Ferromagnetism in the strongly correlated Hubbard model

G. Geipel
Max-Planck-Institut für Plasmaphysik, Boltzmannstrasse 2, D-8046 Garching, Federal Republic of Germany

W. Nolting
Institut für Theoretische Physik II, Wilhelm-Klemm-Strasse 10, D-4400 Münster, Federal Republic of Germany

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We use a self-consistent "spectral-density approach" for the strongly correlated Hubbard model in order to find out under what circumstances spontaneous band ferromagnetism may appear. The magnetic polarization $m=n_\uparrow-n_\downarrow$ is examined for a bcc lattice in terms of the temperature T and the band occupation $n=n_\uparrow+n_\downarrow$ $(0\le n\le 2)$. For $T=0$ and less than half-filled bands $(n<1)$, ferromagnetism becomes possible as soon as n exceeds the critical value $n_{\mathrm{I}}=0.54$ and becomes saturated $(m=n)$ above $n_s^*=0.74$. A further, less polarized ferromagnetic solution appears for $n\ge n_{\mathrm{II}}=0.79$. It turns out that a spin-dependent band shift, which consists of "higher" correlation functions, decisively determines the possibility of spontaneous moment ordering. This is demonstrated by a set of self-consistently calculated quasiparticle densities of states. The Curie temperature T_c appears as strongly n dependent. Starting at 0^+ for $n=0.54$, T_c increases with n, reaching a maximum of about 710 K near $n=0.75$, and decreases again for $n>0.8$ down to 0^+ for $n=1$. According to the free energy F, in cases of more than one solution, that solution with the highest polarization is always stable.

I. INTRODUCTION

The so-called s-band Hubbard model[1-3]

$$H=\sum_{i,j,\sigma}(T_{ij}-\mu\delta_{ij})c_{i\sigma}^{\dagger}c_{j\sigma}+\tfrac{1}{2}U\sum_{i,\sigma}n_{i\sigma}n_{i,-\sigma} \tag{1.1}$$

(notation is as usual) is commonly used to study the magnetic properties of strongly correlated electrons in a narrow energy band. Although this Hamiltonian is surely the simplest one that may be constructed, a general solution of the underlying many-body problem is not yet known. That means that besides the problems which arise with the limited applicability of the model to real systems (neglect of long-range Coulomb forces, of d-band degeneracy, of a possible hybridization with sp bands, and so on), even its inherent properties have not been worked out unambiguously up to now. A controversal question, e.g., is whether the model system can show spontaneous ferromagnetism under certain circumstances.[4] We shall contribute to this question by reporting the results of a self-consistent moment method, which is explained later in the text.

Only a few exactly solvable limiting cases of the model Hamiltonian are known. Some of them refer to the one-dimensional case, which has been solved by Lieb and Wu[5] for $T=0$ and arbitrary band occupation n $(0\le n\le 2)$ and by Beni *et al.*[6] for finite temperatures in the $U\to\infty$ limit. The results, however, can hardly be transferred to three-dimensional lattices. With the use of a proof along the lines of the Mermin-Wagner theorem for the Heisenberg model, it can be shown[7,8] that no collective order is possible in the one- and two-dimensional Hubbard model. For the three-dimensional case Nagaoka[9] has given rigorous $U\to\infty$ results for special band fillings of $n=n_\pm=(1/N)(N\pm 1)$ (N is the number of lattice sites). For the symmetric sc and bcc lattices the ground states turn out to be ferromagnetic for n_+ as well as for n_-; in the fcc lattice only for n_+. In the narrow-band limit, where T_{ij} can be considered as a small perturbation, the Hubbard model can be transformed for exactly half-filled bands $(n=1)$ into an effective Heisenberg model[10] with "exchange integrals" $J_{ij}\to T_{ij}^2/U$. An antiferromagnetic ordering of the momenta is predicted. Kanamori[11] has shown that for low band occupations $(n\to 0)$ a collective magnetic order will not appear.

It is impossible to quote all the approximate theories proposed in the past, aimed mainly at determining the existence of ferro- or anti-ferromagnetic order in the Hubbard model. The claims diverge, so that the situation is far from being unambiguously clarified. We present in this paper a "spectral-density approach" (SDA), which in a certain sense differs from the normal Green's-function decoupling procedures or perturbation methods. A lot of previous applications[12-14] give evidence that the SDA is a very effective method for applying many-body theory. A main advantage of this method, the very simple concept of which is described in the next section, lies in the nonperturbative character of the procedure which therefore makes it useful in particular for systems with phase transitions. In Sec. II we derive within the framework of the Hubbard model by use of the SDA a closed system of equations, which has to be solved self-consistently for the average particle numbers $n_\uparrow$, $n_\downarrow$. Spontaneous magnetization is indicated by $n_\uparrow\neq n_\downarrow$. We discuss our results in Secs. III and IV. This paper is exclusively devoted to the case of ferromagnetism. The possibility of antiferromagnetism will be discussed in a forthcoming paper.[15]

II. SPECTRAL-DENSITY APPROACH

The central function of the procedure is the one-electron spectral density, for which various equivalent representations exist.[16]

$$S_{ij\sigma}(t,t')=\frac{1}{2\pi}\langle[c_{i\sigma}(t),c_{j\sigma}^{\dagger}(t')]_{+}\rangle\ , \tag{2.1}$$

$$S_{\mathbf{k}\sigma}(t,t')=\frac{1}{2\pi}\langle[c_{\mathbf{k}\sigma}(t),c_{\mathbf{k}\sigma}^{\dagger}(t')]_{+}\rangle =\frac{1}{N}\sum_{i,j}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}S_{ij\sigma}(t,t')\ , \tag{2.2}$$

$$S_{ij(\mathbf{k})\sigma}(E)=\int_{-\infty}^{+\infty}d(t-t')e^{(i/\hbar)E(t-t')}\times S_{ij(\mathbf{k})\sigma}(t,t')\ . \tag{2.3}$$

All one-particle properties of the interacting-electron system, which we are interested in, may be derived from $S_{\mathbf{k}\sigma}(E)$. The main goal is, therefore, to find a physically reasonable approximation for this fundamental quantity. Our "spectral-density approach" consists of two steps. First, we try to find out the general structure of the spectral density $S_{\mathbf{k}\sigma}(E)$, guided by exactly solvable limiting cases, series expansions, sum rules, or other physical arguments. This leads to an ansatz for $S_{\mathbf{k}\sigma}(E)$, which contains some parameters, which are fitted in the second step by equating exactly calculable spectral moments. For these moments two completely equivalent relations exist. The one exhibits the connection with the spectral density

$$M_{\mathbf{k}\sigma}^{(n)}=\frac{1}{\hbar}\int_{-\infty}^{+\infty}dE\,E^{n}S_{\mathbf{k}\sigma}(E),\quad n=0,1,2,\ldots, \tag{2.4}$$

while the other can be used to determine, at least in principle, all moments independently from the required spectral density:

$$M_{\mathbf{k}\sigma}^{(n)}=\frac{1}{N}\sum_{i,j}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\left\langle\left[\left[i\hbar\frac{\partial}{\partial t}\right]^{n-p}c_{i\sigma}(t),\left[-i\hbar\frac{\partial}{\partial t'}\right]^{p}c_{j\sigma}^{\dagger}(t')\right]_{+}\right\rangle\Bigg|_{t=t'},\quad 0\le p\le n\ . \tag{2.5}$$

Using the Heisenberg equation of motion for the time-dependent construction operators, the moments can be calculated with the Hubbard-Hamiltonian (1.1) in terms of certain equal-time correlation functions. For the first four moments we get after a lengthy but straightforward procedure

$$M_{\mathbf{k}\sigma}^{(0)}=1\ , \tag{2.6}$$

$$M_{\mathbf{k}\sigma}^{(1)}=\varepsilon(\mathbf{k})-\mu+Un_{-\sigma}\ , \tag{2.7}$$

$$M_{\mathbf{k}\sigma}^{(2)}=[\varepsilon(\mathbf{k})-\mu]^2+2Un_{-\sigma}[\varepsilon(\mathbf{k})-\mu]+U^2n_{-\sigma}\ , \tag{2.8}$$

$$M_{\mathbf{k}\sigma}^{(3)}=[\varepsilon(\mathbf{k})-\mu]^3+3Un_{-\sigma}[\varepsilon(\mathbf{k})-\mu]^2+U^2(2n_{-\sigma}+n_{-\sigma}^2)[\varepsilon(\mathbf{k})-\mu]+U^2n_{-\sigma}(1-n_{-\sigma})(B_{\mathbf{k},-\sigma}-\mu)+U^3n_{-\sigma}\ . \tag{2.9}$$

We have assumed translational symmetry of the lattice

$$\langle n_{i\sigma}\rangle=n_{\sigma}\ \text{for all}\ i\ , \tag{2.10}$$

therewith excluding others than ferromagnetic or paramagnetic order. The term $B_{\mathbf{k},-\sigma}$ in the third moment turns out to be of decisive importance concerning the possibility of ferromagnetic order. It consists of higher correlation functions.

$$n_{-\sigma}(1-n_{-\sigma})B_{\mathbf{k},-\sigma}=B_{S;-\sigma}+B_{W;\mathbf{k},-\sigma}\ . \tag{2.11}$$

$B_{S;-\sigma}$ depends on the electron spin σ, but not on the wave vector $\mathbf{k}$:

$$B_{S;-\sigma}=\frac{1}{N}\sum_{\substack{i,j\\(i\neq j)}}T_{ij}\langle c_{i,-\sigma}^{\dagger}c_{j,-\sigma}(2n_{i\sigma}-1)\rangle +T_0n_{-\sigma}(1-n_{-\sigma})\ . \tag{2.12}$$

T_0 is the center of gravity of the "free" Bloch band.

$$T_0=\frac{1}{N}\sum_{\mathbf{k}}\varepsilon(\mathbf{k})\ . \tag{2.13}$$

The other term is $\mathbf{k}$, but only weakly spin dependent:

$$B_{W;\mathbf{k},-\sigma}=\frac{1}{N}\sum_{\substack{i,j\\(i\neq j)}}T_{ij}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}(\langle n_{i,-\sigma}n_{j,-\sigma}\rangle-n_{-\sigma}^2-\langle c_{j\sigma}^{\dagger}c_{j,-\sigma}^{\dagger}c_{i,-\sigma}c_{i\sigma}\rangle-\langle c_{j\sigma}^{\dagger}c_{i,-\sigma}^{\dagger}c_{j,-\sigma}c_{i\sigma}\rangle)\ . \tag{2.14}$$

It is easy to see that the last two expectation values are spin independent ($T_{ij}=T_{ji}$). The "density correlation" $(\langle n_{i,-\sigma}n_{j,-\sigma}\rangle - n^2_{-\sigma})_{i\neq j}$ vanishes in a mean-field approximation, so that it will be a small correction term, only. Altogether $B_{W;\mathbf{k}-\sigma}$ will not be too strongly spin dependent and therefore not so decisive what concerns the possibility of ferromagnetic order.

The crucial point of the method is the choice of a physically reasonable ansatz for the spectral density. Some hints can be drawn from its spectral decomposition:

$$S_{\mathbf{k}\sigma}(E)=\frac{\hbar}{\Xi}\sum_{n,m} e^{-\beta E_n}\,|\langle E_n\,|\,c^{\dagger}_{\mathbf{k}\sigma}\,|\,E_m\rangle|^2(1+e^{\beta E}) \times\delta(E-(E_n-E_m))\,, \tag{2.15}$$

Ξ is the grand canonical partition function, $|E_m\rangle$ an N-particle, and $|E_n\rangle$ an $(N+1)$-particle eigenstate of the Hamiltonian. The energy differences (E_n-E_m) are therefore just the excitation energies which must be brought up for adding an additional $(\mathbf{k},\sigma)$ electron to the N-electron system. In the zero bandwidth limit [$\varepsilon(\mathbf{k})=T_0$ for all $\mathbf{k}$], only two values come into question, namely $T_0-\mu$ and $T_0+U-\mu$, depending on whether the σ electron is excited at a lattice, where a $(-\sigma)$ electron is already present, or not. The spectral density represents in this limiting case a sum of two positively weighted δ functions, the poles of which are located at $T_0-\mu$ and $T_0+U-\mu$, respectively. When we now "switch on" the electron hopping T_{ij} ($W\neq 0$), some satellite peaks will appear close to the energies $E_d^{(-)}=T_0-dU-\mu$ and $E_d^{(+)}=T_0+(d+1)U-\mu$, respectively, where d is a positive integer. As soon as the additional $(\mathbf{k},\sigma)$ electron appears, the N-electron system may rearrange itself because of the finite hopping. If the actual number of doubly occupied sites changes in this moment, then the excitation energies $E_d^{(\pm)}$ are required. The probability for such a rearrangement is of course the greater the more likely the hopping ($\sim W$), and the smaller the Coulomb-matrix element U. It can exactly be shown[17] that the two satellite peaks $E_1^{(\pm)}$, located next to the two main peaks, have weight factors of order $(W/U)^4$, being therefore negligible in the strong correlation region ($U\gg W$). The weights of the other satellite peaks are still much smaller. Therefore, we can conclude that except for a certain quasiparticle damping, $S_{\mathbf{k}\sigma}(E)$ should have the following structure:

$$S_{\mathbf{k}\sigma}(E)=\hbar\sum_{j=1}^{2}\alpha_{j\sigma}(\mathbf{k})\delta(E-E_{j\sigma}(\mathbf{k})+\mu)\,. \tag{2.16}$$

This ansatz contains four unknown parameters, $\alpha_{(1,2)\sigma}(\mathbf{k})$ and $E_{(1,2)\sigma}(\mathbf{k})$, which are fitted via (2.4) by equating the exactly calculated spectral moments (2.6)–(2.9). After simple manipulations we get the quasiparticle energies,

$$E_{(1,2)\sigma}(\mathbf{k})=\tfrac{1}{2}\{B_{\mathbf{k},-\sigma}+U+\varepsilon(\mathbf{k})\mp[(B_{\mathbf{k},-\sigma}+U-\varepsilon(\mathbf{k}))^2+4Un_{-\sigma}(\varepsilon(\mathbf{k})-B_{\mathbf{k},-\sigma})]^{1/2}\}\,, \tag{2.17}$$

with the corresponding spectral weights:

$$\alpha_{1\sigma}(\mathbf{k})=\frac{E_{1\sigma}(\mathbf{k})-B_{\mathbf{k},-\sigma}-U(1-n_{-\sigma})}{E_{1\sigma}(\mathbf{k})-E_{2\sigma}(\mathbf{k})}\,, \tag{2.18}$$

$$\alpha_{2\sigma}(\mathbf{k})=\frac{B_{\mathbf{k},-\sigma}+U(1-n_{-\sigma})-E_{2\sigma}(\mathbf{k})}{E_{1\sigma}(\mathbf{k})-E_{2\sigma}(\mathbf{k})}\,. \tag{2.19}$$

The quasiparticle energies (2.17) have the same structure as those of the so-called Hubbard I solution,[1] but with the decisive extension of the "band correction" $B_{\mathbf{k},-\sigma}$. It is this term which enables under certain circumstances a ferromagnetic moment ordering. According to (2.11) it consists of two parts, the k-independent $B_{S;-\sigma}$, being responsible for a possibly different shift of the two spin spectra, and the practically spin-independent "bandwidth-correction" $B_{W;\mathbf{k},-\sigma}$.

Most important for realizing spontaneous ferromagnetism is the "band shift" $B_{S;-\sigma}$ (2.12), which contains the higher equal-time-correlation function

$$\langle n_{i\sigma}c^{\dagger}_{i,-\sigma}c_{j,-\sigma}\rangle\,. \tag{2.20}$$

Fortunately, this quantity can be expressed by the one-electron spectral density $S_{\mathbf{k}\sigma}(E)$. This can be seen as follows. With the Hubbard-Hamiltonian we first get

$$[H,c^{\dagger}_{i,-\sigma}]_-=\sum_m(T_{mi}-\mu\delta_{mi})c^{\dagger}_{m,-\sigma}+Un_{i\sigma}c^{\dagger}_{i,-\sigma}\,. \tag{2.21}$$

This means for the expectation value

$$\langle n_{i\sigma}c^{\dagger}_{i,-\sigma}c_{j,-\sigma}\rangle=-\frac{1}{U}\sum_m(T_{mi}-\mu\delta_{mi})\langle c^{\dagger}_{m,-\sigma}c_{j,-\sigma}\rangle +\frac{1}{U}\langle[H,c^{\dagger}_{i,-\sigma}]_-c_{j,-\sigma}\rangle\,. \tag{2.22}$$

Using the spectral theorem[18] and the equation of motion of the time-dependent Heisenberg operators, we can write for the last term in (2.22)

$$\langle[H,c^{\dagger}_{j,-\sigma}]_-c_{j,-\sigma}\rangle=\frac{1}{\hbar}\int_{-\infty}^{+\infty}dE\,f_-(E)\int_{-\infty}^{+\infty}d(t-t')e^{(i/\hbar)(E-\mu)(t-t')}\left(-i\hbar\frac{\partial}{\partial t'}\right)S_{j,i,-\sigma}(t-t')$$

$$=\frac{1}{N\hbar}\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\int_{-\infty}^{+\infty}dE\,f_-(E)(E-\mu)S_{\mathbf{k},-\sigma}(E-\mu)\,, \tag{2.23}$$

$f_-(E)$ is the Fermi function:

$$f_-(E)=\{\exp[\beta(E-\mu)]+1\}^{-1} . \tag{2.24}$$

For the expectation value $\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle$ the spectral theorem yields

$$\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle=\frac{1}{N\hbar}\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \times\int_{-\infty}^{+\infty}dE\, f_-(E)S_{\mathbf{k}\sigma}(E-\mu) . \tag{2.25}$$

With the two-pole ansatz (2.16) we get for the average occupation number

$$n_\sigma=\frac{1}{N}\sum_{\mathbf{k}}\sum_{j=1}^{2}\alpha_{j\sigma}(\mathbf{k})f_-(E_{j\sigma}(\mathbf{k})) . \tag{2.26}$$

The very important spin-dependent band-shift $B_{S;-\sigma}$ (2.12) can now be expressed by (2.22), (2.23), (2.25), and (2.16):

$$B_{S;-\sigma}=\frac{1}{N}\sum_{\mathbf{k}}\sum_{j=1}^{2}\alpha_{j,-\sigma}(\mathbf{k})[\varepsilon(\mathbf{k})-T_0]f_-(E_{j,-\sigma}(\mathbf{k})) \times\left[\frac{2}{U}[E_{j,-\sigma}(\mathbf{k})-\varepsilon(\mathbf{k})]-1\right] +T_0n_{-\sigma}(1-n_{-\sigma}) . \tag{2.27}$$

The evaluation of the bandwidth-correction $B_{W;\mathbf{k},-\sigma}$ cannot be done with the aid of the one-electron spectral density, only. For the determination of the higher equal-time correlation functions in (2.14) one might define "higher" spectral densities, choosing a two-pole ansatz like (2.16) with the same quasiparticle energies $E_{(1,2)\sigma}(\mathbf{k})$ but different spectral weights. The latter are finally fixed by fitting the first two moments of the respective "higher" spectral density. If we apply this method to the expectation value (2.20), e.g., which we treat above in a rigorous manner, we get the correct result. For the bandwidth-correction $B_{W;\mathbf{k},-\sigma}$, however, we found by this method that in the strong correlation region ($U\gg W$) this term plays an unimportant, negligible role. Because of the quasi-spin-independence it does not influence the possibility of ferromagnetism. Furthermore, it disappears when averaged over the whole Brillouin zone:

$$\frac{1}{N}\sum_{\mathbf{k}}B_{W;\mathbf{k},-\sigma}=0 . \tag{2.28}$$

For narrow bands the bandwidth correction does hardly affect the energy spectra. So we neglect it from the very beginning.

Equations (2.17), (2.18), (2.19), (2.26), and (2.25) build a closed system, which must be solved self-consistently for the particle numbers n_σ, $n_{-\sigma}$, and the chemical potential μ, and that for any given total number n,

$$n=n_\sigma+n_{-\sigma} , \tag{2.29}$$

of band electrons per site ($0\le n\le 2$). The interesting question is now, under what conditions the spin degeneracy will be removed ($n_\sigma\neq n_{-\sigma}$), so that a spontaneous magnetization,

$$m=n_\uparrow-n_\downarrow , \tag{2.30}$$

appears. This question is surely influenced by the effective coupling constant U/W, which we consider to be very large, the lattice structure ["free" Bloch density of states $\rho_0(E)$], the degree of band filling n ($0\le n\le 1$; $n>1$ follows by particle-hole symmetry), and of course the temperature T.

If there is ferromagnetism in a certain parameter region, then the electron concentration and the structure dependence of the Curie temperature T_C must be the target of our investigations. T_C can be derived from the magnetization curve $m=m(T)$ as well as from the singularities of the paramagnetic, static susceptibility χ, at least as long as the phase-transition para-ferromagnetism is of second order:

$$\chi=\mu_0\mu_B\frac{N}{V}\left[\frac{\partial m}{\partial B}\right]_{T,B\to 0}^{(0)} . \tag{2.31}$$

The upper index indicates that the calculations are to be done for the paramagnetic system. To calculate χ we have to introduce in the model Hamiltonian (1.1) a field term H_z,

$$H_z=-\mu_B B(n_{i\uparrow}-n_{i\downarrow}) , \tag{2.32}$$

which, however, does not alter or even complicate the above presented theory. When differentiating the dimensionless magnetization m with respect to the field B, we have, however, to take into consideration that all expectation values are implicit functions of B.

The singularities of χ, regarded as a function of n at $T=0$ for a given lattice structure, indicate the instabilities of the paramagnetic electron system against ferromagnetic order. In the strong coupling limit ($U\gg W$) we find the following criterion for ferromagnetism:

$$0=\frac{1-n}{1-n/2}+\varepsilon_F\rho_0(\varepsilon_F)\left[1+\frac{1-n}{(1-n/2)^2}\right] +\eta\rho_0(\varepsilon_F)\frac{4}{2-n} . \tag{2.33}$$

Here we have written for abbreviation

$$\varepsilon_F=\frac{E_F}{(1-n/2)}-\frac{B_{S;0}}{(1-n/2)^2} , \tag{2.34}$$

$$\eta=\int_{-\infty}^{\varepsilon_F}d\varepsilon\,\varepsilon\,\rho_0(\varepsilon) . \tag{2.35}$$

E_F is the Fermi edge ($T=0$) and $B_{S;0}$ the band shift of the interacting, paramagnetic system, both being calculated self-consistently within our above-described procedure.

III. QUASIPARTICLE DENSITIES OF STATES

The complete system of Eqs. (2.17), (2.18), (2.19), (2.26), and (2.27) cannot be solved analytically. It contains some characteristic model parameters, one of which is the Bloch density of states $\rho_0(E)$ of the noninteracting electron system. We present results for a bcc lattice, which according to Jelitto[19] is described in tight-binding

approximation by

$$\rho_0(E)=2\sqrt{1-|E|}\times\ln^2\left(\frac{5.845}{|E|}\right)(16.6791+3.6364|E| +2.4880|E|^2) \text{ if } |E|\leq 1 , \tag{3.1}$$

$$\rho_0(E)=0 \text{ if } |E|>1 . \tag{3.2}$$

The total Bloch bandwidth is $W=2$ eV. We have evaluated our theory in the strong coupling limit for less than half-filled bands, so that for all relevant temperatures the upper quasiparticle subband is always empty:

$$0\leq n\leq 1;\quad f_-(E_{2\sigma})=0 . \tag{3.3}$$

The case $n>1$ follows immediately as a consequence of particle-hole symmetry.

What do we mean by "strong coupling limit?" We have observed that the results of our system of equations practically do not depend on U, when U exceeds a critical value of about $2W-3W$. The structure of the lower quasiparticle subband is then a function of T and n, but not of U. The upper subband is separated from the lower one by a gap of order U. Because of (3.3), however, it is always empty; therefore, it is not interesting for our study. From this reason we have plotted in Figs. 1–6 the lower subband only. In the strong coupling limit ($U\gg W$), the possibility of ferromagnetism is not determined by U.

Temperature T and carrier concentration n are the physical quantities in terms of which we have looked for magnetic solutions. It turns out that the nonmagnetic or paramagnetic situation ($m=0$) represents a mathematical solution for all n and all T. The respective quasiparticle density of states (QDOS)

$$\rho_\sigma(E)=\frac{1}{N\hbar}\sum_{\mathbf{k}} S_{\mathbf{k}\sigma}(E-\mu) , \tag{3.4}$$

which in this case is of course the same for $\sigma=\uparrow$ and $\sigma=\downarrow$, are plotted in Fig. 1 for $T=0$ and for various band occupations n. We have restricted the representation to the lower subband, which is partially occupied by n electrons per site. The main effect of the steady band filling is a band narrowing, roughly according to $(1-n/2)$. For $n=0$ the quasiparticle band is identical to the "free" Bloch band (3.1) because no interaction processes can happen. For $n=1$ the lower subband is completely filled, the bandwidth is half of that in the $n=0$-case.

For band occupations

$$n\geq n_{\mathrm{I}}=0.54 , \tag{3.5}$$

there appears a second solution of our system of equations, which is ferromagnetic. The corresponding quasiparticle densities of states $\rho_\uparrow$ and $\rho_\downarrow$ are plotted in Fig. 2. The minority spinband $\rho_\downarrow(E)$ is shifted to higher energies, so that $n_\uparrow$ becomes greater than $n_\downarrow$. With increasing band occupation n the $\downarrow$ bandwidth decreases substantially, while the width of the $\uparrow$ band becomes broader. The bandwidth of the σ spinband roughly scales with $(1-n_{-\sigma})$. As soon as n exceeds the critical value,

$$n_s^*=0.74 , \tag{3.6}$$

the $\downarrow$ subband lies entirely above the Fermi edge. The system is then ferromagnetically saturated ($m=n$). Since all carriers are now $\uparrow$ spin particles, they cannot interact within the Hubbard model. This is reflected by the fact that for $n\geq n_s^*$ the $\uparrow$ QDOS is again identical to ρ_0.

For band occupations

$$n\geq n_{\mathrm{II}}=0.79 \tag{3.7}$$

a second ferromagnetic solution (FMII) appears. The corresponding quasiparticle densities of states are plotted in Fig. 3. The main difference to the QDOS of FMI (Fig. 2) is that the Fermi edge lies always within the $\downarrow$ subband, therewith excluding ferromagnetic saturation. In the region $0.79\leq n\leq 1$ our system of equations has therefore three different solutions, one is paramagnetic (Fig. 1), and two are ferromagnetic (Figs. 2 and 3). It turns out (see Fig. 12) that always the solution with the highest polarization is stable.

Up to now we have discussed the quasiparticle densities of states $\rho_\uparrow(E)$ and $\rho_\downarrow(E)$ in terms of the band-filling n for the temperature $T=0$ K. Ferromagnetism becomes possible for $n\geq 0.54$. The QDOS of the ferromagnetically ordered system (FMI) exhibits a strong temperature dependence. Figures 4–6 show some typical examples. For $n=0.582$ (Fig. 4) and $n=0.664$ (Fig. 5) the minority subband becomes broader with increasing temperature, simultaneously being shifted to lower energies, where the position of the chemical potential is rather temperature independent. There is a continuous transition into the paramagnetic state ($\rho_\uparrow=\rho_\downarrow$) at about $T=T_C=521$ K for $n=0.582$ and $T=T_C=665$ K for $n=0.664$, respectively. For the higher occupation the temperature reaction of the QDOS is particularly sensitive in the small temperature region 660 K $\leq T\leq$ 665 K, leading to an abrupt but still continuous breaking down of the collective ferromagnetic order. For the example $n=0.749$, however, (Fig. 6) the temperature change between 709 and 710 K is so drastic that the para-ferromagnetic transition must be discontinuous. We shall come back to this point in the next section.

IV. SPONTANEOUS MAGNETIZATION

The self-consistently calculated magnetization m shows a strong T and n dependence (Fig. 7). As already read off

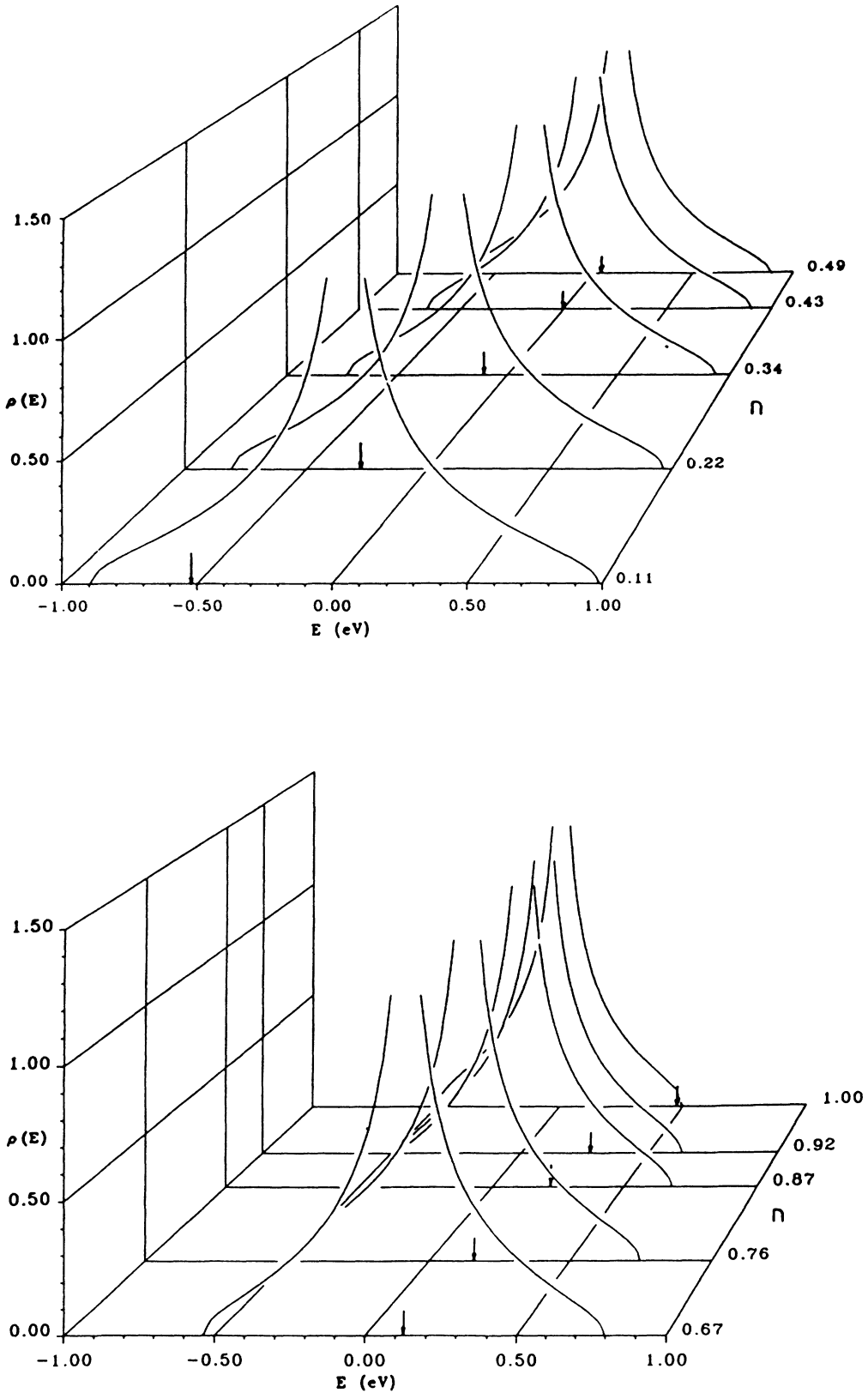

FIG. 1. Quasiparticle density of states $\rho_\uparrow=\rho_\downarrow=\rho$ of the lower "Hubbard subband" for the *paramagnetic* system at $T=0$ as function of energy E, and that for various band occupations n. Arrows indicate the position of the chemical potential μ. The Bloch density of states of the noninteracting system $\rho_0(E)$ is for a bcc lattice (3.1).

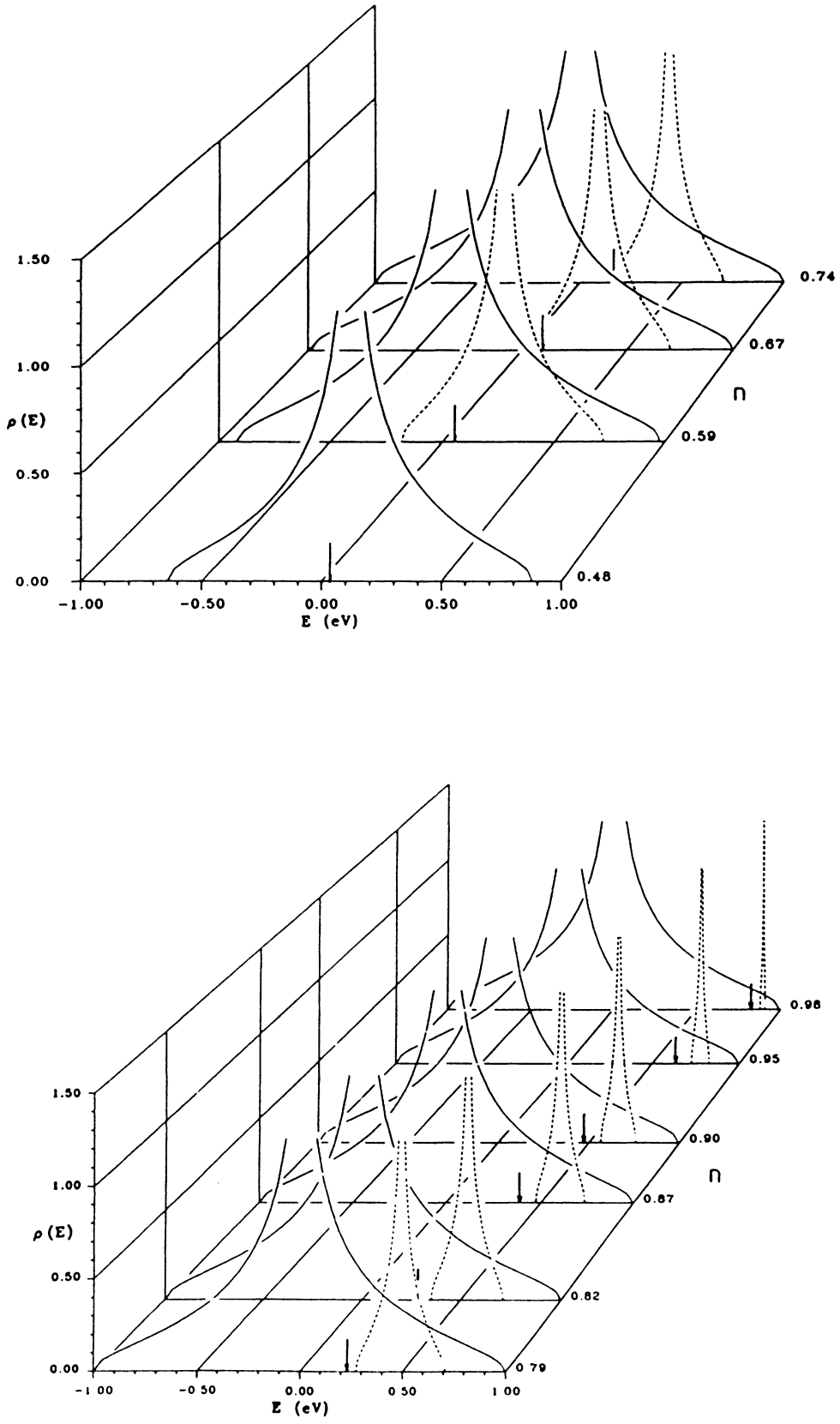

FIG. 2. The same as in Fig. 1, but for the ferromagnetic solution FMI. Solid lines indicate $\rho_\uparrow$, broken lines $\rho_\downarrow$.

from the QDOS at $T=0$ the spontaneous magnetization m of FMI sets in for $n=0.54$, increases very steeply with n, reaching the saturation ($m=n$) at $n=0.74$ (see Fig. 2). It intersects the m-n curve of the second ferromagnetic solution FMII, which starts at $n=0.79$, not before $n=1$. For finite temperatures we observe that this intersection point of the two ferromagnetic solutions shifts with increasing T to lower particle numbers n. It is a common

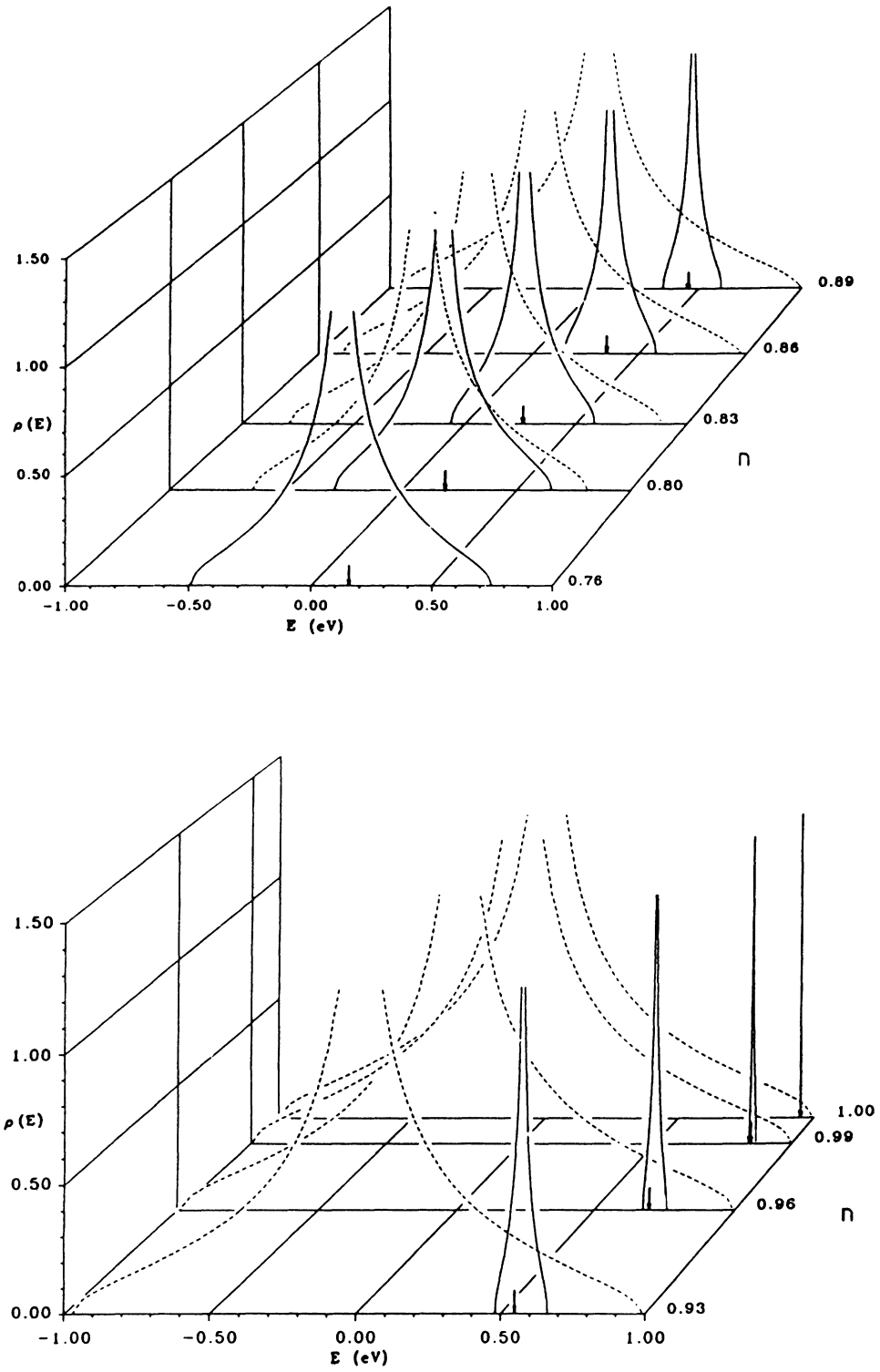

FIG. 3. The same as in Fig. 1, but for the ferromagnetic solution FMII. Broken lines for $\rho_\uparrow$, solid lines for $\rho_\downarrow$.

feature of all our results that for higher n than that of the intersection point ferromagnetism is excluded. The critical band occupation n_{I} and n_{II}, where FMI and FMII, respectively, set in, are functions of temperature. With raising T, n_{I} increases and n_{II} decreases. For $T>650$ K they are coinciding leading therewith to a kind of "magnetic island" in the m-n diagram. The "island" becomes smaller for higher T and disappears completely as soon as T exceeds 710 K.

Figures 3–6 show that finite m results from a relative shift of the two spin subbands $\rho_{\uparrow}$ and $\rho_{\downarrow}$ against one another. As already mentioned in the last section the decisive term for such a shift is the band correction $B_{k\sigma}$, defined in (2.11). In the strong coupled system the center

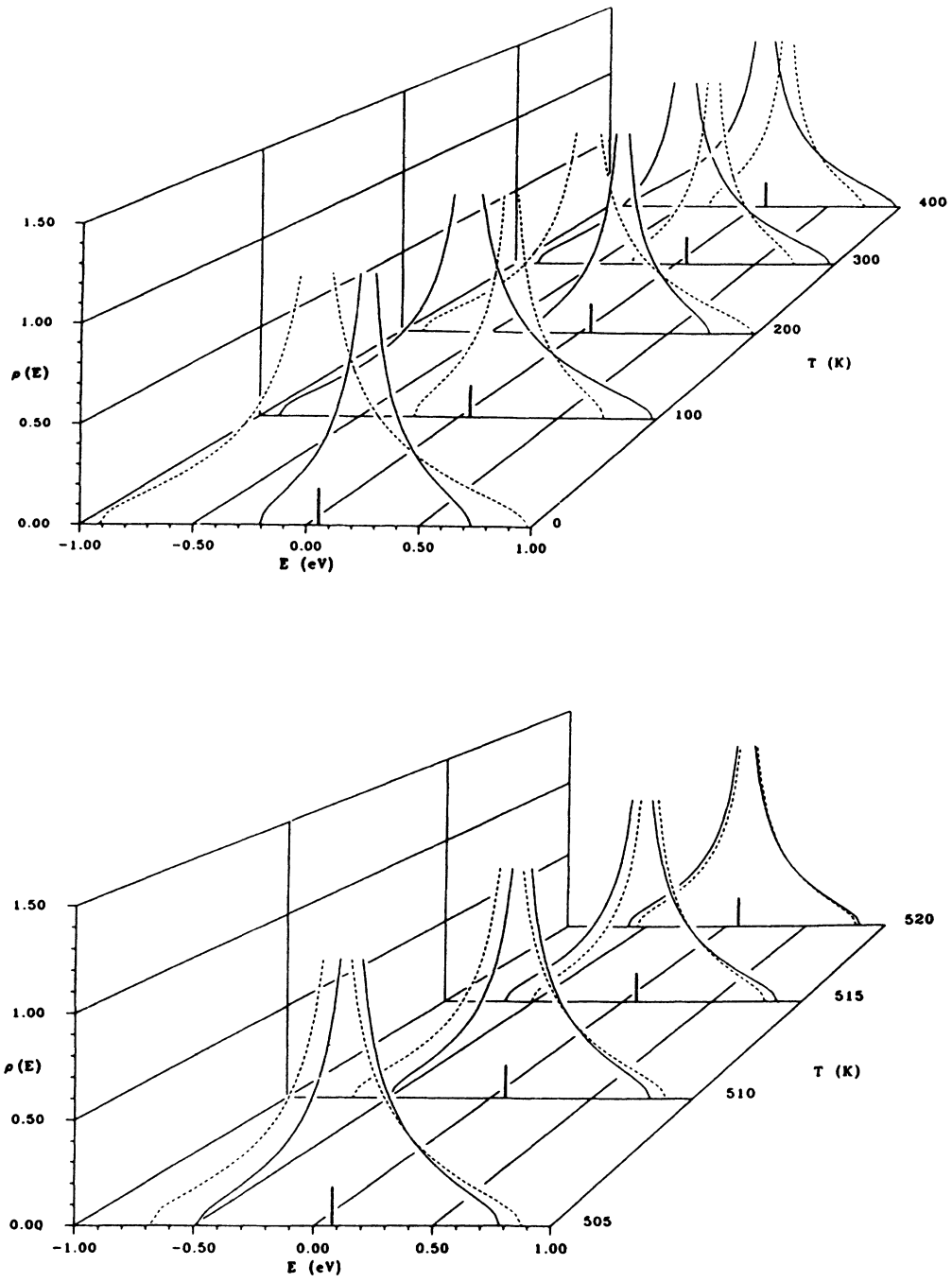

FIG. 4. Quasiparticle density of states ρ_{σ} as function of energy for a band filling $n=0.582$ and various temperature T. The lower-lying curve is always $\rho_{\uparrow}$, the higher-lying one is $\rho_{\downarrow}$. The bar indicates the position of the chemical potential.

of gravity of the σ band is located close to $T_0+n_{-\sigma}B_{-\sigma}$. Because of our assumption that $B_{W;\mathbf{k},-\sigma}\approx 0$, the band correction is k independent ($B_{\mathbf{k},-\sigma}\approx B_{-\sigma}$). The shift $n_{-\sigma}B_{-\sigma}$ is plotted in Fig. 8, explaining directly the appearance of spontaneous ferromagnetism (Fig. 7). In several approaches to the Hubbard model such a spin-dependent band shift is missing, as, e.g., in the Hubbard I solution or in certain coherent potential approximation (CPA) treatments,[20] showing at most some bandwidth effects. As a consequence ferromagnetism is predicted by the Hubbard I solution only for rather exotic Bloch densities of states $\rho_0(E)$ and in the low concentration limit,[21] the latter in clear contradiction to the exact Kanamori result.[11]

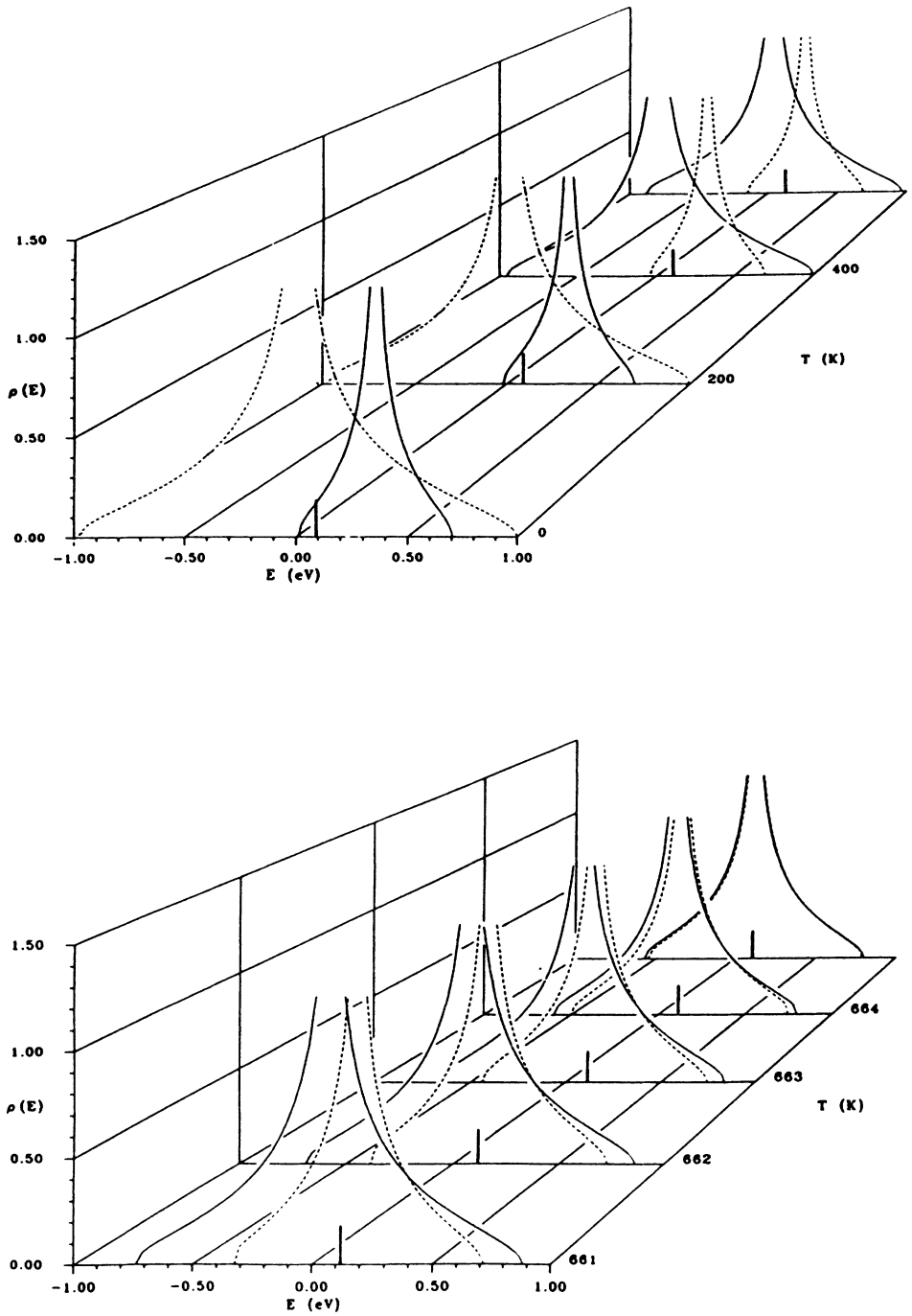

FIG. 5. The same as in Fig. 4 but for $n=0.664$.

The temperature dependence of the FMI magnetization shows for $0.54 \leq n \leq 0.81$ the typical behavior (Fig. 9), where the critical temperature T_C increases up to 710 K, being, therefore, in a rather realistic region. For $n > 0.81$, however, T_C decreases again down to $T_C = 0^+$ for the exactly half-filled band $n = 1$. In addition, the paramagnetic-ferromagnetic phase transition is then discontinuous. Mathematically this fact is due to the ap-

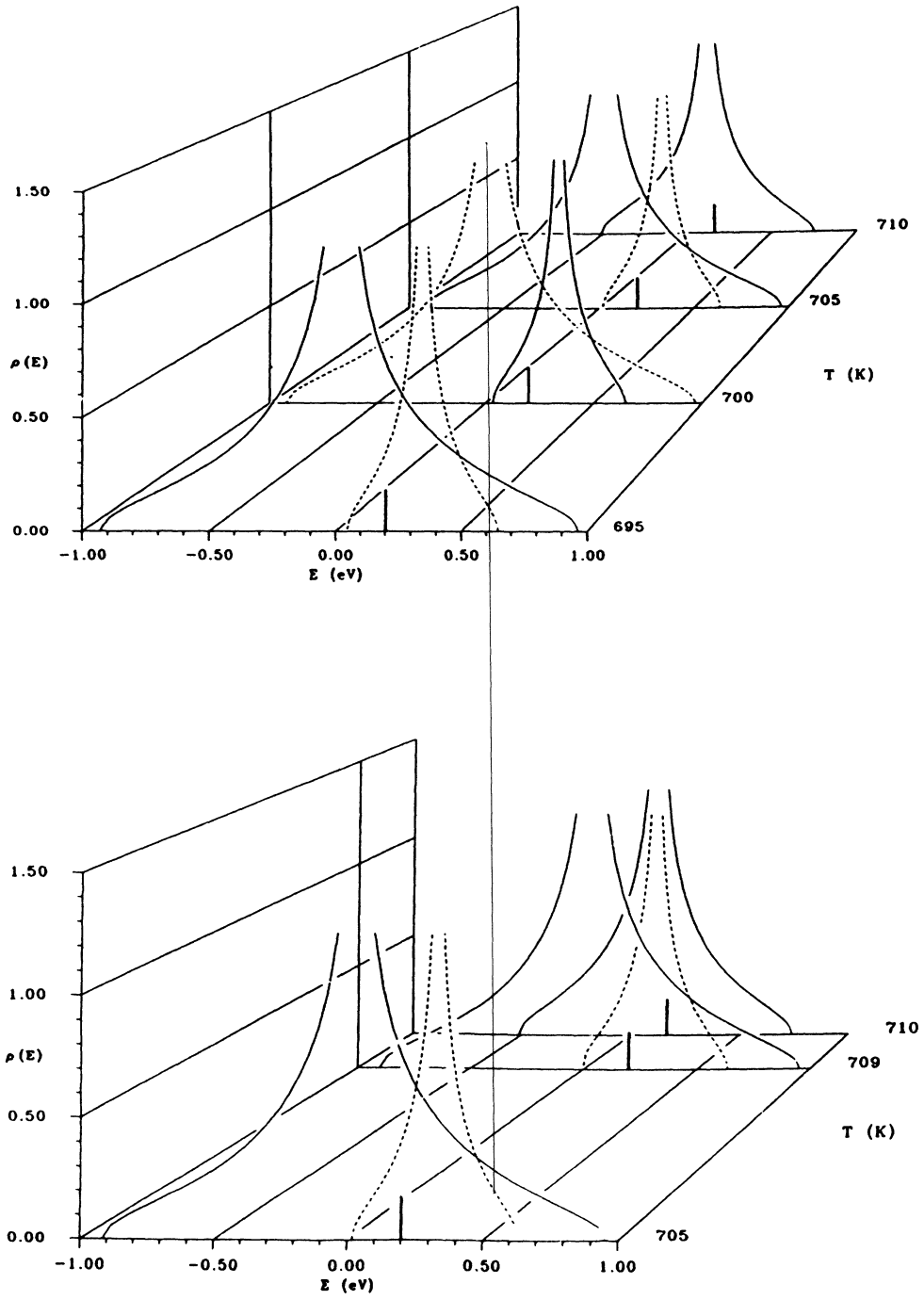

FIG. 6. The same as in Fig. 4 but for $n = 0.749$.

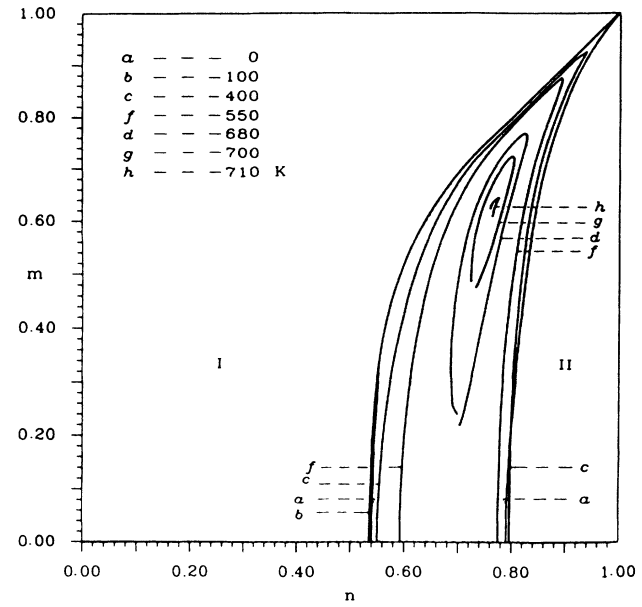

FIG. 7. Dimensionless magnetization $m = n_{\uparrow} - n_{\downarrow}$ as function of the average occupation number n for various temperatures between 0 K (a) and 710 K (h). The left part of the respective curve belongs to the stable ferromagnetic solution FMI, the right wing represents the unstable, second ferromagnetic solution FMII.

pearance of the "magnetic islands" in the m-n plane, as shown in Fig. 7. The T_C results, derived form the $m(T)$ curves, are gathered in Fig. 10. The left part of the graph up to the cross shows the T_C values which are connected with a second-order phase transition, the right part indicates first-order transitions. All (n,T) points *below* the graph belong to a stable ferromagnetic FMI solution,

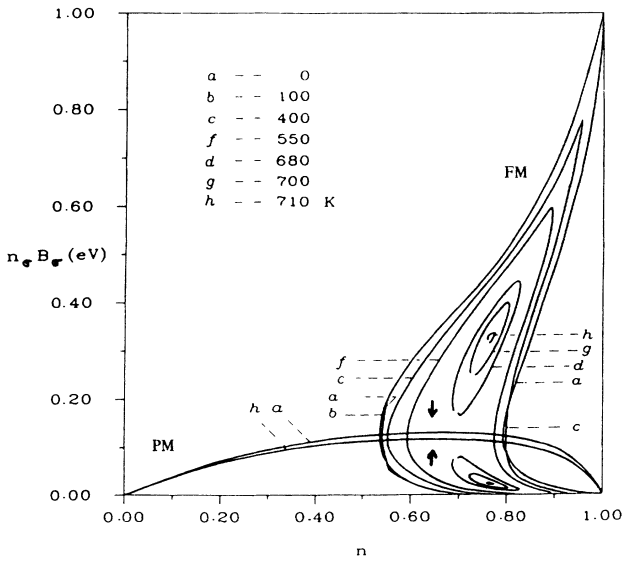

FIG. 8. Spin-dependent band shift $n_{-\sigma}B_{-\sigma}$ as function of band occupation n for various temperatures T (PM: paramagnetic solution, FM: ferromagnetic solution). $n_{-\sigma}B_{-\sigma}$ is the average shift of the lower σ-spin subband. The several curves directly correspond to those of Fig. 7. So the left part of the ferromagnetic solution (FM) belongs to FMI, the right to FMII.

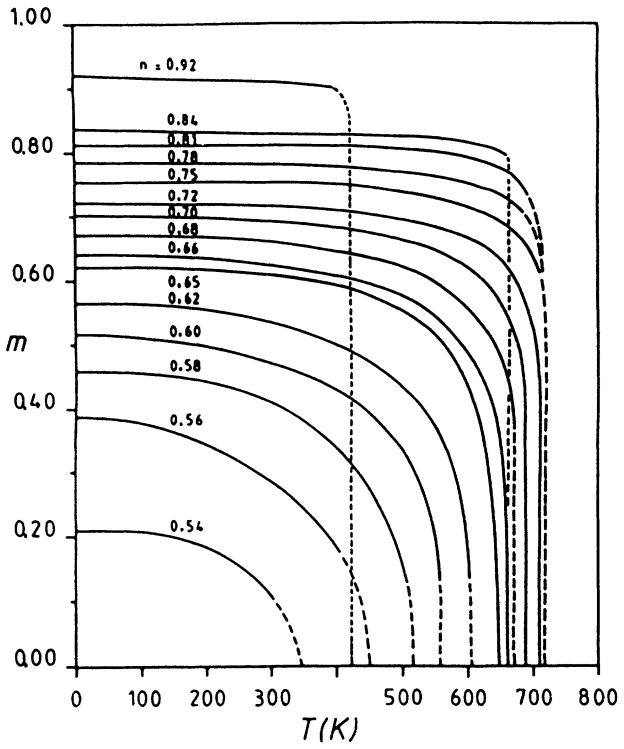

FIG. 9. Magnetization m as function of T for various values of the band occupation n.

outside the system is paramagnetic.

We have seen that there are wide parameter regions in which more than one solution exist. For testing the relative stability we have calculated the internal energy per site U/N, which can be expressed by the spectral density

$$\frac{U}{N} = \frac{1}{2N\hbar} \sum_{\mathbf{k},\sigma} \int_{-\infty}^{+\infty} dE\,[E + \varepsilon(\mathbf{k})] f_{-}(E) S_{\mathbf{k}\sigma}(E - \mu)\,, \tag{4.1}$$

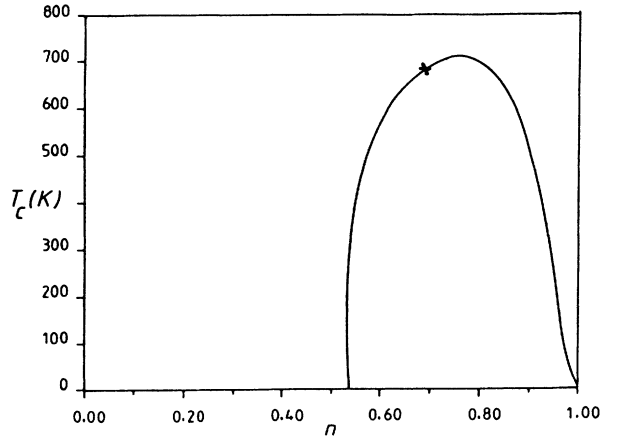

FIG. 10. Curie temperature T_C as function of band-occupation n. The left part of the graph up to the cross belongs to the second-order transitions, the right to first-order transitions.

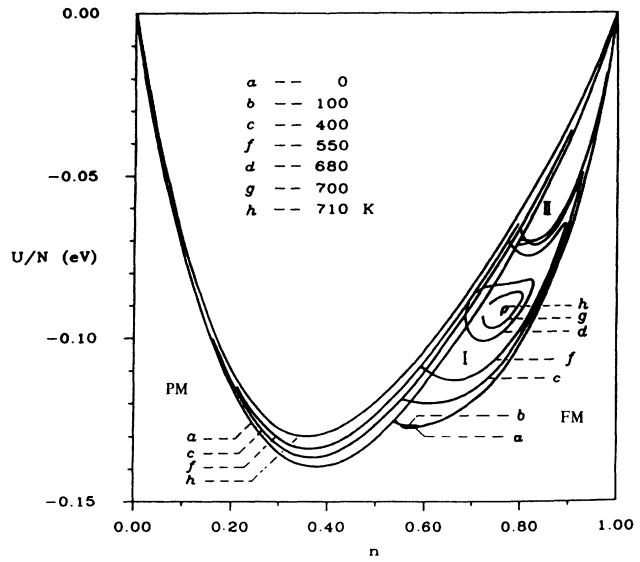

FIG. 11. Internal energy U/N as function of band occupation n for the same temperatures between 0 K (a) and 710 K (h) as in Figs. 7 and 8 (PM: paramagnetic; FM: ferromagnetic). I and II indicate the two ferromagnetic solutions FMI and FMII.

as well as the free energy F/N, which follows by

$$F(T)/N = U(0)/N - T\int_0^T \frac{dT'}{T'^2}\left[\frac{U(T')}{N} - \frac{U(0)}{N}\right]. \tag{4.2}$$

The results are plotted in Figs. 11 and 12. Both ferromagnetic solutions have distinctly smaller internal energies in the n regions, where they exist, than the ever existing paramagnetic solution. In the paramagnetic case U has the expected parabolic shape, while the ferromagnetic cases exhibit deviations, which become smaller with increasing temperature. In any case, the FMI solution is always more stable than the FMII solution.

In the temperature and band occupation regions, where FMI appears as a possible mathematical solution of our system of equations, FMI has the minimal free energy (Fig. 12), is therefore the stable solution. The differences between the free energies of the paramagnetic and the ferromagnetic solutions decrease with increasing temperature and disappear at $T = T_C$.

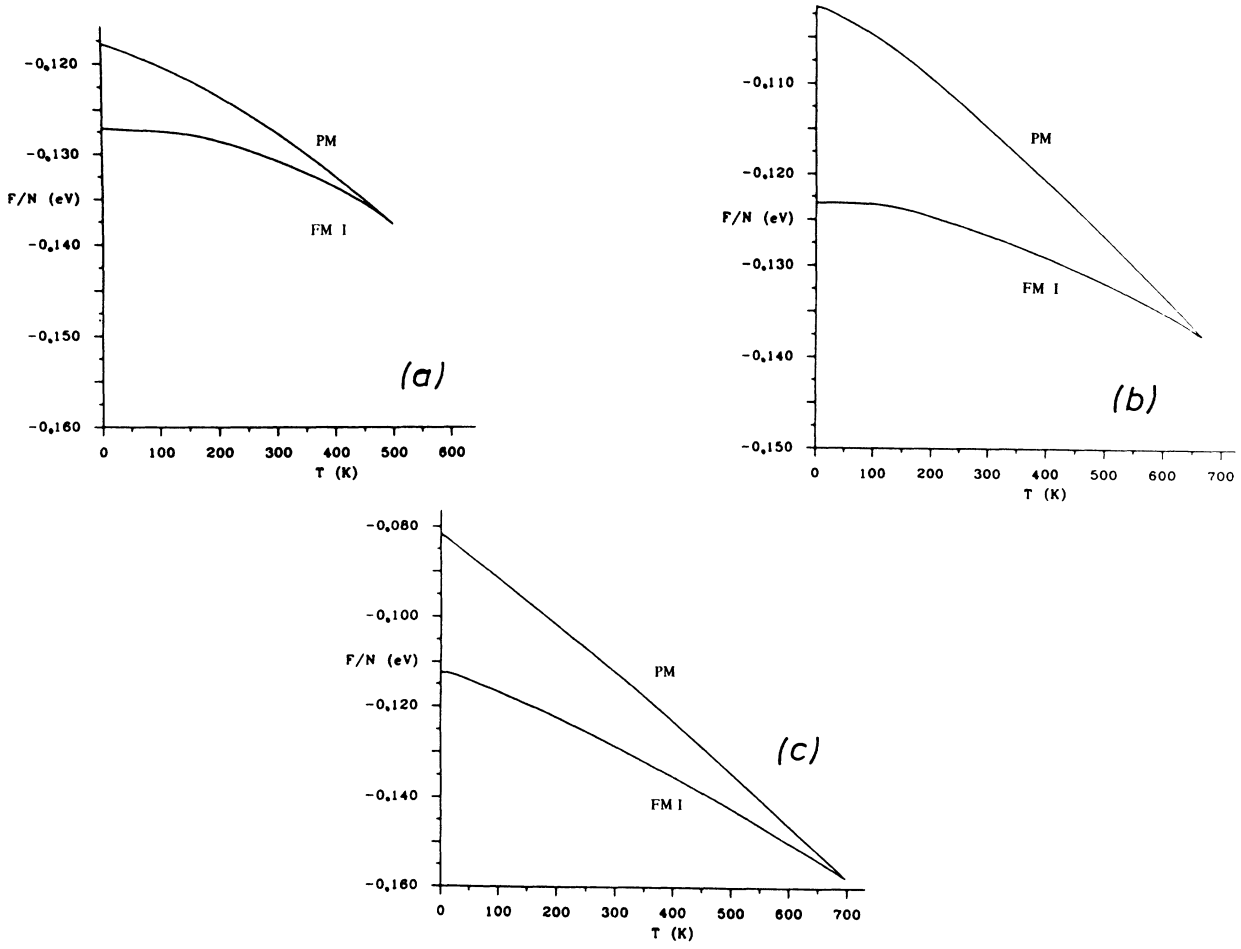

FIG. 12. Free energy per site F/N in dependence of temperature T for the paramagnetic (PM) and the ferromagnetic solution (FMI). (a) $n=0.58$, (b) $n=0.66$, (c) $=0.75$.

V. CONCLUSIONS

Starting with a self-consistent moment method, which needs as input only an "idea" about the general structure of the fundamental one-electron spectral density, being otherwise rigorous, we have inspected the strongly correlated Hubbard model for spontaneous ferromagnetism. As soon as the band occupation exceeds a critical value of $n=0.54$, ferromagnetic order appears as more stable than nonmagnetic disorder, at least at $T=0$. Under certain circumstances a second ferromagnetic solution appears, which is less polarized than the first one. The most polarized phase always has the minimum free energy, and is therefore stable. The Curie temperature T_C turns out to be strongly n dependent. The maximum of T_C for a bcc structure was found to be some 710 K.

The main advantage of our procedure is its very simple concept. We assume a two-pole ansatz for the spectral density, which is absolutely acceptable for the strongly correlated Hubbard model. The approach thus consists of a complete neglection of the electron damping, which could, however, be taken into consideration by applying a two-peak Gaussian ansatz for the spectral density. Such a procedure has been successfully performed for the s-f model of a ferromagnetic $4f$ insulator.[13] But we do not believe that the general question of whether or not spontaneous ferromagnetism is possible is much affected by the inclusion of electron damping.

In this paper we concentrated ourselves from the very beginning on ferromagnetic situations, excluding all antiferromagnetic possibilities. Antiferromagnetism will be studied in a forthcoming paper.[15] There we shall show that antiferromagnetism is stable against ferromagnetism in a small region around $n=1$. In the strong coupling limit ($U \gg W$), which we considered in this paper, this region is even extremely small. Although antiferromagnetic solutions exist in rather the same n range as the ferromagnetic solutions, for n not too close to 1 ferromagnetism appears to be more stable. The phase diagram, following from our moment method, is qualitatively similar to the Hartree-Fock result,[22] but very much more restrictive. For ferromagnetic solutions there exists a critical band occupation n_c and a critical U_c. The special case $n=1$ is antiferromagnetic for all $U \geq U$ (see also Ref. 23). Details will be published elsewhere.[15]

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