Interpolative solution for the Anderson model of an impurity

J. Ferrer, A. Martín-Rodero, and F. Flores
Departamento de Física de la Materia Condensada (C-12), Universidad Autónoma de Madrid, E-28049 Madrid, Spain
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We present calculations for the occupation number, the specific heat, and the density of states of the Anderson model of an impurity using an interpolative approach. The results are compared with the exact solution, showing that the interpolative method can be advantageously used for a periodic Hamiltonian.

Although the problem of a magnetic impurity in a metal has been exhaustively discussed,[1,2] the case of a periodic Anderson Hamiltonian is not so well known.[3,4] In this paper we are concerned with a new approach recently proposed[4] to analyze both the case of an impurity and the periodic Anderson Hamiltonian. In this paper we address the single-impurity problem to discuss the validity and the accuracy of the proposed solution. To this end, we analyze different cases and compare our solution with the exact results of Tsvelick and Wiegmann[2] and other approximate solutions.[5]

In our approach the Anderson Hamiltonian of an impurity,

$$H=\sum_{\sigma}E_f n_{f,\sigma}+\sum_{i,\sigma}E_d n_{d,i,\sigma}+t\sum_{\substack{i,j,\sigma\\(i\neq j)}}c^{\dagger}_{d,i,\sigma}c_{d,j,\sigma}+V\sum_{\sigma}(c^{\dagger}_{d,0,\sigma}c_{f,\sigma}+c^{\dagger}_{d,\sigma}c_{d,0,\sigma})+Un_{f\uparrow}n_{f\downarrow}\ , \tag{1}$$

is solved by using a Green's-function method and by introducing an appropriate self-energy $\Sigma_{ff,\sigma}(\omega)$.

As discussed in Ref. 4, $\Sigma_{ff,\sigma}(\omega)$ is obtained by means of an interpolative scheme; in one limit, we calculate $\Sigma^{(2)}_{ff,\sigma}(\omega)$, the second-order perturbation self-energy of the effective Hamiltonian:

$$H_{\rm eff}=\sum_{\sigma}E_0 n_{f,\sigma}+\sum_{i,\sigma}E_d n_{d,i,\sigma}+t\sum_{\substack{i,j,\sigma\\(i\neq j)}}c^{\dagger}_{d,i,\sigma}c_{d,j,\sigma}+V\sum_{\sigma}(c^{\dagger}_{d,0,\sigma}c_{f,\sigma}+c^{\dagger}_{f,\sigma}c_{d,0,\sigma})\ , \tag{2}$$

where E_0 is introduced in order to have self-consistency between the charges $\langle n_{f,\sigma}\rangle$ as calculated from the final solution and as obtained from Hamiltonian (2).

In a second limit, we calculate the self-energy for the atomic case, with $V\rightarrow 0$ in Eq. (1). The interpolative scheme[4] yields

$$\Sigma_{ff,\sigma}(\omega)=\frac{\Sigma^{(2)}{}_{ff,\sigma}(\omega)}{1-\dfrac{E_f+(1-\langle n_{f,-\sigma}\rangle)U-E_0}{\langle n_{f,-\sigma}\rangle(1-\langle n_{f,-\sigma}\rangle)}\dfrac{\Sigma^{(2)}{}_{ff,\sigma}(\omega)}{U^2}}\ . \tag{3}$$

Notice that Zlatic and co-workers[3,5] have solved the Anderson Hamiltonian considering only the lowest perturbative solution $\Sigma_{ff,\sigma}(\omega)\approx\Sigma^{(2)}{}_{ff,\sigma}(\omega)$. Our solution reduces to this one for the symmetric case: here $E_f+U/2=E_d$, and $E_0=E_d$ (from now on $E_d=0$). In other cases Eq. (3) can represent a significant improvement over $\Sigma^{(2)}{}_{ff,\sigma}(\omega)$ (see below).

Once $\Sigma_{ff,\sigma}(\omega)$ is known, different properties of the Anderson Hamiltonian, density of states, specific heat, etc., can be obtained using well-known Green's-function techniques.[6] We present here different results for the impurity valence $\langle n_f\rangle$, the specific heat at zero temperature, and the density of states.

In Fig. 1, $\langle n_f\rangle$ is displayed as a function of E_f for three different cases: (a) $U=0.2$, $U/\Gamma=4$; (b) $U=0.2$, $U/\Gamma=10$; (c) $U=0.2$, $U/\Gamma=40$. Γ is defined in the usual way: $\Gamma=\pi V^2\rho(0)$, $\rho(0)$ being the d-band density of states at the Fermi level [we take the Fermi level as 0 and $\rho(0)$ as $1/2\pi$]. Notice that for increasing values of U/Γ, electron-correlation effects in the impurity become dominant. This is easily seen in Fig. 1: For $U/\Gamma=4$, $\langle n_f\rangle$ is a smooth function of E_f not far from the Hartree-Fock solution. For $U/\Gamma=10$, $\langle n_f\rangle$ tends to bend around $E_f=-U/2$, and the process is practically completed for $U/\Gamma=40$; in this case, $\langle n_f\rangle\approx 1$ in a region extending approximately from $E_f\approx -U$ to $E_f\approx 0$.

In the same Figs. 1(a)–1(c) we display the results for $\langle n_f\rangle$ as obtained using the exact solution of Tsvelick and Wiegmann,[2] and for the approximate one of Zlatic and Horvatic.[5] From the results shown in these figures, we conclude that a substantial improvement is obtained by using Eq. (3) for the self-energy instead of $\Sigma^{(2)}{}_{ff,\sigma}(\omega)$ for $U/\Gamma\gg 1$; moreover, the results obtained with Eq. (3) for $\langle n_f\rangle$ are in fair agreement with the ones given by the exact solution.[2]

We have also analyzed the specific heat at zero temperature: This is a measure of the impurity density of states at the Fermi level, $\rho_{ff}(0)$. At very low temperature, C_v is given by

$$C_v=2\pi^2 k_B^2\rho_{ff,\sigma}(0)\left[1-\frac{\partial\Sigma_{ff,\sigma}(\omega)}{\partial\omega}\right]_{\omega=T=0}T\ . \tag{4}$$

It is a common practice to define a parameter γ such that (for a nonmagnetic solution)

$$\gamma = \left[1 - \frac{\partial \Sigma_{ff,\sigma}(\omega)}{\partial \omega} \right]_{\omega = T = 0} . \quad (5)$$

In Fig. 2(a) we represent γ as a function of U/Γ for the symmetric case; as mentioned above, in this case the self-energy of Eq. (2) reduces to $\Sigma^{(2)}$, and our analysis coincides with Horvatic Zlatic's results. Notice that for the symmetric case, γ is only well approximated by $\Sigma^{(2)}$ for $U/\Gamma \leq 7$; for larger values, the exact results[2] show an exponential increase with U/Γ while $\Sigma^{(2)}$ yields only a square growth. As discussed by Horvatic and Zlatic,[7] this is related to the scaling behavior appearing in the exact solution for large U/Γ ($U/\Gamma \geq 2\pi$).

In Fig. 2(b) we show the results we have obtained for γ^* [$=\pi\Gamma\rho_{ff,\sigma}(0)\gamma$] as a function of E_f for $U=0.2$ and $\Gamma=0.05$. In the same figure we display the exact results and the ones obtained approximating the self-energy by $\Sigma^{(2)}$. Notice that for $E_f=-U/2$, our results coincide with the ones calculated using $\Sigma^{(2)}$; for $|E_f+U/2|$ larger than zero, our results approach the exact values of γ^*, showing a significant improvement over the results given by $\Sigma^{(2)}$. In Fig. 2(c) we show similar results for $U=0.2$ and $\Gamma=0.02$; in this figure we clearly see how the results obtained for the specific heat using Eq. (3) are much better than the ones given by $\Sigma^{(2)}$. Still, the specific heat for the symmetric case shows the same discrepancy with the exact solution given by Fig. 2(a).

These results can be better understood by analyzing the density of states obtained from Eq. (3). In Figs. 3(a)–3(d) we show that density for $U=0.2$, $\Gamma=0.02$,

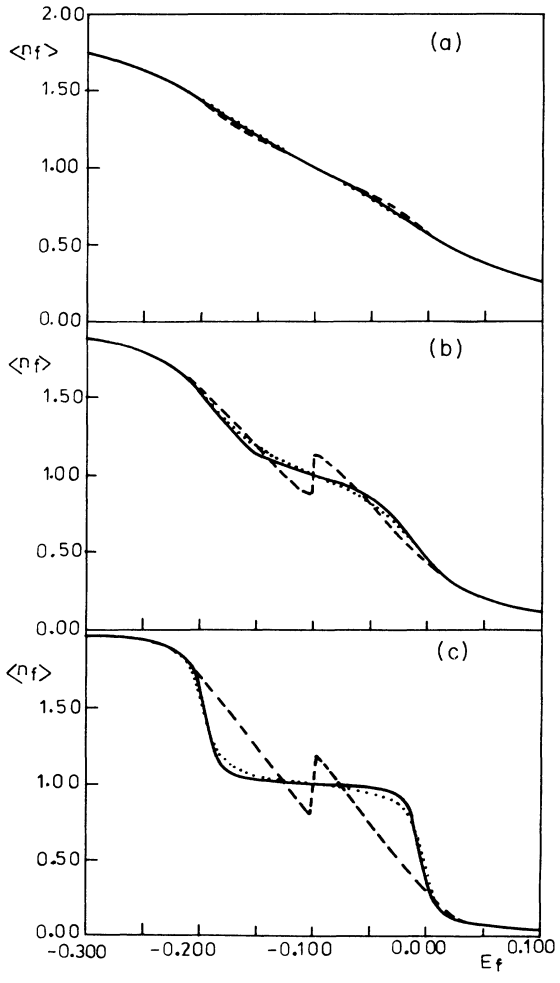

FIG. 1. $\langle n_f \rangle$ is displayed as a function of E_f: (a) $U=0.2$, in arbitrary units, $U/\Gamma=4$; (b) $U=0.2$, $U/\Gamma=10$; (c) $U=0.2$, $U/\Gamma=40$ [$\rho(0)$ is taken $1/(2\pi)$ in all the cases]. Solid line, exact solution;[2] dashed line, second-order perturbation solution[3,5] for Σ; dotted line, present solution. E_f is in arbitrary units, too.

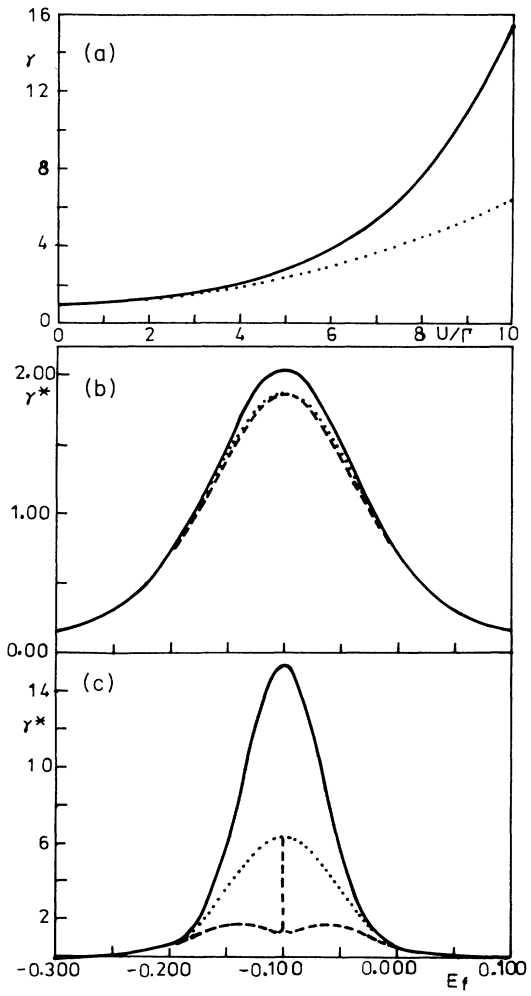

FIG. 2. (a) shows γ as a function of (U/Γ) for the symmetric case. (b) shows γ^* a function of E_f, for $U=0.2$ and $U/\Gamma=10$. Solid line, exact results; dashed line, second-order perturbative solution for Σ; dotted line, present solution. (c), same as (b), for $U=0.2$ and $U/\Gamma=4$.

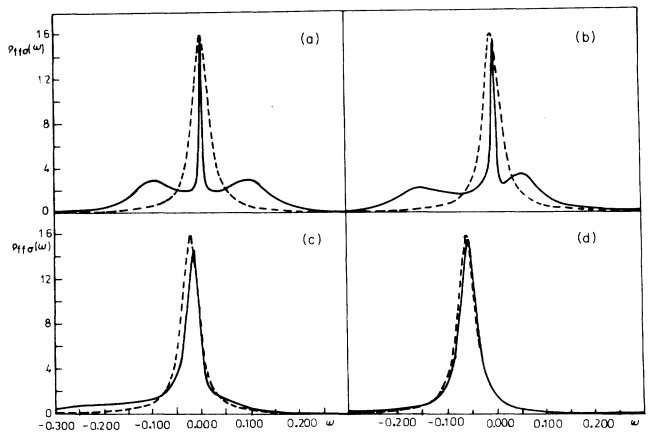

FIG. 3. Local density of states in the f orbital for $U=0.2$, $U/\Gamma=10$, and (a) $E_f=-0.10$, (b) $E_f=-0.15$, (c) $E_f=-0.20$, and (d) $E_f=-0.25$. Solid line, solution obtained using $\Sigma_{ff,\sigma}(\omega)$. Dashed line, solution of the one-electron Hamiltonian given by Eq. (2). ω is in arbitrary units.

and $E_f=-0.10$, -0.15, -0.20, and -0.25. For $E_f=-0.1$ we have the symmetric case and a narrow peak appears at the Fermi level [Fig. 3(a)]; our results for the specific heat suggest that the peak is not narrow enough: According to Fig. 2(b) we expect the exact solution to have a narrow Kondo-like peak at the Fermi level, twice as narrow as Fig. 3(a) shows. For $E_f=-0.15$ we find the results of Fig. 3(b); for this value of E_f the peak is broader than in the symmetric case and, according to Fig. 2(b), we expect the exact solution not to differ very much from the results shown in Fig. 3(b). Figures 3(c) and 3(d) show the cases $E_f=-0.2$ and -0.25, respectively; here, our solution must be quite close to the exact one.

The comparison of Figs. 1(b), 2(b), and 3 suggests that the solution given by $\Sigma_{ff,\sigma}(\omega)$ [Eq. (3)] yields a very satisfactory solution of the Anderson Hamiltonian, except for the narrow Kondo-like peak appearing at the Fermi level. For U/Γ very large, that peak presents an exponential narrowing in the symmetric case, while our solution only shows a $(\Gamma/U)^2$ narrowing behavior. For an unsymmetric case, our solution reproduces much better the Kondo-like peak and, in general, we can expect that any other structure appearing in the density of states is well reproduced by our approximate solution.

In conclusion, our results for the impurity show that the approximate solution of the Anderson model,[4] as discussed in this paper, yields a fair description of the exact solution.[2] In particular, occupation numbers and density of states seem to be well reproduced except for the narrow Kondo-like resonance appearing at the Fermi level. The approximate solution analyzed here does not reproduce adequately the scaling behavior of this peak; this limitation does not seem, however, to be important for the rest of the spectrum as the Kondo-like peak has a very small weight. Accordingly, we think that the method given in Ref. 4 is a fair solution to the Anderson model of an impurity and it can be used advantageously for the periodic Hamiltonian.[4]

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