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On the validity of the static approximation in the spin-fluctuation theory for itinerant electrons

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Received 26 October 1983, in final form 17 April 1984

Abstract. The static approximation in the functional integral theory of itinerant magnetism is critically investigated. For the two-site Hubbard model the local magnetic moment and the specific heat are calculated as functions of temperature and interaction strength. By comparison with the exact results the error in the static approximation is found to be large at low temperatures and for small interaction strengths. It is shown that the subdivision of the ground state into a phase without a local moment (small interaction) and a phase with local moment (large interaction) is induced by the static approximation. The specific heat is underestimated and the zero-point entropy is finite. The implications for the infinite Hubbard model are briefly discussed.

1. Introduction

The magnetism of transition metals and alloys has been the matter of much experimental and theoretical work. Neither the conventional Stoner theory nor the localised spin models yield a satisfactory description of the magnetic properties of transition metals. For example, the non-integral value (in units of μ_B) of the ground-state magnetisation, the Curie–Weiss behaviour of the paramagnetic spin susceptibility, and the temperature dependence of the magnetisation observed in these materials are characteristic features of both localised and band magnetism. The theoretical description of this phenomenon is frequently based on a model proposed by Hubbard (1963) which interpolates between the two limits. The tight-binding Hamiltonian is given by

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{HC}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i, \sigma} n_{i\sigma}. \quad (1)$$

t and U are the nearest-neighbour overlap and on-site Coulomb integrals, respectively. $c_{i\sigma}^{\dagger}$ is the creation operator of an electron in the Wannier state φ_i with spin projection σ and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. The mean electron number n is fixed by the choice of the chemical potential μ .

For $U = 0$ the Hamiltonian (1) describes a single band of non-interacting electrons exhibiting Pauli paramagnetism. In the atomic limit ($t = 0$) the electrons and their magnetic moments are completely localised and the paramagnetic spin susceptibility shows the Curie–Weiss behaviour. The perturbation theory with respect to $t \ll U$ yields an effective antiferromagnetic Heisenberg Hamiltonian and antiferromagnetic long-

range order in three-dimensional lattices. For intermediate parameters no rigorous proof of the existence of magnetic ordering in the Hubbard model is known. However, on the basis of approximate results it is generally assumed that ferromagnetism in transition metals can be described by (1) if the Stoner criterion is fulfilled:

$$U\rho(E_F) > 1 \quad (2)$$

$\rho(E_F)$ is the density of states at the Fermi energy.

In recent years spin-fluctuation theories (SFT) based on the functional integral (FI) representation of (1) have provided an accurate description and a current understanding of itinerant magnetism (Hasegawa 1979, 1980a, b, 1981, Hubbard 1979a, b, 1981, Evangelou *et al* 1982, Evangelou and Edwards 1983). The Hubbard–Stratonovich transformation (Stratonovich 1957) is applied methodically to the interaction in (1) and the partition function is represented as a FI over time-dependent fluctuating fields. Evaluating the FI various approximations are applied. Within the static approximation it is reduced to an ordinary integral. Furthermore, the saddle-point approximation, the self-consistent single-site approximation, etc. are used for the calculation of thermodynamic quantities.

Unfortunately, the validity of the different approximations, especially that of the static one, has not been investigated very thoroughly. For the Anderson model of a magnetic impurity it has been shown that considerable errors may arise due to the violation of the Pauli principle in the static approximation (Amit and Keiter 1973, Macedo *et al* 1982). Recently, the temperature dependence of the local moment in the paramagnetic phase of the Hubbard model has been discussed by one of the authors (Lorenz 1983) and discrepancies in the results of SFT are obtained. The square of the local moment is defined as

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

$\langle \dots \rangle$ denotes the thermodynamic average with respect to (1). According to the results of the SFT quoted above the paramagnetic ground state of the Hubbard model is divided into a phase with vanishing local moment ($U < U_c$) and another phase ($U > U_c$) in which L_0 grows gradually to the atomic limit value with increasing U (Hasegawa 1980a). Consequently, for $U < U_c$, L_0 is an increasing function of temperature T and the proportionality $L_0 \propto T$ holds for low temperatures (Hasegawa 1980a, Evangelou *et al* 1982, Fehske 1983).

However, this qualitative behaviour is in contradiction to exact results and other approximate solutions for the model (1). The exact ground-state solution of the Hubbard chain obtained by Lieb and Wu (1968) yields a local magnetic moment that varies monotonically with U between the band and atomic limits and, in particular, is always larger than zero. The temperature dependence of L_0 for the half-filled band ($n = 1$) as obtained from finite-chain extrapolations (Shiba 1972) and Monte Carlo simulations of the square lattice (Hirsch 1983) deviates qualitatively from the predictions of SFT in the small- U region.

In order to clarify the discrepancies and to test the FI formalism the evaluation of exactly solvable models is of particular interest. Therefore, in the next section (§ 2) we consider the model (1) for two sites only (a Hubbard molecule). The two-site model is treated within the static FI theory and some thermodynamic functions are calculated and compared with the exact solution. In § 3 we discuss the results and present the main conclusions.

2. The two-site Hubbard model

The Hubbard molecule is described by the Hamiltonian

$$H = H^0 + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) - \frac{U}{2} \sum_{\sigma} (n_{1\sigma} + n_{2\sigma}) \quad (4)$$

$$H^0 = -t \sum_{\sigma} (c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma})$$

where we have restricted our considerations to the case $n = 1$ for which $\mu = U/2$.

The model (4) is easily solved and the thermodynamic properties have been discussed by Bernstein and Pincus (1974) and Lorenz (1983). Furthermore, it can be treated within the FI formalism by the application of the static approximation. No further approximation has to be applied unlike, for example, the case for the infinite model (1). This allows us to investigate the effect of the static approach by comparison with the exact solution. However, it has to be pointed out that results obtained for a finite lattice are relevant also for the model (1). Since there is no magnetic long-range order in a finite system this question is outside the scope of this paper. On the other hand it has been shown that some thermodynamic functions, e.g. the specific heat, the entropy and the magnetic moment, are very similar to those of an infinite system in the paramagnetic phase (Bernstein and Pincus 1974, Shiba 1972, Lorenz 1983). The magnetic short-range order that is responsible for the narrow low-temperature peak in the specific heat and that appears at larger values of U as an effect of the hopping-induced effective Heisenberg interaction is well described by the two-site model. The local moment in the model (4) shows the same temperature dependence as that of a larger lattice. Hirsch (1983) has found in two dimensions that L_0 is almost completely insensitive to the size of the lattice. The exactly available limits ($t = 0$ or $U = 0$) for L_0 in the model (1) (Lorenz 1983) are reproduced by the Hubbard molecule (4). Therefore, we investigate the local moment and the specific heat c_v of (4) in the static FI approach and assume that the conclusions are also valid in the paramagnetic phase of (1).

2.1. Exact solution

The partition function of (4) is given by

$$Z = 2 \exp(\beta U/2) [\cosh\{(\beta U/2)[1 + (4t/U)^2]^{1/2}\} + 3 \exp(\beta U/2) + 4 \cosh(\beta t)]. \quad (5)$$

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

The ground-state energy and local moment are obtained as

$$E = U - (k_B T \ln Z)_{T \rightarrow 0} = (U/2) \{1 - [1 + (4t/U)^2]^{1/2}\} \quad (6)$$

$$L_0 = \frac{3}{8} \{1 + [1 + (4t/U)^2]^{-1/2}\} \quad (7)$$

and are shown in figures 1 and 2, respectively.

The temperature dependences of L_0 and c_v represented in figures 3 and 4 are derived from (5) according to

$$L_0 = \frac{3}{8} (1/\beta) \partial \ln Z / \partial U \quad (8)$$

$$c_v = k_B \beta^2 \partial^2 \ln Z / \partial \beta^2. \quad (9)$$

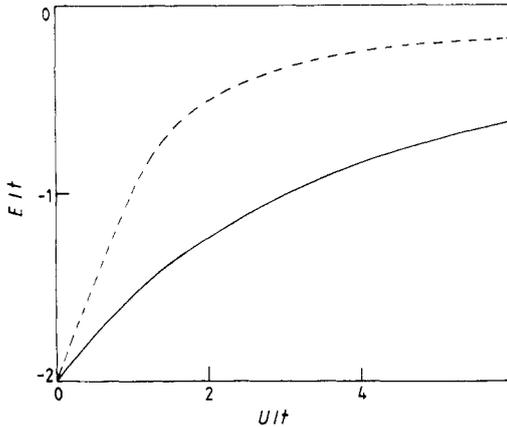


Figure 1. The ground-state energy of the Hubbard molecule. Full curve: exact result; broken curve: static FI theory result.

2.2. Static functional integral theory

For the FI representation of (4) we use the decomposition of the interaction term that introduces the minimal number of fields (Sakoh and Shimizu 1976). The grand partition function is given by

$$Z = \iint \mathcal{D}\xi_1(\tau) \mathcal{D}\xi_2(\tau) \text{Tr} \hat{T}_\tau \exp \left[- \int_0^\beta \left(\frac{U}{2} (\xi_1^2(\tau) + \xi_2^2(\tau)) + H_L(\tau) \right) d\tau \right] \tag{10}$$

$$H_L(\tau) = H^0(\tau) - U \sum_{\sigma=\pm} \sigma (\xi_1(\tau) n_{1\sigma}(\tau) + \xi_2(\tau) n_{2\sigma}(\tau)).$$

$\xi_1(\tau)$ and $\xi_2(\tau)$ are the auxiliary fields connected with the spin fluctuations at sites 1 and 2, respectively. The operators are defined in the interaction representation and \hat{T}_τ is the time-ordering operator.

The partition function (10) is an exact representation of (5). In the static approximation the dependence on τ of the fields and the operators is neglected and performing the trace in (10) we get

$$Z^{\text{st}} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \frac{\beta U}{2\pi} \exp(-\beta F(\xi_1, \xi_2)) \tag{11}$$

with the free-energy functional

$$F(\xi_1, \xi_2) = (U/2)(\xi_1^2 + \xi_2^2) - (2/\beta) \ln [2 \cosh \{ \frac{1}{2} \beta U (\xi_1 + \xi_2) \} + 2 \cosh \{ \frac{1}{2} \beta U [(\xi_1 - \xi_2)^2 + (2t/U)^2]^{1/2} \}]. \tag{12}$$

With (8) the local moment is expressed as

$$L_0^{\text{st}} = \frac{3}{4} (\langle \xi_i^2 \rangle_{\text{st}} - 1/\beta U) \tag{13}$$

where $\langle \dots \rangle_{\text{st}}$ denotes the functional average with the distribution function

$$W(\xi_1, \xi_2) = (\beta U / 2\pi) \exp(-\beta F(\xi_1, \xi_2)) / Z^{\text{st}}.$$

At zero temperature the average (13) is determined by the saddle points of (11), i.e.

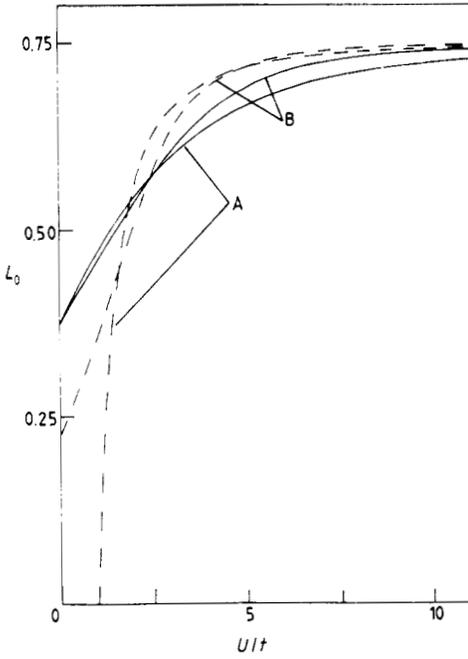


Figure 2. The local magnetic moment of the Hubbard molecule as a function of U for (A) $k_B T = 0$ and (B) $k_B T = 0.5t$. The curves are as in figure 1.

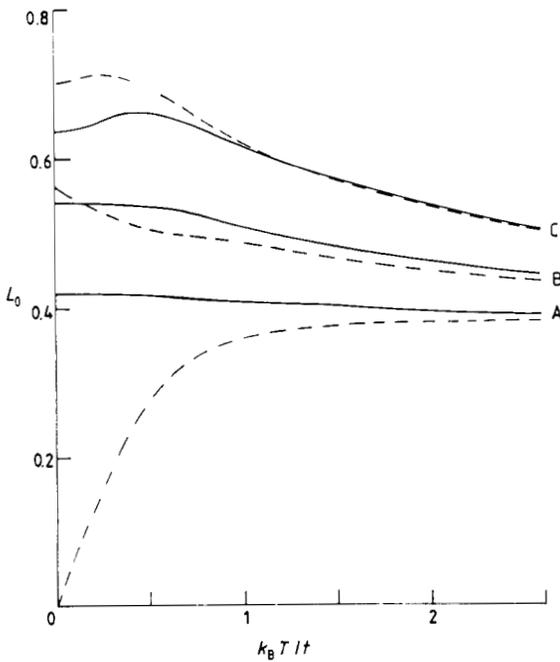


Figure 3. The local magnetic moment of the Hubbard molecule as a function of temperature for (A) $U = 0.5t$, (B) $U = 2t$, and (C) $U = 4t$. The curves are as in figure 1.

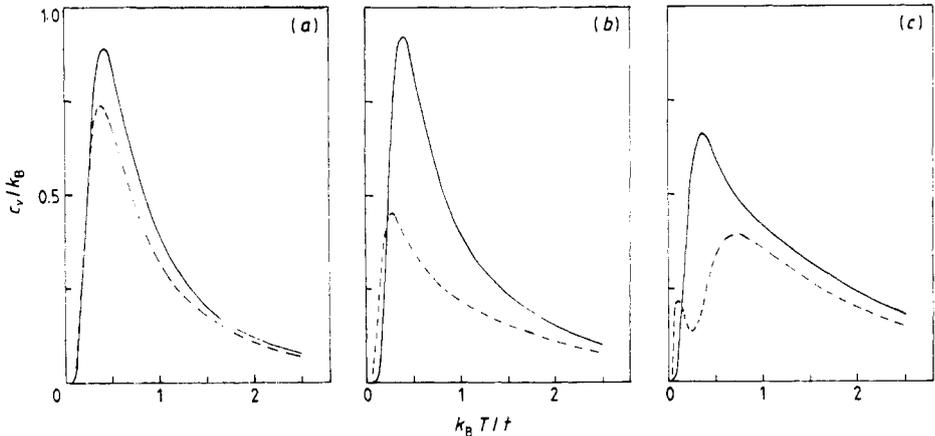


Figure 4. The specific heat of the Hubbard molecule for (a) $U = 0.5t$, (b) $U = 2t$ and (c) $U = 4t$. The curves are as in figure 1.

by the minimum of (12). For $U < t$ the free-energy density (12) has one minimum at $\xi_1 = \xi_2 = 0$. Therefore, the local moment vanishes and the ground-state energy is given by $E(U < t) = U - 2t$. For $U > t$ the two lowest minima appear at $\xi_1 = -\xi_2 = \pm[1 - (t/U)^2]^{1/2}$. Note that the different signs of the fields yield an antiferromagnetic short-range order analogous to the antiferromagnetic spin coupling derived in the perturbation expansion of (1) with respect to $t/U \ll 1$. In the single-site approximation as frequently applied in the SFT this magnetic short-range order is neglected. For L_0 and E in the large-interaction range ($U > t$) we get $L_0 = \frac{2}{3}[1 - (t/U)^2]$ and $E = -(t/U)^2$, respectively.

In figures 1 and 2 the ground-state results are compared with the exact ones. The energy in the static approximation is considerably larger and fails even in the first order in U near the band limit. As discussed by Amit and Keiter (1973) for the Anderson model, the incorrectness of the slope of $E(U)$ at $U = 0$ is probably due to the introduction of one field only and might be corrected by taking into account charge fluctuations. The ground-state moment approaches the exact result (7) at large U . However, for intermediate and smaller values of U the deviation becomes large and the disappearance of L_0 at $U \leq t$ is in qualitative contradiction to the exact moment which is always larger than $\frac{2}{3}$.

For the calculation of thermodynamic quantities we have to evaluate the twofold integral (11). By a proper transformation of the variables one integral can be treated analytically and we get

$$Z^{\text{st}} = 2 \left(\frac{\beta}{\pi U} \right)^{1/2} \int_{-\infty}^{\infty} d\alpha \exp\left(-\frac{\beta}{U} \alpha^2\right) \{2 + \exp(\beta U) + 4 \exp(\beta U/4) \cosh[\beta(t^2 + \alpha^2)^{1/2}] + \cosh[2\beta(t^2 + \alpha^2)^{1/2}]\} \quad (14)$$

with $\alpha = (U/2)(\xi_1 - \xi_2)$. The integral (14) is solved numerically and the local moment and the specific heat are obtained as functions of temperature from (8) and (9), respectively. The results are shown in figures 3 and 4 for various ratios U/t .

Obviously, L_0 and c_v approach the exact curves in the high-temperature range. This is easily understood since the static approximation neglects commutation rules for Fermi

operators, i.e. quantum effects that do not play any significant role for large temperatures. However, in the low-temperature region the quantum fluctuations are not negligible. This is seen in the temperature dependence of L_0 especially for $U < t$ where L_0 tends linearly with T to zero (cf the ground-state analysis). It is interesting to note that the same behaviour has been observed in the infinite Hubbard model (Hasegawa 1980a, Evangelou *et al* 1982). While the temperature dependence of L_0 for small interaction fails qualitatively it reproduces the main characteristics for large U quite reasonably (see figure 3).

The specific heat (figure 4) is underestimated by the static approach. Since the integrated specific heat determines the entropy change ΔS and the high-temperature value of S is given correctly it follows that the ground-state entropy is finite in contradiction to the exact solution where $S(T = 0) = 0$. Calculating the entropy directly from (14) this result is confirmed and it can be shown that S is generally overestimated. A similar result was obtained for the infinite system (cf Sakoh and Shimizu 1976). For $U = 4t$ the specific heat has a low-temperature peak due to the destruction of magnetic short-range order. In the exact solution this peak appears only at larger values of U (not shown in figure 4).

3. Discussion and conclusions

In the previous section we presented some thermodynamic quantities of the Hubbard molecule in the static approximation in comparison with the exact results. Now we will discuss the validity of the approximation and suggest some implications for the N -site system.

The temperature dependence of the specific heat (figure 4) is given qualitatively correctly in the static approximation although c_v is underestimated and the low-temperature peak is resolved at a smaller interaction strength than in the exact solution. The most drastic difference appears in the local magnetic moment (figures 2 and 3). In particular, at $T = 0$ phases with vanishing and non-vanishing local moment are distinguished. This is not the case in the exact solution. As a consequence the temperature dependence of L_0 in the former phase ($U < t$) is given erroneously by the static approach.

It is interesting to note that strictly the same behaviour is obtained in the paramagnetic N -site model within the static FI theory (Sakoh and Shimizu 1976, Cyrot 1972, Hasegawa 1980a, Evangelou *et al* 1982, Evangelou and Edwards 1983). The vanishing ground-state local moment for small U is in contradiction to the exact value in the band limit $L_0(U = 0) = \frac{3}{8}$. The behaviour of thermodynamic functions of the Hubbard molecule and the infinite model is very similar (cf. § 2) and also the results obtained in the static FI theory are qualitatively identical in both systems. Therefore, we suggest that the static approximation has the same effect in the model (1) as in the model (4) discussed above. In particular, the subdivision of the paramagnetic ground state into a phase without local moments (small U) and a phase with local moments (large U) and the qualitative temperature dependence of L_0 in the former phase as predicted by the FI theory are due to the static approximation.

We have to restrict our conclusions to the paramagnetic phase which is assumed to be realised in the region of small U where the Stoner criterion (2) is not fulfilled. Since the static FI method fails just in this case, the results obtained in the SFT for paramagnetic metals should be considered carefully.

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