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Antiferromagnetism within a selfconsistent perturbation treatment of the symmetric periodic Anderson model

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Abstract. We study the infinite-dimensional symmetric periodic Anderson model within the selfconsistent second-order U-perturbation treatment, which is a conserving approximation and the simplest systematic improvement of the Hartree approximation. It is shown that the symmetric model exhibits an antiferromagnetic phase. The phase diagrams, the order of the phase transition and the density of states in the antiferromagnetic and in the paramagnetic phase are calculated and compared with the results obtained using the Hartree–Fock approximation.

1. Introduction

It was established a few years ago that the selfconsistent second-order perturbation treatment (SOPT) of the periodic Anderson model (PAM) in the limit of infinite dimensions is capable of reproducing qualitatively several of the characteristic properties of heavy fermions [1, 2]. This includes the many-body (Kondo) temperature scale, the gradual crossover from a high-temperature region of incoherent scattering to a coherent ground state which has heavy-quasiparticle excitations with long lifetimes near the Fermi surface, and the temperature dependence of quantities such as the specific heat, static magnetic susceptibility, resistivity and thermopower. Even though the temperature scale is not as expected, it appears to give a qualitatively correct picture of the physics of the homogeneous phase, even when the local Coulomb interaction, which is treated as a perturbation, cannot be considered small.

The selfconsistent SOPT is the simplest extension to the Hartree approximation (HA) that is still a conserving approximation. Since these are resummations to infinite order of the perturbation series for the grand canonical potential these approximations can in principle be valid also for large interactions. Both approximations might, however, be considered as truncated perturbation series for the Φ potential in the Kadanoff–Baym formalism (see [3]) (for fixed propagators), and in the absence of other small parameters they would not be expected to work very well unless the Coulomb repulsion is small. When the SOPT is nevertheless able to incorporate such nontrivial features over a wide temperature range in a single theory for the homogeneous phase, it is natural to ask what it will predict for other phases.

To complete the above picture one needs to consider the possibility of magnetically ordered phases in certain regions of the parameter space. This is expected from theoretical treatments of the model in the literature. Leder and Mühlschlegel [4] considered the magnetic phases in the PAM using the Hartree(–Fock) mean-field theory. They used a

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flat model conduction band density of states and found magnetic phases in a variety of parameter regimes. For the symmetric model they found the stable solutions to be either homogeneous or antiferromagnetic. The phase transition between the AF and homogeneous phase was found to be continuous. For other filling fractions they found more complicated situations including a ferromagnetic phase as well. The ground state of the symmetric PAM in one, two and three dimensions was discussed by Yamada and Yosida [5]. Apart from Hartree mean-field theory they used second-order perturbation theory with Coulomb repulsion for the homogeneous phase of the symmetric model, but their argument in favour of AF long-range order in three dimensions was by analogy to the s–d model. A slave-boson study by Möller and Wölfle [6] confirms the above picture of a continuous AF transition for large enough repulsion with half-filled bands. For other filling fractions spiral magnetic phases are stable down to quarter-filled bands for which the ground state is ferromagnetic. Recent quantum Monte Carlo simulations for the symmetric model in infinite dimensions show the same tendency towards AF ordering [7, 8].

In the light of the above discussion it is interesting to consider the AF phase transition in the PAM within the selfconsistent SOPT. Apart from partially completing the SOPT picture of the PAM, it should be able to provide information on the density of states (DOS) in the low-temperature AF phase, which it is not feasible to obtain from quantum Monte Carlo simulations, as well as the low-temperature phase diagram. Furthermore, in comparison with the case for the HA, it is possible to make statements regarding the role of fluctuations in determining the phase diagram and the properties near the transition.

In the following section we present the model and consider the Hartree approximation which already gives a qualitative picture of the phase diagram and serves as a guide for interpreting the SOPT results. The HA is useful because it allows for analytical calculations. The SOPT results are presented and discussed in section 3. The paper is closed with some concluding remarks in section 4. We set $\hbar$ and k_B equal to unity throughout this paper.

2. Basic equations and the Hartree approximation

We consider the simplest form of the PAM with only a spin degeneracy of the localized f-electron states, a simple tight-binding conduction band and only on-site hybridization between the conduction and f electrons. In our notation the Hamiltonian reads

$$H = -\frac{t}{\sqrt{2d}} \sum_{\langle r,r'\rangle,\sigma} c^{\dagger}_{r,\sigma} c_{r',\sigma} + V \sum_{r,\sigma} (f^{\dagger}_{r,\sigma} c_{r,\sigma} + c^{\dagger}_{r,\sigma} f_{r,\sigma}) + E_f \sum_{r,\sigma} f^{\dagger}_{r,\sigma} f_{r,\sigma} + U \sum_{r} f^{\dagger}_{r,\uparrow} f_{r,\uparrow} f^{\dagger}_{r,\downarrow} f_{r,\downarrow} \tag{1}$$

where $c_{r,\sigma}$ ($c^{\dagger}_{r,\sigma}$) annihilates (creates) a conduction band electron with spin σ at site r of the d-dimensional hypercubic lattice and $f_{r,\sigma}$ ($f^{\dagger}_{r,\sigma}$) is the similar operator for the f electron. The scaling of the hopping matrix element $-t/\sqrt{2d}$ ensures a nontrivial limit when $d \to \infty$ [9]. The local Coulomb repulsion is denoted by U, and V is the hybridization. Since we consider only the symmetric PAM, the local f level is at $E_f = -U/2$ and the chemical potential μ is pinned to zero.

In the limit of high dimensions the selfenergy becomes site diagonal [9], but it may depend on the site r. Here we allow for an antiferromagnetic ordering in a hypercubic lattice, so the selfenergy's spatial variation can only depend on the sublattice. We will, without loss of generality, assume that the spontaneous (staggered) magnetization will occur parallel to the spin quantization axis such that the one-particle Green function and selfenergy are

spin diagonal. Furthermore we have by symmetry that the up-spin f-electron selfenergy on one sublattice is equal to the down-spin selfenergy on the other sublattice. Together these simplifications imply that we need only consider the site-diagonal matrix elements of the Green function and selfenergy on one of the sublattices. We can therefore drop the coordinate indices, but keep spin, time (or frequency) and particle (c or f) indices. The selfenergy has nonzero matrix elements only between f-electron states, so for this quantity we will not write the particle indices explicitly.

On an AB lattice the site-diagonal matrix elements of the Green function read

$$G_\sigma^{cc}(z) = \left(z_c - \frac{V^2}{z_{f,-\sigma}}\right)\frac{g_0(Z)}{Z} \tag{2}$$

$$G_\sigma^{ff}(z) = \frac{1}{z_{f,\sigma}}\left(1 + \frac{V^2}{z_{f,\sigma}}G_\sigma^{cc}(z)\right) \tag{3}$$

where

$$z_c = z + \mu \tag{4}$$

$$z_{f,\sigma} = z + \mu - E_f - \Sigma_\sigma(z) \tag{5}$$

$$Z = \sqrt{\left(z_c - \frac{V^2}{z_{f,\uparrow}}\right)\left(z_c - \frac{V^2}{z_{f,\downarrow}}\right)}. \tag{6}$$

The quantity g_0 is the Green function for tight-binding electrons on a hypercubic lattice of infinite dimension:

$$g_0(z) = -\mathrm{i}\sqrt{\frac{\pi}{2t^2}}\,\mathrm{sgn}(\mathrm{Im}\ z)\exp\left(-\frac{z^2}{2t^2}\right)\mathrm{erfc}\left(-\mathrm{i}\frac{\mathrm{sgn}(\mathrm{Im}\ z)z}{\sqrt{2t^2}}\right) \tag{7}$$

and corresponds to a Gaussian DOS. It is convenient to split the f-electron self-energy into instantaneous (Hartree) and frequency-dependent (correlation) parts:

$$\Sigma_\sigma(z) = \frac{1}{2}n_f U - \sigma m_f U + \Sigma_\sigma^c(z). \tag{8}$$

In the symmetric PAM the f-electron filling fraction $n_f = 1$ and the spin-independent Hartree contribution will cancel against E_f in all equations. The staggered f-electron magnetization per site m_f is given by

$$m_f = \frac{T}{2}\sum_n \left(G_\uparrow^{ff}(\mathrm{i}\omega_n) - G_\downarrow^{ff}(\mathrm{i}\omega_n)\right) \tag{9}$$

where $\omega_n = (2n+1)\pi T$ denotes the Matsubara frequencies (T is the temperature). Assuming a continuous phase transition one can look for the parameter values that give a divergent antiferromagnetic susceptibility in the homogeneous phase. This occurs when

$$1 = T\sum_n g(\mathrm{i}\omega_n) \tag{10}$$

where

$$g(z) = \lim_{m_f\to 0}\frac{G_\uparrow^{ff}(z) - G_\downarrow^{ff}(z)}{2m_f}. \tag{11}$$

When Σ_σ^c is explicitly given as a functional of $G_\uparrow^{ff}$ and $G_\downarrow^{ff}$ in equation (8) one can solve equations (3)–(9). Besides the Hartree approximation $\Sigma_\sigma^c = 0$ we will here employ self-consistent second-order perturbation theory in which the selfenergy is given (in the imaginary-time representation) by

$$\Sigma_\sigma^c(\tau) = -U^2 G_\sigma^{ff}(\tau)G_{-\sigma}^{ff}(\tau)G_{-\sigma}^{ff}(-\tau). \tag{12}$$

When there are magnetic solutions of the selfconsistent equations they always appear in pairs as required by symmetry and one always finds a homogeneous solution. To judge the stability of the solutions it is then convenient to add to the Hamiltonian a term $H_{\rm ext}$ with an external staggered field h coupled linearly to the f-electron spin:

$$H_{\rm ext} = -\frac{h}{2}\sum_r (-1)^{\sum_i |r_i|}(f^\dagger_{r,\uparrow} f_{r,\uparrow} - f^\dagger_{r,\downarrow} f_{r,\downarrow}). \tag{13}$$

One can still find several solutions in some ranges of h, such that $m_f = m_f(h)$ is multivalued, but when inverting the different branches of solutions one can construct a hypothetical $h = h(m_f)$ isotherm which is single valued. For high temperatures it is a valid physical isotherm and for low temperature we obtain a physical isotherm from a Maxwell construction.

Equation (10) above can be converted to real frequencies as

$$1 = \int_{-\infty}^{\infty} {\rm d}\omega \; f(\omega)\rho_g(\omega) \tag{14}$$

where f is the Fermi function $f(x) = 1/(\exp(x/T)+1)$ and $\rho_g(\omega)$ is the spectral function of $g(\omega)$ from equation (11). In the Hartree approximation it reduces to

$$1 = -U\int_{-\infty}^{\infty} {\rm d}\omega \; f(\omega)\frac{2\omega^2 - V^2}{\omega(\omega^2 - V^2)}\rho_0(\omega) \tag{15}$$

where the integral should be understood as a principal value and

$$\rho_0(\omega) = \frac{V^2}{\omega^2}\exp\left(-\frac{1}{2t^2}\left(\omega - \frac{V^2}{\omega}\right)^2\right)\Big/\sqrt{2\pi t^2} \tag{16}$$

is the f-electron spectral function for $U = 0$. The integral is finite, and can be evaluated exactly for $T = 0$, so there is a critical value $U = U_c$ at which AF order sets in:

$$\left(\frac{U_c}{t}\right)^{-1} = {\rm e}^{(V/t)^2}\left[K_1((V/t)^2) - \frac{1}{2}K_0((V/t)^2)\right]\Big/\sqrt{2\pi}\ . \tag{17}$$

$K_n(x)$ is a modified Bessel function (see [10]).

In the limit of large V/t we have $U_c \sim 4V$. To obtain the AF phase, U will then be the largest parameter in the Hamiltonian, and we cannot expect our approximation to be valid. For small hybridization we obtain $U_c \sim \sqrt{2\pi}V^2/t$. In this limit we can also find a relation between the dimensionless critical temperature $\theta = tT_N/V^2$ and $u = U/U_c$ near $u = 1, \theta = 0$:

$$u - 1 = \sqrt{\frac{8\pi}{3}}\left(\frac{1}{\theta}\right)^{1/3}\exp\left(-\frac{3}{2}\left(\frac{1}{\theta}\right)^{2/3}\right). \tag{18}$$

Thus θ drops very quickly to zero when $u \to 1^+$.

For $u < 1$ the system is in the homogeneous phase and the Hartree electron spectral functions f and c are identical to the noninteracting ones. See the example in figure 1—it shows two subbands separated by a hybridization 'gap'. The gap is not a true gap, as can be seen from equation (16), but the DOS is zero at the Fermi level and dies exponentially as it is approached. This is an artifact of hypercubic lattices in high dimensions. When the spontaneous symmetry breaking occurs, the Brillouin zone halves, and each subband breaks into two new subbands, with inverse-square-root divergencies at one of the gap edges as in figure 1. The gap around the Fermi level now becomes a true gap with edges at $\omega = \pm m_f U$. The other band edges are located at $\omega = \pm m_f U/2 - \sqrt{(m_f U/2)^2 + V^2}$ and $\omega = \pm m_f U/2 + \sqrt{(m_f U/2)^2 + V^2}$.

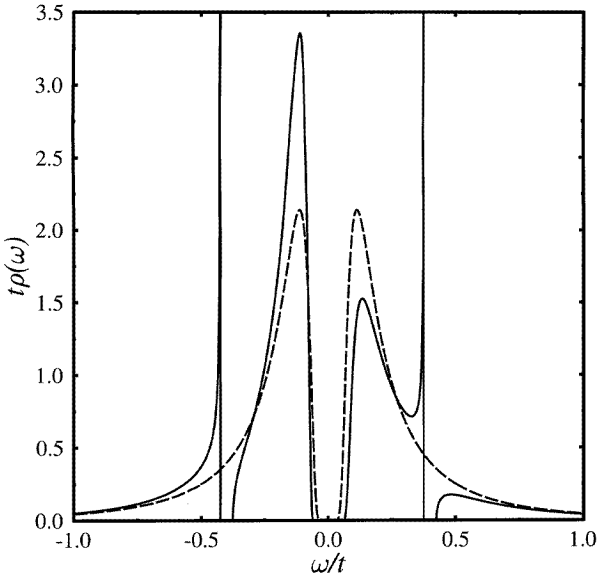

Figure 1. Hartree f-electron spectral functions for $V = 0.4t$. Dashed line: the homogeneous phase (like a noninteracting one). Solid line: the antiferromagnetic phase with $m_f U = 0.05t$.

3. Numerical SOPT

To judge the effects of fluctuations we have investigated the instabilities towards AF ordering numerically within the SOPT approximation described in the previous section. The finite-temperature calculations were done in the Matsubara frequency or imaginary-time representation. The high-frequency tails of the Green functions and selfenergies were then approximated by terminated continued fractions that are exact (for SOPT) up to and including the third and first moment respectively. Spectral functions and selfenergies for real frequencies were calculated directly for real frequencies. In both cases FFT methods were employed, together with interpolation techniques to ensure correct results for the highest frequencies stored. Cubic spline interpolation was used for transformations from imaginary time to Matsubara frequencies, and simple linear interpolation for the real-frequency calculations. In the latter case the staggered magnetization from a Matsubara frequency calculation was used as the input to the calculation.

Figure 2 shows the temperature of the divergence of the AF susceptibility as a function of U/t for various values of V/t. The form is qualitatively what one could expect from the Hartree result. For U smaller than some $U_c(V)$ there is no AF phase, whereas for $U > U_c$ the susceptibility diverges for some temperature T_c, and the system must be in the AF phase below this temperature. When the f electrons order antiferromagnetically, so do the conduction electrons, but with the opposite direction of the moments on the same site. Because T_c goes to zero so quickly when $U \to U_c$, we can estimate $U_c = U_c(V, t)$ from these calculations just by taking the result for some low enough temperature; see also below. Using these results we have also checked the quantity $\ln(\theta^3(u-1))$ versus $\theta^{-2/3}$ for various values of V/t in the range 0.02–0.4 (not shown here). The dimensionless quantities θ and u are the same as in the previous section, but using the SOPT U_c in the definition of u. We find a linear dependence within the numerical accuracy. Thus the relation between

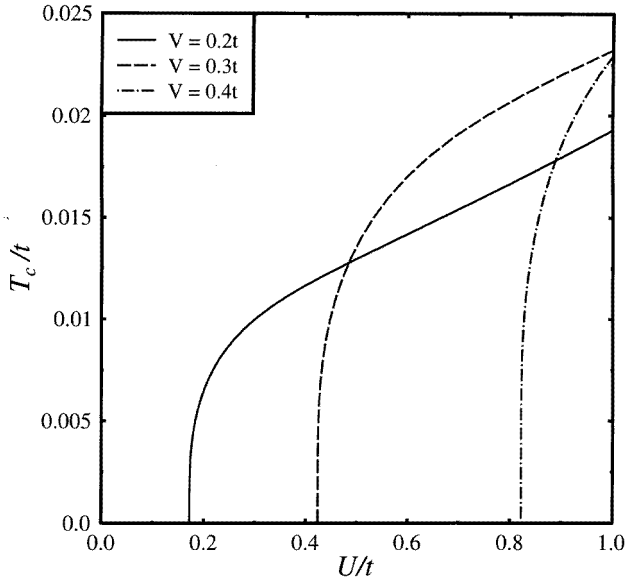

Figure 2. The temperature where the antiferromagnetic f-electron susceptibility diverges.

u and θ appears to be the same as for the HA (see equation (18)), except for the changes in scale. The linear behaviour of T_c as a function of U/t for large values of this parameter is contradictory to recent QMC results [7, 8] which show a decreasing T_c for large U/t. The SOPT does not reproduce this behaviour—which is not surprising, as the SOPT is a weak-coupling expansion for small U/t and does not properly describe the strong-coupling limit of large U/t.

In order to check whether or not the predicted phase transition really is continuous we have calculated $h = h(m_f)$ isotherms for various values of U and V. Upon lowering the temperature the AF phase becomes more stable at zero field than the homogeneous phase, and this happens at a temperature ($T_c \approx 0.0072t$ for $U = V = 0.2t$) which is larger than the critical temperature determined from the condition that the (zero-field) susceptibility diverges. Therefore, the transition found here within the SOPT must be first order as indicated in figure 3. Actually it is first order for a wide range of parameter choices except possibly for U very close to U_c or for V/t larger than the values that we have considered. This is similar to the prediction of the SOPT for the Hubbard model [11] for large enough U. First-order transitions have not been obtained within other investigations of AF for the PAM in finite dimensions mentioned in the introduction. Therefore, one cannot exclude the possibility that the first-order transition may be an artifact of the SOPT, though to our knowledge there is no rigorous argument against the existence of AF first-order transitions. Even if it is an artifact, this means only that the SOPT fails to describe the finite-temperature phase transition correctly, but it does not remove the approximation's relevance to the low-temperature ordered phase or to the homogeneous phase.

The zero-temperature phase diagram arising from extrapolating the T_c-curves discussed above is shown in figure 4. For small V/t the ratio $U_c t/(\sqrt{2\pi}V^2)$ does not approach unity, but is rather about 1.5. The dependency on V/t is also much stronger in the case of the SOPT than for the HA. Thus the fluctuations quantitatively influence the phase diagram considerably, and are nowhere negligible along the phase transition line.

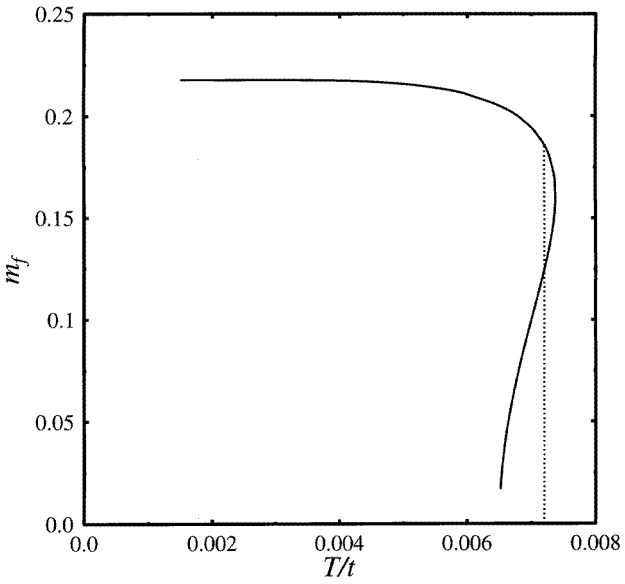

Figure 3. The staggered f-electron magnetization, m_f. Solid line: SOPT solutions to $h(m_f) = 0$. Dotted line: the first-order transition.

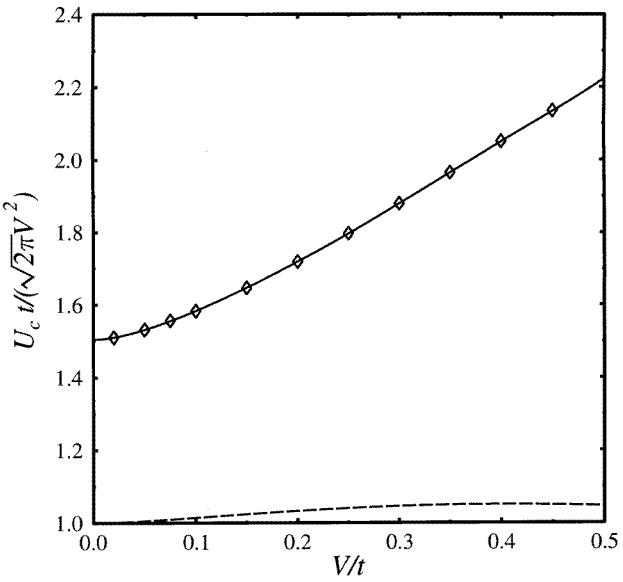

Figure 4. The critical interaction $U_c t/\sqrt{2\pi}V^2$ versus V/t. Solid line: the SOPT. Dashed line: the HA.

Figures 5 and 6 show the f-electron DOS and selfenergies respectively of one sublattice for two temperatures, one above and one below the phase transition, when $U = V = 0.2t$. In the ordered phase the most apparent difference from the HA spectral function is that the inverse-square-root singularities have disappeared completely and the additional gaps

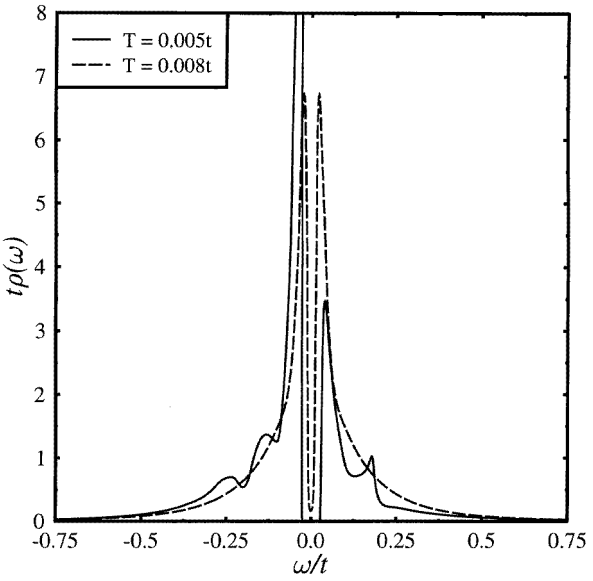

Figure 5. The f-electron DOS for $U = 0.2t$, $V = 0.2t$.

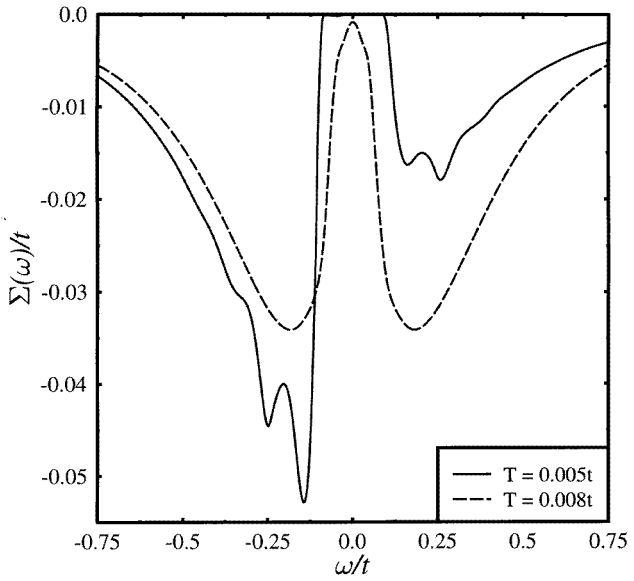

Figure 6. The f-electron selfenergy for $U = 0.2t$, $V = 0.2t$.

are smeared out. If one looks at the selfenergy it is clear that this effect is simply due to the finite lifetime resulting from the selfenergy imaginary part, which is finite even at zero temperature this far away from the Fermi level in the central gap. The temperature is quite low, the staggered magnetization is almost saturated and the gap around the Fermi level is quite distinct. Therefore the state should be representative for the low-temperature phase including the ground state, and the smearing is not a finite-temperature effect. Comparing

to the homogeneous phase we see that apart from the obvious shifting of spectral weight to the lower subband there are some structures left that are not present in the homogeneous solution and can be attributed to the symmetry breaking.

4. Concluding remarks

In summary we have investigated the symmetric PAM, which is a model relevant for the description of heavy-fermion systems. Treating the PAM within the Hartree approximation and within its simplest systematic improvement we investigated if and where AF solutions are obtained. Defining T_c as the temperature where the susceptibility diverges, we calculated the dependence of T_c on the model parameters, finding a vanishing T_c below a lower critical value U_c and a linear dependence on U for large U. When calculating the staggered magnetization as a function of a staggered magnetic field h for different temperatures, a finite order parameter (finite magnetization for $h = 0$) and thus a stable AF solution was already obtained for temperatures larger than the above-mentioned T_c, which is a clear indication of a first-order phase transition. We cannot exclude the possibility that this may be an artefact of the SOPT, because such first-order transitions are not obtained within other investigations of AF within the PAM and are usually not seen in experiment. Furthermore we have calculated the dependence of the critical interaction U_c on the hybridization, and found strong corrections in the SOPT as compared to the Hartree result. Finally we have calculated the f-electron density of states in the homogeneous phase and the ordered phase and found, besides the opening of an antiferromagnetic gap (larger than the hybridization pseudo-gap), additional fine structures in the subbands within the AF phase.

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