tilde{V}(\tau_3)\tilde{V}(\tau_4)\}\ .$$

Now the trace can be written as a sum over states

$$\mathrm{Tr}\{\ \}=\sum_{ijkl}e^{i\beta E_i}e^{\tau_1(E_i-E_j)}e^{\tau_2(E_j-E_k)}\times e^{\tau_3(E_k-E_l)}e^{\tau_4(E_l-E_i)}V_{ij}V_{jk}V_{kl}V_{li}\ ,$$

where the E_i's are unperturbed energies. Note that, since the hopping term conserves electron number and electron spin, the energy differences which appear in the exponentials are always $0,\pm U$.

The computation then proceeds in the following steps.

(i) The states and unperturbed energies are enumerated. There are 4^v states (v = number of vertices in the diagram), and these are conveniently represented as $2v$-bit binary integers.

(ii) The matrix elements V_{ij} are computed and stored. This is done by keeping, for each initial state, a list of all possible final states together with the matrix element (± 1) and the bond of the diagram which corresponds to the particular electron transfer.

(iii) The multiple sum is then evaluated with the constraint that the system return to the initial state and that all bonds of the diagram be used. The terms are grouped according to the powers of $\tau_1,\tau_2,\ldots$.

(iv) The multiple integrals are evaluated using an efficient computer routine.

(v) Finally, the terms are grouped according to powers of the variables x, y, ω, and $(\beta U)^{-1}$ to give a contribution of the form

$$(\beta t)^{\text{order}}z_0^{-v}\sum_k C_k x^{n_1}y^{n_2}(\beta U)^{-n_3}w^{n_4}\ ,$$

where the variables are as defined in the text.

Various tricks are used to speed up the program, but the essential steps are as described above.

APPENDIX B

Coefficients f_{rpml} in the expansion of the free energy for the sc lattice to order $r=6$ with $y=1$ [see Eq. (10)].

p	m	l	$f_{2pml}(1)$
1	2	0	12
1	2	1	-12
2	1	0	6
2	3	1	6

p	m	l	$f_{4pml}(1)$
1	2	0	60
1	6	2	60
1	2	1	-60
1	4	2	120
1	4	1	-120
1	6	3	-60
2	2	0	-144
2	4	1	144
2	4	0	72
2	6	2	-144
2	2	1	84
2	4	2	-96
2	6	3	84
3	2	0	114
3	3	0	-108
3	3	1	108
3	4	1	-228
3	5	2	108
3	5	1	-108
3	6	2	114
4	1	0	15/2
4	2	0	-52
4	3	1	33/2
4	3	0	24
4	4	1	-88
4	5	2	33/2
4	5	1	24
4	6	2	-52
4	7	3	15/2

p	m	l	$f_{6pml}(1)$
1	2	0	912
1	2	1	-912
1	3	0	6624
1	3	1	-6624
1	4	0	35664
1	4	1	-37728
1	4	2	2064
1	5	0	48000
1	5	1	-6624
1	5	2	-41376
1	6	0	13920
1	6	1	78912
1	6	2	-76608
1	6	3	-16224
1	7	1	48000
1	7	2	-6624
1	7	3	-41376
1	8	2	35664
1	8	3	-37728
1	8	4	2064
1	9	3	6624
1	9	4	-6624
1	10	4	912
1	10	5	-912
2	2	0	-1920
2	3	0	-600
2	3	1	-6024
2	4	0	-13536
2	4	1	-14112
2	5	0	-21648
2	5	1	-52104
2	5	2	-15624
2	6	1	-64320
2	6	2	-59328
2	7	1	-21648
2	7	2	-52104
2	7	3	-15624
2	8	2	-13536
2	8	3	-14112
2	9	3	-600
2	9	4	-6024
2	10	4	-1920
2	4	2	-5952

p	m	l	$f_{6pml}(1)$
2	6	0	-4608
2	6	3	5280
2	8	4	-5952
2	2	1	1008
2	10	5	1008
3	2	0	1896
3	3	0	-4784
3	3	1	2072
3	4	0	-456
3	4	1	-13112
3	5	0	2224
3	5	1	4784
3	5	2	-4296
3	6	1	9232
3	6	2	14112
3	7	1	2224
3	7	2	4784
3	7	3	-4296
3	8	2	-456
3	8	3	-13112
3	9	3	-4784
3	9	4	2072
3	10	4	1896
3	6	0	192
3	6	3	-3904
3	4	2	2288
3	8	4	2288
3	2	1	-432
3	10	5	-432
4	2	0	-1088
4	3	0	5220
4	3	1	-1240
4	4	0	-2312
4	4	1	9200
4	5	0	-828
4	5	1	-2364
4	5	2	412
4	6	1	5824
4	6	2	-15024
4	7	1	-828
4	7	2	-2364
4	7	3	412
4	8	2	-2312

p	m	l	$f_{6pml}(1)$
4	8	3	9200
4	9	3	5220
4	9	4	-1240
4	10	4	-1088
5	2	0	422
5	3	0	-3214
5	3	1	210
5	4	0	3426
5	4	1	-2338
5	5	0	-422
5	5	1	3214
5	6	1	436
5	7	1	-422
5	7	2	3214
5	8	2	3426
5	8	3	-2338
5	9	3	-3214
5	9	4	210
5	10	4	422
5	6	2	-3456
5	5	2	212
5	7	3	212
6	1	0	155/30
6	2	0	-3374/15
6	3	0	14512/15
6	4	0	-10118/15
6	5	0	143/3
6	7	1	143/3
6	8	2	-10118/15
6	9	3	14512/15
6	10	4	-3374/15
6	11	5	155/30
6	4	1	-9092/15
6	5	1	32918/15
6	6	1	-16704/15
6	7	2	32918/15
6	8	3	-9092/15
6	3	1	485/30
6	5	2	79/3
6	6	2	-12008/15
6	7	3	79/3
6	9	4	485/30

Coefficients f_{rpml} in the expansion of the free energy for the fcc lattice to order $r=6$ with $y=1$ [see Eq. (10)].

p	m	l	$f_{2pml}(1)$
1	2	0	24
1	2	1	-24
2	1	0	12
2	3	1	12

p	m	l	$f_{3pml}(1)$
1	2	0	-96
1	2	1	96
1	4	1	96
1	4	2	-96
2	2	0	96
2	4	1	-96
3	1	0	16
3	2	0	-16
3	4	1	16
3	5	2	-16

p	m	l	$f_{4pml}(1)$
1	2	0	696
1	3	0	144
1	4	0	144
1	5	1	144
1	6	2	696
1	2	1	-696
1	3	1	-144
1	4	2	1248
1	4	1	-1392
1	5	2	-144
1	6	3	-696
2	2	0	-1008
2	3	0	-72
2	4	1	1440
2	4	0	144
2	5	1	-72
2	6	2	-1008
2	2	1	312
2	3	1	-72
2	4	2	-480
2	5	2	-72
2	6	3	312
3	2	0	660
3	3	0	-576

p	m	l	$f_{4pml}(1)$
3	3	1	576
3	4	1	-1320
3	5	2	576
3	5	1	-576
3	6	2	660
4	1	0	45
4	2	0	-272
4	3	1	69
4	3	0	114
4	4	1	-368
4	5	2	69
4	5	1	114
4	6	2	-272
4	7	3	45

p	m	l	$f_{5pml}(1)$
1	2	0	5760
1	3	0	-480
1	4	1	-17280
1	4	0	-480
1	6	2	17280
1	2	1	-5760
1	3	1	480
1	4	2	17760
1	6	3	-17760
1	6	1	480
1	7	2	480
1	8	3	-5760
1	7	3	-480
1	8	4	5760
2	2	0	-8640
2	3	0	4800
2	4	1	20064
2	4	0	7968
2	6	2	-20064
2	2	1	2880
2	3	1	-4320
2	4	2	-9792
2	6	3	9792
2	6	1	-7968
2	7	2	-4800
2	8	3	8640
2	7	3	4320

p	m	l	$f_{5pml}(1)$
2	8	4	-2880
3	2	0	5760
3	3	0	-7776
3	4	1	-28272
3	4	0	1872
3	6	2	28272
3	6	1	-1872
3	7	2	7776
3	8	3	-5760
3	3	1	3216
3	7	3	-3216
4	2	0	-2400
4	3	0	7168
4	4	1	4432
4	4	0	-2352
4	6	2	-4432
4	6	1	2352
4	7	2	-7168
4	8	3	2400
4	3	1	-1712
4	7	3	1712
5	1	0	-72
5	2	0	1152
5	3	1	-88
5	3	0	-1524
5	4	1	844
5	4	0	204
5	6	2	-844
5	6	1	-204
5	7	2	1524
5	8	3	-1152
5	7	3	88
5	9	4	72

p	m	l	$f_{6pml}(1)$
1	2	0	54624
1	3	0	45216
1	4	1	-510432
1	4	0	284112
1	5	1	-74400
1	6	2	-328608
1	5	0	386304
1	6	1	642816
1	7	2	-74400
1	8	3	-510432
1	6	0	101664
1	7	1	386304
1	8	2	284112
1	9	3	45216
1	10	4	54624
1	2	1	-54624
1	3	1	-45216
1	4	2	226320
1	5	2	-311904
1	6	3	-415872
1	7	3	-311904
1	8	4	226320
1	9	4	-45216
1	10	5	-54624
2	2	0	-84960
2	3	0	63192
2	4	1	95520
2	4	0	-6240
2	5	1	-495096
2	6	2	-729216
2	5	0	-175344
2	6	1	-739392
2	7	2	-495096
2	8	3	95520
2	6	0	-32256
2	7	1	-175344
2	8	2	-6240
2	9	3	63192
2	10	4	-84960
2	2	1	30336
2	3	1	-108408
2	4	2	-147072
2	5	2	-27768
2	6	3	238848
2	7	3	-27768
2	8	4	-147072
2	9	4	-108408
2	10	5	30336
3	2	0	60592
3	3	0	-127152
3	4	1	-412136
3	4	0	-4360
3	5	1	139952
3	6	2	659376
3	5	0	23120
3	6	1	103632
3	7	2	139952
3	8	3	-412136
3	6	0	-1152
3	7	1	23120
3	8	2	-4360
3	9	3	-127152
3	10	4	60592
3	2	1	-2944
3	3	1	41352
3	4	2	20448
3	5	2	-52696
3	6	3	-35904
3	7	3	-52696
3	8	4	20448
3	9	4	41352
3	10	5	-2944
4	2	0	-27216
4	3	0	108884
4	4	1	165296
4	4	0	-73464
4	5	1	-122876
4	6	2	-282736
4	5	0	3420
4	6	1	148288
4	7	2	-122876
4	8	3	165296
4	3	1	-20864
4	5	2	28828
4	7	3	28828
4	9	4	-20864
4	7	1	3420
4	8	2	-73464
4	9	3	108884
4	10	4	-27216
5	2	0	8804
5	3	0	-61946
5	4	1	-42598
5	4	0	63278
5	5	1	66970
5	6	2	-42116
5	5	0	-7306
5	6	1	-8916
5	7	2	66970
5	8	3	-42598
5	3	1	4222
5	5	2	2028
5	7	3	2028
5	9	4	4222
5	7	1	-7306
5	8	2	63278
5	9	3	-61946
5	10	4	8804
6	1	0	352/3
6	2	0	-68348/15
6	3	1	3319/15
6	3	0	249974/15
6	4	1	-32852/5
6	5	2	1194/5
6	4	0	-149018/15
6	5	1	315988/15
6	6	2	-85636/15
6	7	3	1194/5
6	5	0	9509/15
6	6	1	-150656/15
6	7	2	315988/15
6	8	3	-32852/5
6	9	4	3319/15
6	7	1	9509/15
6	8	2	-149018/15
6	9	3	249974/15
6	10	4	-68348/15
6	11	5	352/3

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