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The one-dimensional periodic Anderson model: A mean field study

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Abstract

The ground-state properties of the symmetric Anderson lattice model in one dimension have been studied using a local mean-field decoupling approach and a renormalized perturbation expansion for the self-energy. The total energy, the local moment, the effective hybridization, the density of states, and the momentum distribution function have been calculated as a function of the Coulomb interaction U, the hybridization V, and the band filling. At half-filling, the mean-field results for the antiferromagntic state are in good agreement with those of quantum Monte Carlo simulations. t quarter filling and at relatively large $U/2t$ values, the antiferromagnetic state is favored compared to the ferromagnetic state.

Keywords: Heavy fermions; Periodic Anderson model

The periodic Anderson model (PAM) is thought to describe the general behavior of "heavy-fermions" systems, and has thus been an object of great theoretical interest. At low temperatures, the heavy fermions exhibit different kinds of ground states: antiferromagnetic, superconducting, spin density waves, charge density waves, Kondo-like, and semiconducting [1]. A variety of approximate and perturbative techniques [2–4] have been applied to the PAM. Quantum Monte Carlo simulations [5] and density-renormalization-group (DMRG) [6] calculations of finite PAM chains at half-filling have provided physical insight into the ground-state properties. Steiner et al. [7] have applied the second-order perturbation theory in the fluctuations around the mean-field result and found good agreement with the Monte Carlo results.

In this paper we report results for the ground-state properties of the one-dimensional symmetric nondegenarate PAM, employing a local mean-field approximation (LMFA) and a renormalized perturbation expansion for the self-energy [8]. The ground-state properties, i.e. the total energy, the f-magnetic moment, the effective hybridization, the f- and c-projected spectral weight function are in good agreement with quantum Monte Carlo simulations [5] and DMRG calculations [6] under the extreme conditions of the one dimensionality. The good agreement of the LMFA results puts the LMFA on a firmer basis in two and three dimensions, where no results are available and other approaches may be limited. Even though the method is not an exact one, it has the advantage that the problem becomes simple enough to generalize it to the calculation of finite-temperature properties and that it allows the study of all regimes in parameter space.

Although we have examined a range of different parameters, most of the results presented in this paper have been obtained for one-dimensional PAM in the symmetric case ($E_f = -U/2$) at half-filling with $V = 0.375$ and $\varepsilon_k = -2t\cos k$ ($t = 0.5$), in order to be able to compare them directly with those of Monte Carlo and DMRG calculations. In Fig. 1 we show the LMFA results (solid curve) for the ground-state energy of the antiferromagnetic structure (solid line) versus the Coulomb

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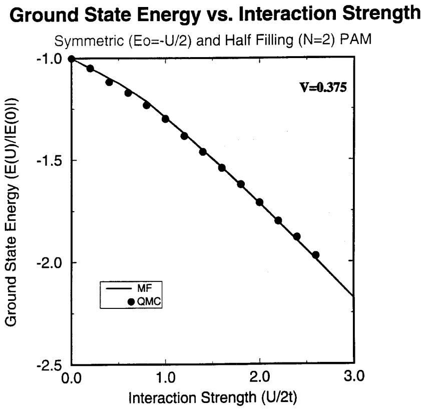

Fig. 1. The normalized ground-state energy (solid line) for the antiferromagnetic structure $E(U)/E(0)$ plotted versus $U/2t$. Here $t = 0.5$ and $V = 0.375$. The closed circles are the Monte Carlo results.

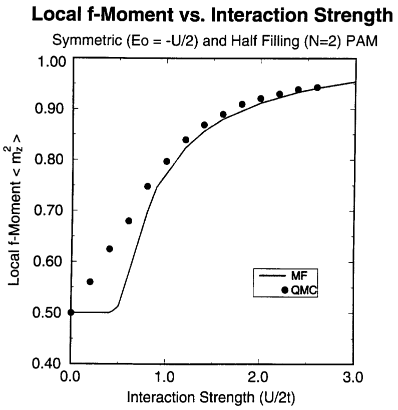

Fig. 2. The square of the f-orbital magnetic moment $\langle m_{\rm f}^2 \rangle$ versus $U/2t$ for $t = 0.5$ and $V = 0.375$. The closed circles are the Monte Carlo results.

interaction $U/2t$ and compare them with the Monte Carlo results (closed circles). The excellent agreement of the LMFA results with previous calculations in the entire $U/2t$ range indicates that the LMF approach yields accurate energetics. As a further corroboration of the validity of our approach, we also compare our results for the square of the local f moment, $\langle m_{\rm f}^2 \rangle = 1 - 2\langle n_{{\rm f}\uparrow} n_{{\rm f}\downarrow} \rangle$. The LMF f moment (solid curve), $\langle m_{\rm f}^2 \rangle$ is plotted versus $U/2t$ in Fig. 2 and compared with the Monte Carlo results (solid circles). For large $U/2t$, the double occupancy is reduced by the Coulomb repulsion and $\langle m_{\rm f}^2 \rangle$ approaches unity. The agreement between the LMFA and the Monte Carlo results is very good for $U/2t \geqslant 1$. Note that as expected, for small $U/2t$ values ($U \leqslant U_{\rm c} = 1.2t$) the

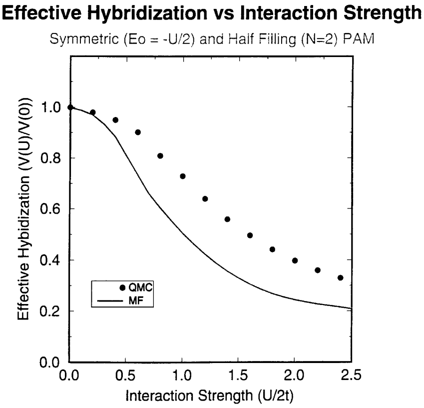

Fig. 3. The normalized hybridization matrix element $\langle f_{i\sigma}^{\dagger} c_{i\sigma} + {\rm h.c.} \rangle$ versus $U/2t$ for $t = 0.5$ and $V = 0.375$. The closed circles are the Monte Carlo results.

LMFA gives a paramagnetic solution and $\langle m_{\rm f}^2 \rangle = \frac{1}{2}$ is constant. Here, $U_{\rm c}$ is the critical value of the Coulomb interaction for the onset of long-range antiferromagetic order, which decreases as V decreases. The induced conduction-electron moment $\mu_{\rm c}$ is small (~ 0.1) and is aligned antiferromagnetically with the local f moment, in agreement with the Monte Carlo simulations [5].

In the presence of U, the effective hybridization $\langle f_{i\sigma}^{\dagger} c_{i\sigma} + c_{i\sigma}^{\dagger} f_{i\sigma} \rangle = \frac{1}{2} \vartheta E_0 / \vartheta V$ is reduced as a result of the Coulomb correlations [5]. The LMFA results for the normalized effective hybridization is plotted versus $U/2t$ in Fig. 3 and compared with the Monte Carlo results (closed circles). The effective hybridization decreases as $U/2t$ increases with the LMFA results being consistently underestimated by about 10–20%.

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