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Critical Study of the Static Functional Integral Method in the Hubbard Model

By

B. LORENZ and H. FEHSKE

The effect of the static approximation in the functional integral representation of the paramagnetic Hubbard model is critically investigated. The exactly solvable two-site model is treated within the one- and two-field static functional integral method and some thermodynamic properties (local magnetic moment, specific heat c_v) are compared with the exact solution for various interaction strengths and electron densities. It is shown that the static functional integral theory yields unphysical results for c_v in the strong interacting system at small densities. The two-field and one-field methods are preferable in the low- and high-temperature regions, respectively.

Der Einfluß der statischen Näherung in der Funktionalintegraldarstellung des paramagnetischen Hubbardmodells wird kritisch untersucht. Das exakt lösbare Zweiplatzmodell wird mit der Ein- und Zweifeldmethode behandelt und einige thermodynamische Eigenschaften (lokales magnetisches Moment, spezifische Wärme c_v) werden für verschiedene Werte der Wechselwirkung und der Elektronendichte mit der exakten Lösung verglichen. Im Bereich großer Wechselwirkung und kleiner Teilchendichten liefert die statische Näherung falsche und unphysikalische Ergebnisse für c_v . Die Zweifeldmethode ist bei tiefen und die Einfeldmethode bei hohen Temperaturen geeigneter.

1. Introduction

In recent years the magnetic properties of transition metals and alloys have attracted increasing attention. Despite much experimental and theoretical work a current understanding of itinerant magnetism has not been achieved. Neither the conventional Stoner theory nor the localized spin models yield a satisfactory description of the magnetic behaviour of these materials. The non-integral value (in units of μ_B) of the ground state magnetization, the Curie-Weiss behaviour of the paramagnetic spin susceptibility, and the temperature dependence of the magnetization observed in the transition metals are characteristic features of both localized and band magnetism.

As the theoretical basis for an interpolating description the Hubbard model [1] in its functional integral (FI) representation is frequently used [2 to 6]. These spin fluctuation theories have provided a fairly accurate description of itinerant magnetic phenomena. Methodically, the Hubbard-Stratonovich transformation is used to linearize the interaction and to express the partition function of the Hubbard model by a functional integral over time-dependent auxiliary fields. The FI is evaluated within various approximations. In the static approximation it is reduced to an ordinary integral which is treated by further approximations, e.g. the saddle point approximation [2], the self-consistent single-site approximation [3], etc.

Unfortunately, the FI representation of the Hubbard Hamiltonian depends on the number and kinds of auxiliary fields introduced by the Hubbard-Stratonovich transformation. Usually, local charge and spin fields connected with the charge density

¹⁾ Karl-Marx-Platz, DDR-7010 Leipzig, GDR.

operator $n_{i\uparrow} + n_{i\downarrow}$ and the spin density operator $n_{i\uparrow} - n_{i\downarrow}$, respectively, are used in the two-field method. However, with the identity for Fermi operators $n_{i\sigma}^2 = n_{i\sigma}$ the FI can be expressed by only one field per site (charge or spin field). This one-field method yields a simpler expression for the partition function [7]. In an exact FI representation both methods are equivalent but evaluating the FI approximately different results can be obtained. Until now the effects of the various approximations, especially that of the static one, have not been investigated very thoroughly. For the Anderson model of a magnetic impurity it has been shown that there may arise considerable errors due to the violation of the Pauli principle in the static approximation [8]. Furthermore, in this model the two-field static FI scheme is superior to the one-field methods since it represents the first corrections to some exactly solvable limits rigorously [8]. A similar statement is obtained for the Anderson model treated in the static and saddle point approximations [9] where the Hartree-Fock result is reproduced by the two-field method only.

In order to investigate the effect of the static approach in the FI theory of the Hubbard model the evaluation of exactly solvable problems is of particular interest. Therefore, we consider the two-site Hubbard model for various electron densities. In the next section the two-site problem is treated rigorously and in the static FI theory using the one- and two-field methods. The results for some thermodynamic functions are given in Section 3 and compared with the exact solution. The main conclusions are presented in Section 4.

2. Two-Site Hubbard Model

The two-site Hamiltonian is written as

$$H = H^{(0)} + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}),$$

$$H^{(0)} = -t \sum_{\sigma} (c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma}) - \left(\mu + \frac{U}{2}\right) \sum_{\sigma} (n_{1\sigma} + n_{2\sigma}). \quad (1)$$

$n_{i\sigma}$ is the occupation number operator for an electron at the site i with spin projection σ , U is the intraatomic Coulomb integral, and $H^{(0)}$ describes the hopping of electrons between the two sites with the overlap parameter t . Since we are working in the grand-canonical ensemble the chemical potential μ is introduced in order to fix the mean electron density per site n . It is convenient to shift the chemical potential by the constant $U/2$. Hence, for $n = 1$ we have $\mu = 0$.

The exact solution and the thermodynamic properties of (1) are discussed in [10, 11]. In the FI formalism the two-site model has the advantage that it can be treated in the static approach without applying additional approximations. Hence, in contrast to the infinite model we are able to investigate the effect of the static approximation separately. If the results of this paper should be relevant also for the infinite Hubbard model, we have to consider those physical quantities which are qualitatively insensitive to the size of the system. Since there is no magnetic long-range order in a finite lattice we restrict our discussion to the behaviour in the paramagnetic phase. The approximate treatment of finite and infinite Hubbard chains for $n = 1$ has shown that some thermodynamic functions, e.g. the specific heat, the entropy, the local magnetic moment, etc. of the model (1) are very similar to those of the infinite system [10 to 13]. The local magnetic moment $L_0 = \frac{3}{4} \langle (n_{i\uparrow} - n_{i\downarrow})^2 \rangle$ of (1) shows the same qualitative temperature dependence as that of a large lattice. Hirsch [14] has found only a weak size dependence of L_0 in two dimensions. Furthermore, some available limits ($t=0$ or $U=0$) for L_0 in the infinite model are reproduced by the model (1) [11]. The specific heat of (1) shows the temperature dependence which is characteristic of the infinite

lattice. Especially, at larger U -values there appears a typical low-temperature peak due to the destruction of magnetic short-range order which is known for the infinite model to be an effect of the hopping-induced effective Heisenberg interaction. Therefore, we investigate the local magnetic moment and the specific heat of (1) in the static FI approach and compare the results with the exact solution.

2.1 Exact solution

The grand partition function of (1) is expressed as

$$Z = 1 + (x + x^3) S_1 + x^2 S_2 + x^4, \tag{2}$$

with

$$S_1 = 4e^{\beta U/2} \cosh \{ \beta t \}, \quad x = e^{\beta \mu},$$

$$S_2 = 1 + 3e^{\beta U} + 2e^{\beta U/2} \cosh \left\{ \frac{1}{2} \beta \sqrt{U^2 + 16t^2} \right\}.$$

$\beta = 1/k_B T$ is the inverse temperature.

The chemical potential μ is determined by the condition

$$\frac{\partial}{\partial \mu} \left(- \frac{1}{\beta} \ln Z \right) = 2n, \tag{3}$$

from which we get the equation of fourth degree

$$x^4(2 - n) + x^3(1.5 - n) S_1 + x^2(1 - n) S_2 + x(0.5 - n) S_1 - n = 0. \tag{4}$$

The local magnetic moment can be expressed by the local correlation function

$$L_0 = \frac{3}{4} \langle (n_{i\uparrow} - n_{i\downarrow})^2 \rangle = \frac{3}{4} (n - 2 \langle n_{i\uparrow} n_{i\downarrow} \rangle) \tag{5}$$

and is calculated from (2) according to

$$L_0 = \frac{3}{4} \frac{1}{\beta} \frac{\partial \ln Z}{\partial U}. \tag{6}$$

Let us note that in (5) we have used the identity $n_{i\sigma}^2 = n_{i\sigma}$. An alternative formula for L_0 is given by

$$L_0 = \frac{3}{4} \frac{1}{\beta^2 Z} \frac{\partial^2 Z}{\partial h_i^2} \Big|_{h_i=0}. \tag{7}$$

h_i denotes an external field that couples to the local spin. Formulas (6) and (7) are equivalent definitions of L_0 . However, in an approximate treatment of Z this equivalence can be destroyed. In a previous paper [15] we have shown that in the static FI theory better results are obtained from (6) rather than from (7).

The specific heat per particle in the grand-canonical ensemble is given by

$$\frac{c_v}{k_B} = \frac{\beta^2}{2n} \left\{ \frac{\partial^2 \ln Z}{\partial \beta^2} - \frac{\left(2n - \frac{\partial^2 \ln Z}{\partial \beta \partial \mu} \right)^2}{\frac{\partial^2 \ln Z}{\partial \mu^2}} \right\}. \tag{8}$$

2.2 Static one-field theory

Rewriting the interaction term of (1) as

$$n_{i\uparrow} n_{i\downarrow} = \frac{1}{2} (n_{i\uparrow} + n_{i\downarrow}) - \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})^2 \tag{9}$$

and applying the Hubbard-Stratonovich transformation the partition function of (1) in the static approximation takes the form

$$Z^{\text{st}} = \int \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \frac{\beta U}{2\pi} e^{-\frac{\beta U}{2}(\xi_1^2 + \xi_2^2)} \text{Tr} e^{-\beta H_{\text{L}}} . \quad (10)$$

H_{L} is a one-particle Hamiltonian describing the coupling of the fields ξ_i to the local spin operator and is given by

$$H_{\text{L}} = H^{(0)} - U \sum_{j=1}^2 \sum_{\sigma=\pm} (\sigma \xi_j - \frac{1}{2}) n_{j\sigma} . \quad (11)$$

Note that in the infinite Hubbard model further approximations have to be applied in order to evaluate the trace and the integrals for the calculation of Z^{st} [7]. For the model (1) the trace in (10) can be performed and we get

$$\text{Tr} e^{-\beta H_{\text{L}}} = 4 \left[\cosh \left\{ \frac{\beta U}{2} (\xi_1 + \xi_2) \right\} + \cosh \left\{ \frac{\beta U}{2} \sqrt{(\xi_1 - \xi_2)^2 + \left(\frac{2t}{U} \right)^2} \right\} \right]^2 . \quad (12)$$

Inserting (12) into (10) and calculating one integral after a proper substitution analytically the partition function (10) is represented in the form (2) with

$$S_1 = 4e^{\beta U/4} \sqrt{\frac{\beta}{\pi U}} \int_{-\infty}^{\infty} d\alpha e^{-\beta \alpha^2 / U} \cosh \{ \beta \sqrt{\alpha^2 + t^2} \} , \quad (13)$$

$$S_2 = 2 \left[1 + e^{\beta U} + \sqrt{\frac{\beta}{\pi U}} \int_{-\infty}^{\infty} d\alpha e^{-\beta \alpha^2 / U} \cosh \{ 2\beta \sqrt{\alpha^2 + t^2} \} \right] .$$

The integrals in (13) are easily calculated numerically. The chemical potential, the local moment, and the specific heat are determined according to (4), (6), and (8), respectively.

It is worth noting that besides (9) there is an alternative one-field representation given by

$$n_{i\uparrow} n_{i\downarrow} = -\frac{1}{2} (n_{i\uparrow} + n_{i\downarrow}) + \frac{1}{2} (n_{i\uparrow} + n_{i\downarrow})^2 . \quad (14)$$

Using (14) two auxiliary fields are introduced which couple to the charge density operators at sites 1 and 2. The partition function in the static approximation is expressed in an analogous way as above by (2) with

$$S_1 = 4e^{3\beta U/4} \sqrt{\frac{\beta}{\pi U}} \int_{-\infty}^{\infty} d\alpha e^{-\beta \alpha^2 / U} \cosh \{ \beta \sqrt{t^2 - \alpha^2} \} , \quad (15)$$

$$S_2 = 2e^{\beta U} \left[2 + \sqrt{\frac{\beta}{\pi U}} \int_{-\infty}^{\infty} d\alpha e^{-\beta \alpha^2 / U} \cosh \{ 2\beta \sqrt{t^2 - \alpha^2} \} \right] .$$

2.3 Static two-field theory

In the representations (9) and (14) the identity $n_{i\sigma}^2 = n_{i\sigma}$ has been used. As shown for the Anderson model [8, 9] in this scheme considerable errors arise in the static approxi-

mation. The relation

$$n_{i\uparrow}n_{i\downarrow} = \frac{1}{4}(n_{i\uparrow} + n_{i\downarrow})^2 - \frac{1}{4}(n_{i\uparrow} - n_{i\downarrow})^2 \quad (16)$$

does not employ the Fermi character of the operators and was preferred by many authors [2 to 6]. With (16) two kinds of fields are introduced by the transformation to the FI. One field is connected with the local spin operator and the other one couples to the charge density operator. Then the static partition function becomes

$$Z^{\text{st}} = \int_{-\infty}^{\infty} d\xi_1 d\xi_2 d\eta_1 d\eta_2 \left(\frac{\beta U}{4\pi}\right)^2 e^{-\frac{\beta U}{4}(\xi_1^2 + \xi_2^2 + \eta_1^2 + \eta_2^2)} \text{Tr} e^{-\beta H_{\text{L}}}, \quad (17)$$

$$H_{\text{L}} = H^{(0)} - \frac{U}{2} \sum_{j=1}^2 \sum_{\sigma=\pm} (\sigma\xi_j + i\eta_j) n_{j\sigma}. \quad (18)$$

i denotes the imaginary unit.

The Hamiltonian (18) is non-hermitian. The complex eigenvalues of H_{L} are given by

$$E_{1/2} = -z_1 \pm \sqrt{z_2^2 + t^2} - \left(\mu + \frac{U}{2}\right), \quad E_{3/4} = -E_{1/2}^* - (2\mu + U), \quad (19)$$

with

$$z_{1/2} = \frac{U}{4} [\xi_1 + i\eta_1 \pm (\xi_2 + i\eta_2)],$$

from which we get

$$\text{Tr} e^{-\beta H_{\text{L}}} = \sum_{j=1}^4 e^{-\beta E_j}. \quad (20)$$

Inserting (20) into (17) two of the four integrals are solved analytically and by a suitable transformation of the integration variables the partition function (17) is expressed by (2) with

$$S_1 = 32 e^{\beta U/2} \frac{\beta}{\pi U} \int_0^{\infty} dr \int_0^{\pi/2} d\varphi r e^{-2\beta r^2/U} \cosh\{\beta a\} \cos\{\beta b\},$$

$$S_2 = 2 e^{\beta U} + 16 e^{\beta U/2} \frac{\beta}{\pi U} \int_0^{\infty} dr \int_0^{\pi/2} d\varphi r e^{-2\beta r^2/U} (\cosh\{2\beta a\} + \cos\{2\beta b\}), \quad (21)$$

with

$$a = \sqrt{(R_1 + R_2)/2}, \quad b = \sqrt{(R_1 - R_2)/2},$$

and

$$R_1 = \sqrt{r^4 + 2t^2 r^2 \cos(2\varphi) + t^4}, \quad R_2 = |t^2 + r^2 \cos(2\varphi)|.$$

The twofold integrals (21) can be solved numerically with sufficient accuracy and the thermodynamic quantities of interest are calculated from (4), (6), and (8).

3. Results and Discussion

In order to investigate a broad spectrum of the model parameters we calculate the temperature dependences of the local moment and the specific heat for different interaction strengths ($U/t = 0.5; 4; 8$) and electron densities ($n = 1; 0.6; 0.2$). The

parameters $U/t = 0.5, 4,$ and 8 are representative for the small, intermediate, and large interaction regions, respectively. Because of the symmetry properties of the Hubbard model we can restrict our calculations to $n < 1$, where $n = 1$ corresponds to the half-filled band case in the infinite system. The particle densities $n = 1$ and $n < 1$ will be discussed separately.

3.1 $n = 1$

In Fig. 1 the temperature dependence of L_0 as obtained in the FI approaches described in Section 2 is compared with the exact solution. Obviously, in the low-temperature region the two-field static approximation yields the best result, whereas the one-field methods are even qualitatively incorrect for small U . For instance, the zero-temperature limit of L_0 calculated from (13) is zero in contrast to the exact result (Fig. 1a). This behaviour is confirmed by a ground-state analysis. The U -dependence of $L_0(T = 0)$ and the ground-state energy E_0 are shown in Fig. 2 and 3, respectively. The correct value of L_0 in the band limit ($U = 0$) is only reproduced by the two-field approach which also yields the best fit to the exact ground-state energy. Especially, the first-order corrections to E_0 near the band limit are given correctly by the two-field method only. A similar statement has been obtained for the Anderson model [8]. The results of the one-field approach according to (13) are discussed more extensively in [16].

At larger temperatures the local moments in the one-field approximations tend rapidly to the exact one. However, in the two-field approach L_0 deviates appreciably and the exact high-temperature limit $L_0(T = \infty) = 3/8$ is not obtained. We have calculated this limiting value analytically from (21) and get $L_0(T = \infty) = 3(1 + 1/\pi)/8$. That is, in the high-temperature region the static two-field scheme is not superior to the one-field schemes as one should from claim the ground-state discussion. Note that the alternative calculation of L_0 in the two-field scheme according to (7) yields the high-temperature limit $L_0 = 3(1/2 + 1/\pi)/8$ which is smaller than the exact value. A similar behaviour is also observed in the infinite lattice [17]. In the one-field method (13) the formulas (6) and (7) yield identical results and the correct limit $L_0(T = \infty) = 3/8$.

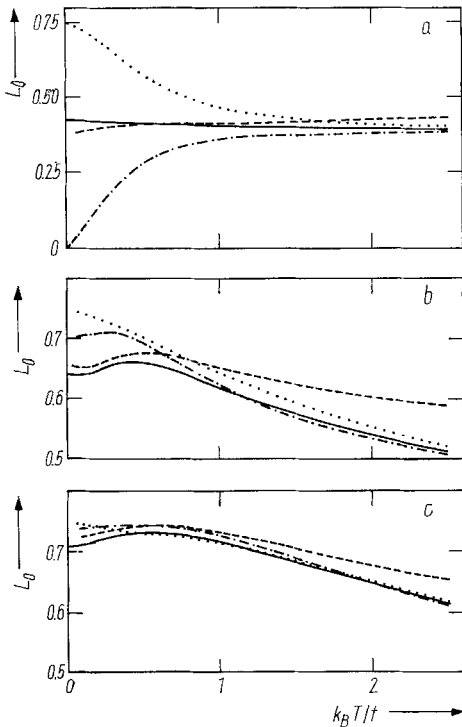


Fig. 1. Local magnetic moment L_0 of the two-site Hubbard model vs. temperature for $n = 1$ and a) $U = 0.5t$, b) $4t$, and c) $8t$. — exact result, - - - two-field static approximation according to (16), - · - · - spin-field static approximation according to (9), ····· charge-field static approximation according to (14)

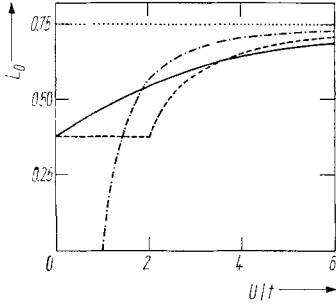


Fig. 2. Ground-state local moment as function of interaction strength U . Notations as in Fig. 1

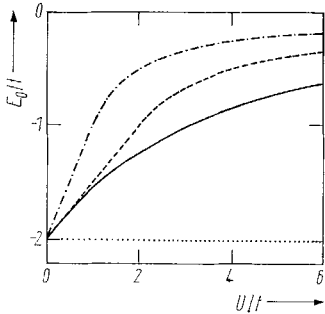


Fig. 3. Ground-state energy of the two-site model. Notations as in Fig. 1

The specific heat is shown in Fig. 4. For small values of U there is a reasonable agreement of all approximate methods with the exact result (Fig. 4a). In the case of intermediate and large U (Fig. 4 b, c) there is a considerable overestimation of c_v in

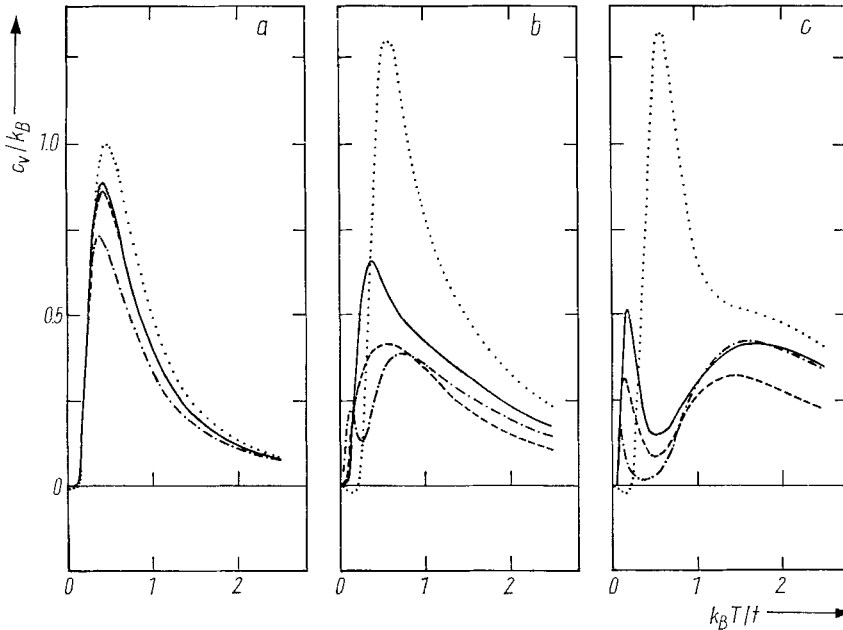


Fig. 4. Temperature dependence of the specific heat per particle c_v for $n = 1$ and a) $U = 0.5t$, b) $4t$, c) $8t$. Notations as in Fig. 1

the one-field approach using the charge fields (15). This yields a negative low-temperature entropy and a negative c_v at very low T . Furthermore, the characteristic two-peak structure of c_v at $U = 8t$ is not well resolved. In the one-field approximation (13) and in the two-field scheme two peaks are obtained (Fig. 4c). The latter method results in a better low-temperature description and the former one resolves the low-temperature peak of c_v already at $U = 4t$ (Fig. 4b). Obviously, this behaviour is strongly connected with the excitation spectrum. In the one-field approach (13) the excitation energy due to the destruction of magnetic short-range order is too small compared with the exact one resulting in a shift of the narrow peak of c_v to lower temperatures (Fig. 4b, c). In the high-temperature region the specific heat in the static two-field method is considerable smaller than the exact one confirming the conclusion that the high-temperature description in this scheme is not very accurate.

3.2 $n < 1$

For $n = 0.6$ and $n = 0.2$ the temperature dependence of L_0 is shown in Fig. 5 and 6, respectively. The results of the comparative study of the different FI schemes are

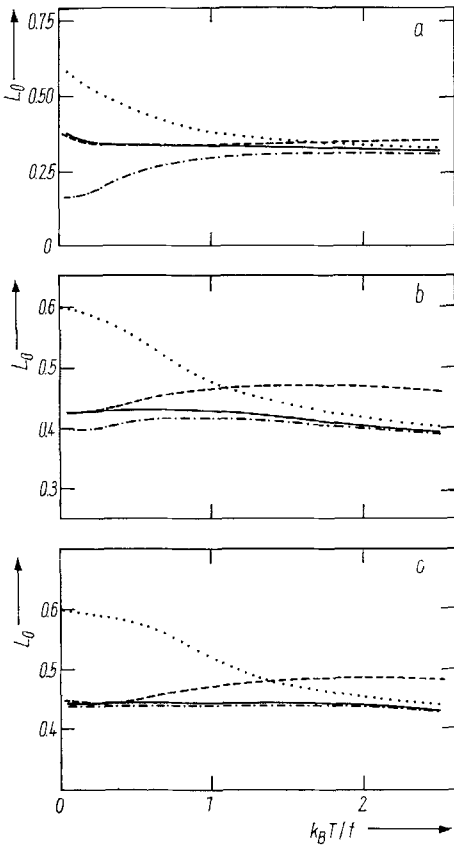


Fig. 5

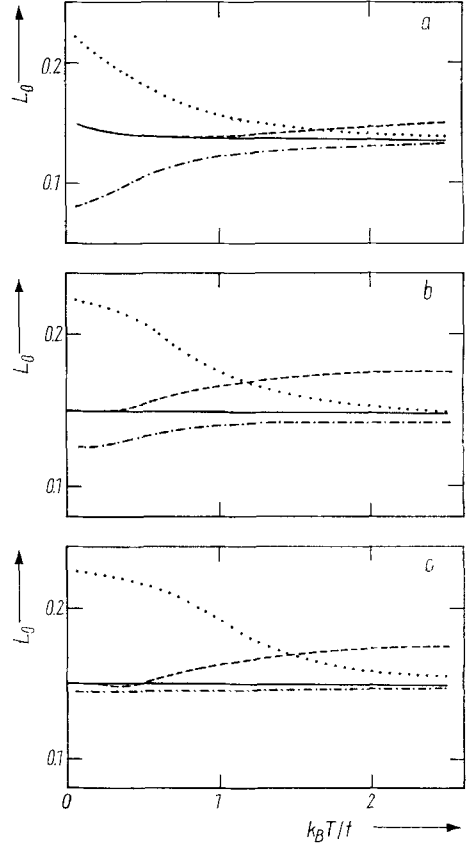


Fig. 6

Fig. 5. Local magnetic moment vs. temperature for $n = 0.6$ and a) $U = 0.5t$, b) $4t$, c) $8t$. Notations as in Fig. 1

Fig. 6. Local magnetic moment vs. temperature for $n = 0.2$ and a) $U = 0.5t$, b) $4t$, c) $8t$. Notations as in Fig. 1

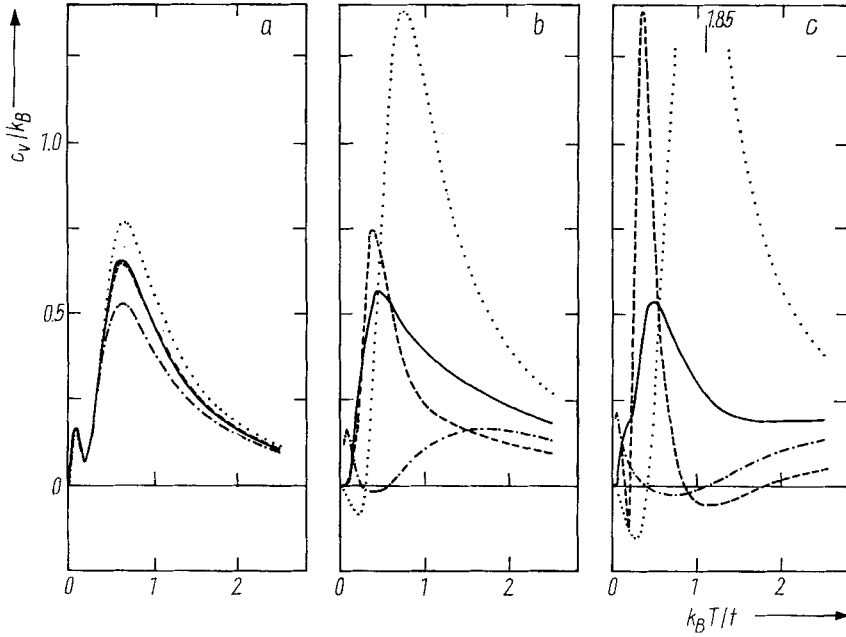


Fig. 7. Specific heat c_v vs. temperature for $n = 0.6$ and a) $U = 0.5t$, b) $4t$, c) $8t$. Notations as in Fig. 1

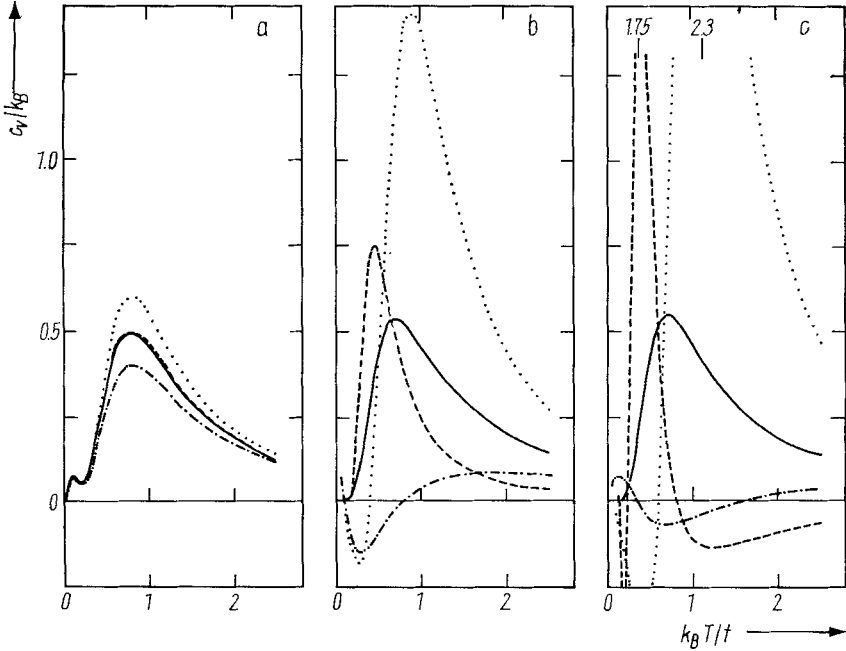


Fig. 8. Specific heat c_v vs. temperature for $n = 0.2$ and a) $U = 0.5t$, b) $4t$, c) $8t$. Notations as in Fig. 1

very similar to the case $n = 1$. The two-field method describes L_0 rather accurately in the low-temperature region. However, considerable deviations and a false limiting value are obtained for intermediate and high temperatures. The results of the one-field approximations are bad for low T and agree quite well at high T . Especially, the high-temperature limit is given correctly.

As to the specific heat the situation is not so clear. The specific heat versus temperature curves are represented in Fig. 7 and 8. In the small U -region (Fig. 7a, 8a) c_v is qualitatively well described. The curve of the two-field approach nearly coincides with the exact one. Note that the small peak at very low T is an effect of the smallness of the system (1) and is a consequence of a discrete low-lying excitation due to the noninteger value of n . In an infinite lattice these excitations are gapless and cause a faster increase of c_v at low T .

For $U = 4t$ the specific heat is only qualitatively well described by the two-field scheme. The peak of c_v is overestimated and shifted to lower T (Fig. 7b, 8b). For intermediate and larger T c_v is appreciably underestimated. In the one-field approximations c_v becomes negative at smaller T and the overall behaviour of the exact specific heat is not reproduced. Hence, the one-field method is not able to describe the thermodynamics of (1). The same statement is true also for larger interaction (Fig. 7c, 8c). Moreover, the two-field scheme yields for $U = 8t$ negative c_v values in the low- and intermediate temperature regions (Fig. 7c, 8c) indicating the break-down of the static FI theory as applied to the model (1).

4. Conclusions

On the basis of the results discussed in the previous section we can estimate the range of validity of the various static FI approximations. Since we have considered physical quantities which do not depend strongly on the size of the lattice (cf. Section 1) and some results for the two-site model in the static approximation are also obtained in the paramagnetic phase of the infinite Hubbard model (e.g. negative low-temperature entropy [6]), we expect the main statements to be valid also in the latter case. Our conclusions are summarized as follows:

(i) The static two-field approach describes the thermodynamic behaviour of the model (1) quite well for small interaction strengths. In the intermediate and large interaction regions the results are qualitatively correct for $n = 1$ although considerable deviations from the exact result appear at higher temperatures. For $n < 1$, however, the approach is bad and thermodynamic stability conditions are violated at large U (negative specific heat).

(ii) The static one-field approximations for small U yield qualitatively good results for c_v but not for the low-temperature local moment. For intermediate and large interactions there are appreciable quantitative errors and, for $n < 1$, the specific heat becomes negative in some temperature regions. However, in contrast to the two-field method, the results for c_v and L_0 in the high-temperature region are fairly accurate and the correct limits for L_0 are reproduced.

(iii) As a general tendency all the static FI approaches give unphysical results for c_v in the strong interacting system with small electron densities. The two-field and one-field methods yield the best results in the high- and low-temperature regions, respectively.

It is worth noting that besides the representations of the Hubbard interaction (9), (14), (16) considered in Section 2 there are other possibilities which introduce the square of the vector spin operator $(\mathbf{S}_i)^2$ [18, 19]. However, the latter method yields incorrect results even in the atomic limit ($t = 0$) whereas with (9), (14), or (16) the static approximation

is an exact procedure for $t = 0$. The static approximation neglects the anticommutativity of the Fermi operators. In the atomic limit of (1) with (9), (14), or (16) there appear only occupation number operators which are commutative. Using the vector spin decomposition, however, the components of the spin operator S_i do not commute and the static approach does not reproduce the limit $t = 0$.

Hubbard [4] has proposed a representation which combines the vector character of the spin with the commutative properties of the atomic-limit operators and which is able to give the correct atomic-limit result in the static approximation. In this method the spin vector is projected onto an arbitrary unit vector e and the partition function is averaged over all directions of e in order to preserve the spin rotational invariance of the Hubbard Hamiltonian. For this method we can show that the ground-state results are identical to those of the corresponding scalar representations (9) or (16). Within the single-site approximation for the infinite system it has been pointed out [20] that the scalar and projected vector field methods are equivalent in the paramagnetic state. Differences appear in the description of long-range magnetic ordering which is not considered here.

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