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Ferromagnetism in the Single-Band Hubbard Model: An Exact High-Temperature Expansion

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The first ten terms of the high-temperature expansion of the susceptibility of the single-band Hubbard model in the strong correlation limit are obtained for arbitrary electron density. The series is analyzed by ratio methods and Padé approximants. A critical temperature is found for $0.2 \leqslant \rho \leqslant 0.8$; for $\rho > 1$ further terms in the series are required.

KEY WORDS: Hubbard model; ferromagnetism; high-temperature expansion; phase transition.

1. INTRODUCTION

The single-band Hubbard model[1] has been the subject of many theories and speculations both in the context of metal–insulator phase transitions and of the magnetism found in the 3*d* transition metals. Few exact results exist. Lieb and Wu[2] found the ground-state energy exactly in one dimension for one electron per atom and Shiba[3] has extended their solution to arbitrary electron concentration and has also calculated the zero-temperature susceptibility. In three dimensions the only exact result is Nagaoka's[4] proof that in the strong correlation limit for $n = N - 1$ the ground state is ferromagnetic in the simple cubic and body-centered cubic lattices and nonferromagnetic

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in the face-centered cubic and hexagonal close-packed lattices. He also showed that for $n = N + 1$ all four lattices have a ferromagnetic ground state. Here N is the number of lattice sites, n the number of electrons.

The question remains whether for macroscopic deviations from the half-filled lattice magnetic ordering can occur. Some authors[5] have conjectured that ferromagnetism can only exist in the presence of orbital degeneracy. Several approximate theories,[6–9],[2] on the other hand, do predict ferromagnetism in the single-band model at least for some range of electron density. Recently Fukuyama and Ehrenreich[11] have shown that in the coherent potential approximation the susceptibility at $T = 0$ is nonsingular for any electron density. We remark that this question of the existence of ferromagnetism in the absence of Hund's rule coupling is of more than academic interest. Kanamori,[6] for example, argues that a model of non-interacting d bands is appropriate for nickel.[3]

In this paper we apply the method of exact high-temperature expansions to the single-band Hubbard model on the fcc lattice in the limit $U \to \infty$ and present evidence that for $0.2 \leqslant \rho \leqslant 0.8$ the susceptibility diverges at a non-zero critical temperature. High-temperature expansions have been carried out in one dimension for this model by Beni *et al.*[13] These authors also obtained the first two significant terms for the simple cubic lattice. In Section 2 the high-temperature expansions for the quantities of interest are developed. The analysis of the series is presented in Section 3. Section 4 contains a discussion of this work.

2. THEORY OF THE HIGH-TEMPERATURE EXPANSION

The method we use to derive the expansion is a modification of the method of Betts *et al.*[14],[4] for the high-temperature expansion of the XY model partition function and we shall closely follow their notation and terminology.

The Hubbard model has the Hamiltonian

$$\mathscr{H} = -\tfrac{1}{2} \sum_{i,j,\sigma} t_{ij}(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - h \sum_{i} m_i \tag{1}$$

where $t_{ij} = t > 0$ for i, j nearest-neighbor lattice sites and zero otherwise. The c and $c^{\dagger}$ are electron annihilation and creation operators, $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, $m_i = n_{i\uparrow} - n_{i\downarrow}$, and we specify that the number of electrons $\sum_{i,\sigma} n_{i\sigma} = n < N$, where N is the number of sites in the lattice. In the strong correlation limit $U/kT \to \infty$ we need only consider the subspace of at most singly

[2] See Ref. 10 for a critical review of various approximate techniques.

[3] Also see Ref. 12 for a discussion of Hund's rule in nickel.

[4] Also see Ref. 15 for a review of series expansion results on the XY model.

occupied sites and henceforth neglect the interaction term. We note that in this limit the Hubbard model is similar to the XY model; instead of a hard-core Bose lattice gas we have a hard-core Fermi lattice gas. For this reason the method of Betts *et al.*[14] is an appropriate starting point. Since the XY model considered by these authors represents a half-filled lattice—a somewhat simpler situation than a lattice at arbitrary density—a generalization of the procedure is necessary.

The grand partition function of the system is given by

$$\Xi_N(\beta, z, h) = \sum_{n=0} z^n \operatorname{tr}_{\{n\}} e^{-\beta \mathscr{H}_0} \tag{2}$$

where $\mathscr{H}_0$ is the Hamiltonian (1) without the interaction term and $\operatorname{tr}_{\{n\}}$ indicates a trace over all n particle states with double occupancy of any site excluded. In the limits $|\beta \mathscr{H}_0| \ll 1$, $N \to \infty$,

$$\lim_{N\to\infty} (1/N) \log \Xi_N(\beta, z, h) = \log(1 + 2z) + \lim_{N\to\infty} (1/N) \sum_{j=1}^{\infty} (-\beta)^j \langle \mathscr{H}_0^j \rangle / j! \tag{3}$$

where

$$\langle \mathscr{H}_0^j \rangle = (1 + 2z)^{-N} \sum_{n=1}^{N} z^n \operatorname{tr}_{\{n\}} \mathscr{H}_0^j \tag{4}$$

From the partition function (3) all thermodynamic functions may be obtained. In particular the density ρ is given by

$$\rho = \lim_{N\to\infty} (1/N) z(\partial/\partial z) \log \Xi \tag{5}$$

Instead of evaluating the partition function series in a finite magnetic field and differentiating, we obtain the zero-field susceptibility $\chi(\beta, z)$ per atom from a separate series,

$$\chi(\beta, z) = \beta\left(\rho + \lim_{N\to\infty} 2/N \sum_{i>j} \sum_{l=0}^{\infty} \frac{(-\beta)^l}{l!} \langle \mathscr{H}_0^l m_i m_j \rangle\right) \tag{6}$$

To eliminate the fugacity z from Eq. (6), we use relation (5) and series (3) to obtain a high-temperature series for $z(\beta, \rho)$ which is substituted into (6), thus yielding a series $\chi(\beta, \rho)$. Our task is therefore to evaluate $\langle \mathscr{H}_0^l \rangle$ and $\langle \mathscr{H}_0^l m_i m_j \rangle$.

The general term in $\mathscr{H}_0^l$ is of the form $\prod t_{ij} c_{i\sigma_i}^\dagger c_{j\sigma_i}$. Each factor $t_{ij} c_{i\sigma_i}^\dagger c_{j\sigma_i}$ is graphically represented by an arrow from site j to site i labeled with the spin direction σ_i. The trace of the product depends on the order of the operators, which is specified by an associated "time" variable, earliest time indicating that an operator is furthest to the right. To obtain the net contribution of a *shadow graph*,[14] i.e., the same set of arrows with their time

ordering neglected, we must sum over all time orderings consistent with the constraints (a) arrow heads and tails must alternate at every site, (b) a spin σ tail may not follow a $-\sigma$ head, (c) equal numbers of heads and tails of both spin types must exist at each vertex.

The shadow graphs appearing in this calculation are, except for spin labelings, the same as those appearing in the calculation of the partition function of the XY model. In performing the average (4) for a given time ordering, one associates with each site i appearing in the product a factor $p = z(1 + 2z)^{-1}$ if an annihilation operator $c_{i\uparrow}$, $c_{i\downarrow}$ appears to the right of the first creation operator $c_{i\uparrow}^{\dagger}$, $c_{i\downarrow}^{\dagger}$, and a factor $1 - 2p = (1 + 2z)^{-1}$ if a creation operator appears first. The sum over time orderings constitutes the *vertical weight*[14] $V(g, \{\sigma\})$ of the labeled shadow graph g, the notation indicating that the vertical weight depends on the spin labeling. We define the *spin weight* $W(g, \{\sigma\})$ as the number of equivalent spin labelings of the graph g and the horizontal weight $H(g)$ as the number of equivalent renumberings of the vertices of the unlabeled shadow graph g.[14] The corresponding bare graph g' is obtained by replacing all connections between sites i, j by a single line and its lattice constant $\mathcal{N}(g', L)$ is defined as the number of weak embeddings[16] of the graph g' in the lattice L. In terms of these quantities the partition function series is written

$$\lim_{N\to\infty} \frac{1}{N} \log \Xi = \log(1 + 2z) + \sum_{l=0}^{\infty} \frac{(-K)^l}{l!} \sum_{g'} \mathcal{N}(g', L) \sum_{g} H(g) \times \sum_{\sigma} W(g, \sigma) V(g, \sigma) \tag{7}$$

where $K = \beta t$. The susceptibility is calculated in the same way. The operators m_i and m_j are traceless and contribute only if they arise in combinations with other operators referring to site i. They act as decorations of the partition function graphs and change the vertical weight calculation only by the added constraint that a tail must occur at a decorated site before a head. In the evaluation of the trace, a factor ± 1 is associated with a decorated site depending on whether an up or down spin arrow occurs first.

We obtain series of the form

$$(1/N) \log \Xi(\beta, z, h = 0) = \log(1 + 2z) + p(1 - 2p) \sum_{j\geq 2} K^j \sum_{l=0}^{j-2} a_{jl} p^l \tag{8}$$

$$kT\chi(\beta, z) = \rho + p^2(1 - 2p) \sum_{j\geq 3} K^j \sum_{l=0}^{j-3} b_{jl} p^l \tag{9}$$

The numbers a_{jl}, b_{jl} are displayed in Table I up to $j = 6$ for a_{jl}, and to $j = 9$ for b_{jl}.

Table I[a]

	$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$	$l = 5$	$l = 6$
a_{2l}	12	—	—	—	—	—	—
a_{3l}	16	−16	—	—	—	—	—
a_{4l}	45	−276	486	—	—	—	—
a_{5l}	72	−720	2,100	−1,692	—	—	—
a_{6l}	$117\frac{1}{3}$	−2,405.6	14,907.6	−37,138	32,647	—	—
b_{3l}	32	—	—	—	—	—	—
b_{4l}	176	−220	—	—	—	—	—
b_{5l}	864	−3,048	3,328	—	—	—	—
b_{6l}	3,089.6	$-16{,}665\frac{1}{3}$	35,665.6	−27,332	—	—	—
b_{7l}	9,603.2	$-75{,}569\frac{1}{3}$	290,598.4	−541,198.4	376,826.4	—	—
b_{8l}	25,743.1427	−259,967.664	1,495,667.72	−4,531,333.93	6,589,117.49	−3,669,134.04	—
b_{9l}	61,786.3069	−760,897.4	6,576,156.88	−30,982,337.5	76,657,425.9	−95,627,516.5	47,687,748.3

[a] The coefficients M_l of the moment expansion of $[\omega - \mathscr{H}(-t)]^{-1}$ for a single hole in an otherwise half-filled band can be obtained from Table I by the prescription $M_l = l! \sum_{j=0}^{l-2} a_{lj} 2^{-j-1}$. We have found discrepancies of up to 7%, which we have not been able to resolve, between our moments and those tabulated by Sokoloff[8] for the fcc lattice for $l > 3$. Our procedure, adapted to the simple cubic lattice, does yield the same moments as those found by Brinkman and Rice.[17]

We evaluated the partition function series only to sixth order since we intend to use it only to eliminate the fugacity z in terms of the density ρ. This is achieved by using the relation (5), the series (8), and the ansatz $p = \rho/2 + \sum_{l=2}^{\infty} A_l(\rho)K^l$. We then obtain a high-temperature expansion of χ of the form

$$kT\chi = \rho + \rho^2(1 - \rho) \sum_{j \geq 3} B_j(\rho)K^j \tag{10}$$

in which each term is exact in the density variable ρ. The analysis of this series is discussed in the next section.

3. ANALYSIS OF THE SUSCEPTIBILITY SERIES

We analyzed the series (10) by ratio and Padé approximant methods.[5] While Padé approximants to $\chi^{1/\gamma}$, for various values of γ, were fairly well converged, the ratios B_{n+1}/B_n of successive terms in the series showed marked irregularities. Examination of the poles of Padé approximants to $(d/dK) \log \chi(K, \rho)$ showed the consistent appearance of a pair of poles almost on the imaginary axis at a comparable distance from the origin as the physical singularity. We tried transformations of the form

$$K = \alpha\bar{K}/(1 - \beta\bar{K}^2) \tag{11}$$

which have the effect of stretching the imaginary axis and contracting the real axis. Transformations of this type have been successfully applied to the two-dimensional XY model by Betts *et al.*[19] We found that the transformation (11) for $\alpha = 0.75$ and $\beta = 0.65$ had a smoothing effect on the series. In Fig. 1 the ratio $\bar{B}_n/\bar{B}_{n-1}$ of the transformed series is plotted against $1/n$ for several densities. Extrapolating to $1/n = 0$ yields an estimate of the critical temperature $\bar{K}_c^{-1}$. It can be seen that for $\rho = 0.4, 0.55, 0.65$ (curves B, C, D) the ratios seem to have settled down and may readily be extrapolated to $1/n = 0$. Curve A ($\rho = 0.25$) is noisier but we still expect a finite intercept. In all cases the results of series extrapolation are consistent with Padé analysis of both the transformed and untransformed series.

Table II lists real poles of Padé approximants to $\chi(\bar{K}, \rho)$ for $\rho = 0.5$. An entry "c" indicates that only complex poles exist. In our opinion the entries are converged well enough to indicate the existence of a critical point but not well enough to allow better than two figure determination of its location $\bar{K}_c$. As Hunter and Baker[18] have pointed out, functions for which ratio methods are more accurate than Padé approximants for a given number of terms in the expansion can easily be constructed. We believe χ to be such a function.

[5] See Ref. 18 for a review of methods of series analysis.

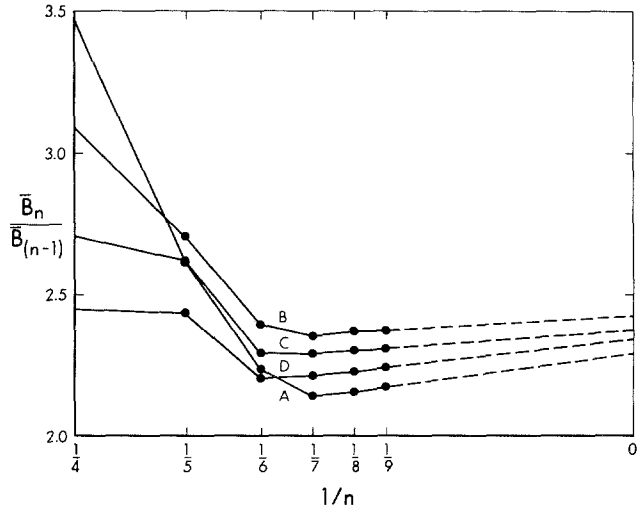

Fig. 1. Plot of ratios of terms in the transformed susceptibility series $\bar{B}_n/\bar{B}_{n-1}$ as function of $1/n$. (A) $\rho = 0.25$, (B) $\rho = 0.4$, (C) $\rho = 0.55$, (D) $\rho = 0.65$. The dashed lines show extrapolation to $1/n = 0$.

For densities $\rho < 0.2$ and $\rho > 0.75$ the series is very noisy and it is difficult to extract information. We conjecture that the critical densities below and above which ferromagnetism does not exist are in the vicinity or $\rho = 0.15$ and $\rho = 0.8$. This result is consistent with the exact proof of Nagaoka[4] that for $n = N - 1$ the ferromagnetic state is not the ground state.

Figure 2 shows a plot of kT_c/t as function of ρ as determined by the ratio method. In all cases Padé approximants to $\chi(\bar{K}, \rho)$ yield a figure within 5% of the point plotted in the figure.

Table II

N/D	0	1	2	3	4	5	6	7	8
1					0.383	0.432	0.433	0.430	0.427
2				0.402	c	0.433	0.432	0.425	
3			0.369	0.492	0.445	0.429	0.427		
4		0.366	c	0.443	0.411	0.427			
5	0.603	0.414	0.424	0.428	0.427				
6	0.544	0.422	0.430	0.427					
7	0.510	0.426	0.427						
8	0.489	0.427							
9	0.475								

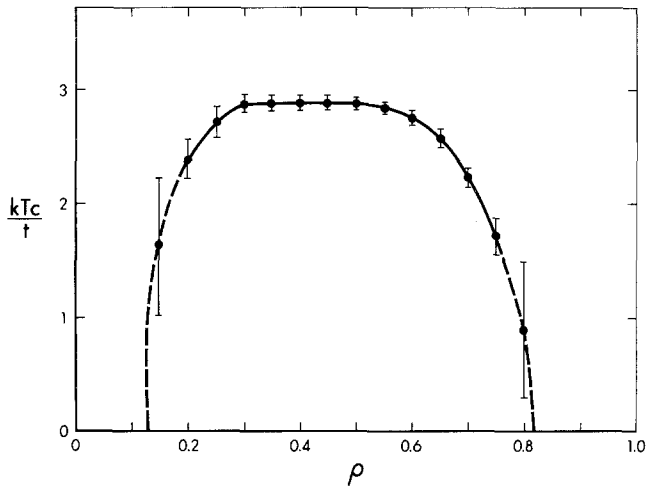

Fig. 2. Plot of the critical temperature kT_c/t as function of the density ρ. The dashed lines represent a crude estimate in a region in which the series is quite noisy.

We have also attempted to determine the critical exponent γ of the susceptibility. Padé approximants to $(d/d\bar{K}) \log \chi(\bar{K}, \rho)$ tielded $\gamma \simeq 1$ with very poor convergence. Plots of the location of real poles of Padé approximants to $(1/\bar{K}^2)(d/d\bar{K})\chi(\bar{K})^{1/\gamma+1}$ and to $\chi^{1/\gamma}$ had the highest density of intersections for $\gamma \simeq 2/3$, again with poor convergence. As in the determination of the critical point, we favor the ratio method for determination of γ. The slope of ratio plots $\bar{B}_n/\bar{B}_{n-1}$ as function of $1/n$ yields a value $\gamma \simeq 1.5$ for ρ close to 0.5. This value of γ is the one closest to results on other magnetic models, but more terms in the series will be required before one can have any confidence in the result.

Finally we note that the series for $\rho > 1$ can be generated from our series on this lattice by letting $t \to -t$. The density ρ then corresponds to density of holes, i.e., $2 - \rho$ electrons per atom. Nagaoka[4] has shown that for $n = N + 1$ the ground state is ferromagnetic and we have attempted to analyze our series in this region. While for $\rho < 1$ the terms $B_j(\rho)$ are generally all positive, they alternate in sign for $\rho > 1$. Morevoer, the first nontrivial coefficient B_3 is negative. Since we expect a positive divergence of χ at the Curie point, this negative term effectively shortens the series. Neither ratio methods nor Padé approximants to both the original series and series obtained by various transformations yielded a critical point. We conjecture that on this lattice the critical temperature for $n > N$, if finite, is substantially lower than for $n < N$.

4. DISCUSSION

We believe that we have presented strong evidence for the existence of ferromagnetism in the Hubbard model even in the absence of Hund's rule coupling and orbital degeneracy. As noted earlier, this model may be appropriate for nickel. While different estimates of the critical temperature are consistent, it seems that more terms in the series are required for a determination of the critical exponent γ.

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REFERENCES

1. J. Hubbard, *Proc. Roy. Soc. A* **276**:238 (1963); **277**:237 (1964); **281**:401 (1964).
2. E. Lieb and F. Wu, *Phys. Rev. Letters* **20**:1445 (1968).
3. H. Shiba, *Phys. Rev. B* **6**:930 (1972).
4. Y. Nagaoka, *Phys. Rev.* **147**:392 (1966).
5. J. H. Van Vleck, *Nuovo Cimento (Suppl.)* **6**:886 (1957); M. C. Gutzwiller, *Phys. Rev. Letters* **10**:159 (1963).
6. J. Kanamori, *Progr. Theoret. Phys. (Kyoto)* **30**:275 (1963).
7. D. R. Penn, *Phys. Rev.* **142**:350 (1966).
8. J. Sokoloff, *Phys. Rev. B* **2**:3707 (1970); **3**:3826 (1971).
9. L. M. Roth, *Phys. Rev. Letters* **20**:1431 (1968).
10. D. M. Esterling and H. C. Dubin, *Phys. Rev. B* **6**:4276 (1972).
11. H. Fukuyama and H. Ehrenreich, *Phys. Rev. B* **7**:3266 (1973).
12. C. Herring, in *Magnetism*, Vol. IV, G. T. Rado and H. Suhl, eds., Academic Press, New York (1966), Chapters 9, 10.
13. G. Beni, P. Pincus, and D. Hone, *Phys. Rev. B* **8**:3389 (1973).
14. D. D. Betts, C. J. Elliott, and M. H. Lee, *Can. J. Phys.* **48**:1556 (1970).
15. D. D. Betts, in *Phase Transitions and Critical Phenomena*, Vol. III, C. Domb and M. S. Green, eds., Academic Press, London, in press.
16. M. F. Sykes, J. W. Essam, B. R. Heap, and B. J. Hiley, *J. Math. Phys.* **7**:1557 (1966).
17. W. F. Brinkman and T. M. Rice, *Phys. Rev. B* **2**:1324 (1970).
18. D. L. Hunter and G. A. Baker, *Phys. Rev. B* **7**:3346 (1973).
19. D. D. Betts, C. J. Elliott, and R. V. Ditzian, *Can. J. Phys.* **49**:1327 (1971).