On the ground state energy of the periodic Anderson model: exact results for $d = 1$

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Abstract

We derive the exact ground state energy of the asymmetric periodic Anderson model for $d = 1$ in several different parameter regimes, for example in the Kondo limit, and find that exponentially small terms do not exist. Obviously the appearance of a low, Kondo-like energy scale is *not generic* for the periodic Anderson model. The exact ground state energy is compared with the results obtained from slave-boson mean-field theory and the Gutzwiller approximation.

The periodic Anderson model (PAM) is commonly used to investigate, and understand, basic properties of heavy-fermion and intermediate valence systems. Its Hamiltonian

$$\hat{H} = \sum_{k,\sigma} \varepsilon_k^c \hat{n}_{k\sigma}^c + \sum_{k,\sigma} \varepsilon_k^f \hat{n}_{k\sigma}^f + \sum_{k,\sigma} V_k (\hat{f}_{k\sigma}^+ \hat{c}_{k\sigma} + \hat{c}_{k\sigma}^+ \hat{f}_{k\sigma}) + \frac{U}{2} \sum_{i,\sigma\sigma' \atop (\sigma \neq \sigma')} \hat{n}_{i\sigma}^f \hat{n}_{i\sigma'}^f \tag{1}$$

describes a band of non-interacting conduction electrons with dispersion ε_k^c, a narrow band of f-electrons with dispersion ε_k^f, a hybridization V_k between c and f-electrons and a strong, repulsive Hubbard interaction between the f-electrons. In Eq. (1) wave vectors are denoted by k and lattice sites by i. The spin index $\sigma = 1, \ldots, N$ defines an angular momentum quantum number which combines the orbital angular momentum and the actual spin. Typically, the maximal f-degeneracy is $N = 14$; it is reduced to $N = 6.8$ by spin–orbit interaction [1]. In a tight-binding approximation the dispersions are given by

$$\varepsilon_k^c = -2t \sum_{i=1}^{d} \cos k_i, \qquad \varepsilon_k^f = E_f + 2t' \sum_{i=1}^{d} \cos k_i, \tag{2}$$

with $t, t' \geq 0$ and lattice spacing $a \equiv 1$. The orbitals of c- and f-electrons have a different symmetry with respect to parity operations; hence t and t' enter with different signs. The matrix element t' is much smaller than t and, therefore, is often neglected altogether. One should note, however, that the symmetry property of the orbitals does not permit a purely local hybridization [2]. This fact is often ignored and V_k is set constant ($V_k \simeq V = \text{const.}$). Taking the symmetry property into account one has, for example, for a hypercubic lattice, $V_k = 2V \sum_{i=1}^{d} \sin k_i$. The particle density is given by $n = n^c + n^f$; in general, $n^c \neq n^f$.

It was recently shown by one of us [3] that for $d = 1$ and in the limit $U = \infty$ the ground state energy of Eq. (1) can be calculated exactly for *arbitrary* spin degeneracy in a certain subspace of the full parameter space spanned by (t, t', E_f, V). This is achieved by calculating upper and lower bounds on the energy which coincide in a certain

parameter range. The method was previously applied to the Hubbard model and the PAM with $N = 2$ in the case of special Perovskite-like lattices [4] and recently to a general Hubbard model on lattices with arbitrary coordination number [5]. It may also be used in the case of the Emery model in $d = 1$ [3].

As shown in Ref. [3], the exact ground state energy of (1) in $d = 1$, E_N, may be obtained for the parameter range

$$t' = \frac{V^2}{t}, \qquad E_f = 2t - 2N\frac{V^2}{t}, \quad n = N, \tag{3}$$

with arbitrary N; in this case, one finds $E_N = -2NLV^2/t$, where L is the number of lattice sites. The corresponding ground state wave function is nonmagnetic, since it can be written as a product over the spin index. We note that for $N = 8$ this solution applies in the case of $t = 1\,\text{eV}$, $V = 0.4\,\text{eV}$, $E_f = -0.56\,\text{eV}$, $t' = 0.16\,\text{eV}$, which appears to be a physically reasonable choice. In particular, setting $V = V^*/\sqrt{N}$, the limit $N \to \infty$ may be performed. It yields the nontrivial result $E_\infty = -2LV^{*2}/t$; in this case $E_f = 2t - 2V^{*2}/t$ and $t' = 0$.

Using the above exact result we are in a position to evaluate and qualify previously obtained *approximate* results for the PAM, e.g. results from slave-boson mean-field theory (SBMFT) [1], and the Gutzwiller approximation (GA) for the appropriate correlated wave function [6,7]. For $N \to \infty$ and in the parameter range (3) both mean-field methods yield an energy $E_{MF} = E_\infty$, i.e. they become exact. How about finite N? For $N \leqslant \infty$ the energy renormalization factor q is given by $q = 1 - n^f$ and $q = (1 - n^f)/(1 - n^f/N)$ within SBMFT [1] and GA [6,7], respectively. The results coincide for $N \to \infty$. However, so far, it was not possible to decide which one of the two approximations gives a better description of the ground state for *finite* N. Within the parameter range (3), we are able to provide an exact answer for $d = 1$. In this case the GA can be evaluated analytically for arbitrary N. It leads precisely to an energy $E_{N,GA} = E_N$, i.e. the GA yields the *exact* result for the ground state *energy* of the PAM for arbitrary N. The results from the SBMFT have to be evaluated numerically. A comparison between the exact result, GA and SBMFT for $N = 2$ and t', E_f given by Eq. (3) is shown in Fig. 1. Obviously, the results from the SBMFT differ from those of the GA and hence from the exact result. This is true for all values of N we investigated. For large N and/or small V this difference decreases. This is clear in the case of $N \to \infty$ when the q-factors become equal. For $V \to 0$ the local f-level, E_f, *is close to* $2t$, the upper band edge of the conduction band, and hence $n^f \to 0$, such that the q-factors become equal, too.

Finally there is an interesting, controversial point concerning the existence of exponentially small energy scales

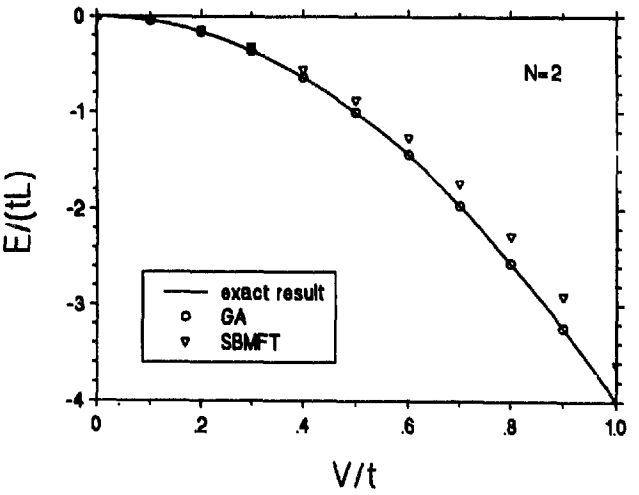

Fig. 1. Ground state energy of the PAM in $d = 1$.

in the ground state energy of the PAM. For the asymmetric PAM with $U = \infty$ both the SBMFT [1] and the GA [7] lead to such non-analytic, Kondo-like contributions ($\sim \exp[-\alpha t(\varepsilon_F + |E_f|)/V^2]$) which have the form known from the single-impurity Kondo problem (here ε_F is the Fermi energy). In the exact solution discussed above they do *not* appear at all for any N, although for large N, $E_f = 2t - 2NV^2/t$ lies far below the Fermi energy (Kondo regime). From this one might conclude that the exponential contributions are due to the approximations. However, we saw that in the parameter range (3) the GA did *not* lead to exponentially small terms, while such terms appeared in the GA used in Refs. [6,7]. We note that the approximations finding such terms always made use of a purely local hybridization, a constant density of states for the conduction electrons and $t' = 0$. By contrast, we worked with a (physically more reasonable) nearest-neighbor hybridization, a cosine conduction band and a small but finite dispersion for the f-electrons. For this more general case our exact solution shows that such terms do not exist. At present it is not clear whether in the exact solution the exponential terms are absent even outside the parameter range (3).

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