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Abstract. The densities of states for the periodic Anderson model are evaluated by means of a non-standard perturbation expansion in the kinetic term of the conduction electrons. The calculations are performed at finite temperature, taking into account in an exact way the effect of the on-site Coulomb repulsion U and the hybridization coupling V. We reproduce most of the properties that are usually expected for the correlated electrons, especially the peaks in the density of states at energies ϵ_f and $\epsilon_f + U$ and the double peak structure with the hybridization gap in the region around the chemical potential.

1. Introduction

The physics of systems containing isolated magnetic impurities is an active field of research. Indeed, the striking anomalies shown by these systems, especially in the response functions such as resistivity, susceptibility and specific heat, still cannot be completely reproduced by suitable mathematical models [1]. Besides, one of the essential properties of these systems, i.e. the existence of strong electronic correlations, seems to play a fundamental role in the phenomenon of high T_c superconductivity [2].

It is known that the best experimental realization of these systems is obtained by diluting rare earth or actinide atoms in a host metal. This is due to the fact that the magnetic moments of these ions are generated by inner core 4f (rare earth) or 5f (actinide) shells which retain their atomic character when the atom is implanted into a metal.

The resulting compounds show a large variety of behaviours which are not easy to interpret in terms of a unique underlying interaction mechanism. Depending on their properties, these compounds are usually divided in two large classes: the intermediate valence (IV) systems (mainly rare earth compounds) and the heavy fermions (HF) systems (mainly actinide compounds), which show different physical responses which in some cases are quite remarkable. It is worth recalling, for instance, that a few HF compounds even become superconductors at very low temperatures [3].

In spite of that, it now seems clear that the behaviour of IV and HF systems is controlled by the same interactions in different parameter regimes. This would allow the use of a unique theoretical model for both kinds of system.

For a theoretical analysis there are two basic features that must be taken into account. The first one is the experimental evidence that two f-electrons belonging to the same ion experience a very high Coulomb repulsion because of their strong localization; this implies that the multi-occupancy of an f-level is energetically unfavourable.

The other one is the fact that in most of these compounds the configuration with n f-electrons and $n - 1$ f-electrons plus one electron in the conduction band are nearly degenerate; this gives rise to the phenomenon of hybridization corresponding to the possibility of transitions from f-states into the band and *vice-versa*.

Bearing this in mind, these compounds can be idealized as systems of uncorrelated conduction electrons hybridizing with highly correlated electrons localized at the same lattice sites. This description is similar to the one provided by the periodic version of the single impurity Anderson model [4].

As is well known, this model cannot be solved exactly unless one of the following limits is considered:

(a) zero hybridization energy: the model is exactly solvable because the conduction and localized electrons behave as independent systems;

(b) zero on-site correlation energy: the absence of many-body correlations allows the diagonalization of the Hamiltonian by means of a suitable canonical transformation; or

(c) vanishing conduction bandwidth: the model is again exactly solvable because different sites are not coupled.

Although the results obtained by solving the model in these limits are non-physical, they have often been used as zeroth-order approximations in perturbative approaches.

We recall, for instance, a perturbation expansion with respect to the on-site Coulomb repulsion (usually denoted by U), which makes use of the determinant perturbation expansion in the form first introduced by Yosida and Yamada [5]. In this approach one has the advantage that the Wick theorem holds and the Feynman diagram method can be used.

However, in most of the rare earth and actinide compounds which are usually studied the correlation energy U is much larger than the impurity level width $\Gamma = \pi V^2 \rho(E_F)$ ($\rho(E_F)$ is the conduction electrons' density of states at the Fermi level), which is a measure of the hybridization strength. Therefore, in spite of some reliable results obtained within the framework of the previously mentioned approach, a perturbative expansion with respect to the hybridization coupling V seems to be more realistic.

In this case, however, the presence of the on-site Coulomb repulsion term in the unperturbed Hamiltonian forbids the application of the Wick theorem [6], so that the standard Feynman diagram technique cannot be used.

In order to deal with this problem, many ingenious non-standard methods have been proposed, among which for brevity we only recall the diagrammatic expansion developed by Keiter and Kimball [7] (a summary of other techniques can be found in Czycholl [1]).

In this paper we propose an approach based on a perturbation expansion in the conduction electrons' kinetic term. The 'free' Green functions, which exactly take into account the effect of both the hybridization and the on-site Coulomb repulsion, have been calculated by means of a path integral technique developed in [8]. The full propagators have then been expressed in terms of the free ones by means of a suitable approximate Dyson equation [9]. We stress that our calculations are performed at finite temperature and for finite values of the correlation energy U.

In our opinion, the main properties of systems with magnetic impurities in which band effects are not very relevant can be successfully investigated within the framework of the approach presented here. This could be the case, for instance, for the HF systems in normal phase, the properties of which seem to be strongly dependent on

the behaviour of the nearly localized f-electrons, rather than on that of the conduction electrons.

In section 2 we specify the model and the approximate Dyson equation used to evaluate of the full propagators. The corresponding densities of states (DOSs) are studied in section 3 as functions of the temperature and the parameters of the theory.

2. The model

Let us study the periodic Anderson Hamiltonian

$$H = H_f + H_c + H_{fc} \tag{1}$$

where

$$H_f = \sum_{i,\sigma} \epsilon_f f_{i\sigma}^\dagger f_{i\sigma} + U \sum_i f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow} \tag{2a}$$

$$H_c = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} \tag{2b}$$

$$H_{fc} = V \sum_{i,\sigma} (f_{i\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger f_{i\sigma}). \tag{2c}$$

Here H_f is the Hamiltonian of a set of localized electrons with a strong Coulomb repulsion U at the same site, H_c describes a system of uncorrelated itinerant electrons and H_{fc} is the term accounting for the hybridization between localized and conduction states. Standard second quantization notation is used, with the operators f and c referring to the localized and conduction electrons, respectively.

We introduce a perturbative approach regarding the conduction electron kinetic term H_c as the perturbation H_I which in turn implies

$$H_0 = H_f + H_{fc}. \tag{3}$$

The temperature Green functions of the full Hamiltonian are obtained by means of the following Dyson equation in (k, ω_ν)-space (ω_ν is the Matsubara frequency)

$$\widehat{\mathcal{G}}(k, \omega_\nu) = \widehat{\mathcal{G}}^0(\omega_\nu) + \widehat{\mathcal{G}}^0(\omega_\nu)\widehat{\Sigma}(k, \omega_\nu)\widehat{\mathcal{G}}(k, \omega_\nu). \tag{4}$$

Here

$$\widehat{\mathcal{G}}(k, \omega_\nu) = \begin{pmatrix} G_{ff}(k, \omega_\nu) & G_{fc}(k, \omega_\nu) \\ G_{cf}(k, \omega_\nu) & G_{cc}(k, \omega_\nu) \end{pmatrix} \tag{5}$$

is the exact matrix propagator, $G_{ab}(k, \omega_\nu)$ being the Fourier transform of

$$G_{ij}^{ab}(\tau - \tau') = -\text{Tr}\left[e^{-\beta H} a_i(\tau) b_j(\tau')\right] \equiv -\langle T[a_i(\tau) b_j(\tau')]\rangle \tag{6}$$

(*i* and *j* are site indices). $\widehat{\mathcal{G}}_0(\omega_\nu)$ is the unperturbed matrix propagator, showing no dependence on k because of the absence of a band of finite width in H_0. The self-energy matrix $\widehat{\Sigma}(k, \omega_\nu)$ is assumed to be

$$\widehat{\Sigma}(k, \omega_\nu) \equiv \widehat{\Sigma}(k) = \begin{pmatrix} 0 & 0 \\ 0 & \epsilon_k \end{pmatrix}. \tag{7}$$

As the Wick theorem cannot be applied, equation (4) with self-energy (7) must be regarded as an approximation. It is exact in the limit $U \to 0$: in this case every n-point unperturbed Green function can be factorized by use of the Wick theorem and equation (4) is a consequence of this factorization.

Nonetheless, we are confident that this approximation is not as drastic as it could appear. Indeed, the fluctuations neglected in factorizing the unperturbed propagators can be expected to be small in our approach, because they are fluctuations around mean values computed by taking exactly into account the effect of the largest term in the Hamiltonian, the correlation energy U. For a better investigation of this point, we have also explicitly evaluated the contributions neglected in factorizing the four-point free propagators in terms of two-point free ones. Preliminary results seem to indicate that for physical choices of the parameters our approximation is a good one.

We point out that the same assumption on the form of the self-energy can be found in a similar context in [10] for zero-temperature calculations and in [11] at $T \neq 0$.

Returning to equation (4), we see that from assumption (7) we obtain the following equations

$$G_{ff}(k, \omega_\nu) = G_{ff}^0(\omega_\nu) + \epsilon_k\, G_{fc}^0(\omega_\nu) G_{fc}(k, \omega_\nu) \tag{8a}$$

$$G_{fc}(k, \omega_\nu) = G_{cf}(k, \omega_\nu) = \frac{G_{fc}^0(\omega_\nu)}{\left[1 - \epsilon_k G_{cc}^0(\omega_\nu)\right]} \tag{8b}$$

$$G_{cc}(k, \omega_\nu) = \frac{G_{cc}^0(\omega_\nu)}{\left[1 - \epsilon_k G_{cc}^0(\omega_\nu)\right]}. \tag{8c}$$

These equations have been used to evaluate the full propagators starting from the results given in [12], where the Green functions for the Hamiltonian (3) have been exactly computed at finite temperature. The DOSs for localized and conduction electrons have then been obtained from the well-known relationships

$$\rho_f(\omega) = -\frac{1}{\pi N} \sum_k \operatorname{Im} G_{ff}(k, i\omega_\nu \to \omega + i\eta)$$

$$\rho_c(\omega) = -\frac{1}{\pi N} \sum_k \operatorname{Im} G_{cc}(k, i\omega_\nu \to \omega + i\eta).$$

Instead of specifying the form of the energy spectrum, we have computed ρ_f and ρ_c assuming a parabolic DOS for the unperturbed conduction electrons [10, 11]:

$$\rho_c^0(\omega) = \begin{cases} (\frac{3}{4}W)\left[1 - (\omega/W)^2\right] & \text{if } |\omega| \leq W \\ 0 & \text{otherwise} \end{cases}$$

where W is the half-width of the conduction band.

3. Results and discussion

The DOSs have been evaluated as functions of the energy for different choices of the temperature and the parameters V, ϵ_f and U. The chemical potential has been fixed in such a way as to have two electrons per site. All the energy values are measured with respect to W.

The general structure of the DOS for localized electrons is the one showed, for instance, in figure 3. We always find two peaks, one around ϵ_f and one around $\epsilon_f + U$, together with two other peaks in the region of the chemical potential, separated by a small hybridization gap. Having fixed an even number of electrons per site, we always find the chemical potential falling in this gap. This result is in agreement with the one obtained by Martin and Allen [13].

We have evaluated the DOS for localized and conduction electrons varying the parameters for two fixed positions of the f-level, well below the conduction band ($\epsilon_f/W = -2$) and inside it ($\epsilon_f/W = -0.5$) (note that in the figures given here different scales are used).
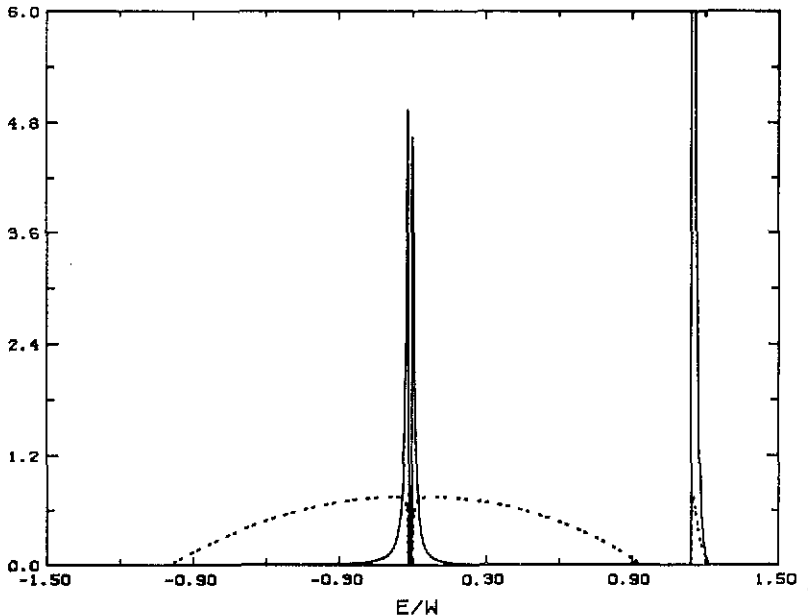

Figure 1. DOSs of localized (full curve) and conduction (broken curve) electrons for $\epsilon_f/W = -2$, $V/W = 0.2$, $U/W = 3$ and $k_B T/W = 0.00086$ (the peak near ϵ_f is not shown).

In figures 1–4 two values of the hybridization are considered ($V/W = 0.2$ and 0.3), the temperature being fixed at $k_B T/W = 0.00086$ (for $W = 1$ eV this corresponds to $T = 10$ K). An inspection of the figures clearly shows that an increase in V always makes the f-peaks lower, wider and further apart. It is interesting to note (see figures 2 and 4) that when the f-level is in the conduction band a second gap within the corresponding peak in f-DOS is created (the same gap is also found in the c-DOS). Owing to the high value of the chosen Coulomb repulsion ($U/W = 3$), in these cases we always find f and c occupation numbers very close to one, regardless of the position
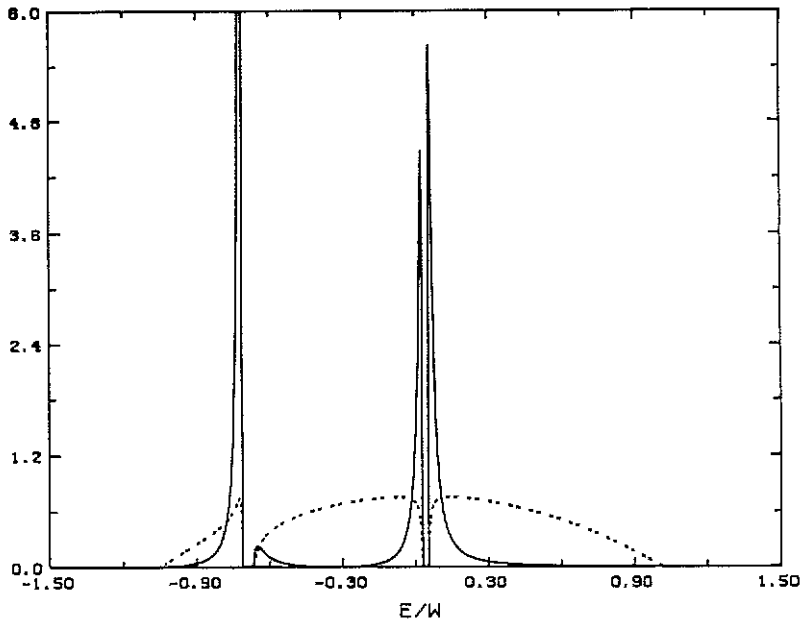
Figure 2. Same as in figure 1, with $\epsilon_f/W = -0.5$ (the peak near $\epsilon_f + U$ is not shown).

of the f-level. Referring to figures 1–4, we find for $\langle n_f \rangle$ the values 1.014, 0.952, 1.034 and 0.892, respectively.
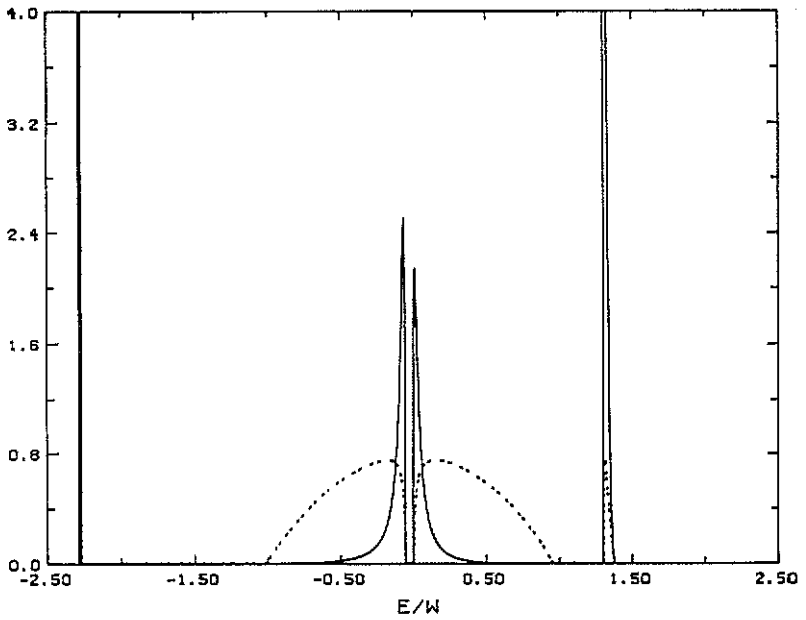

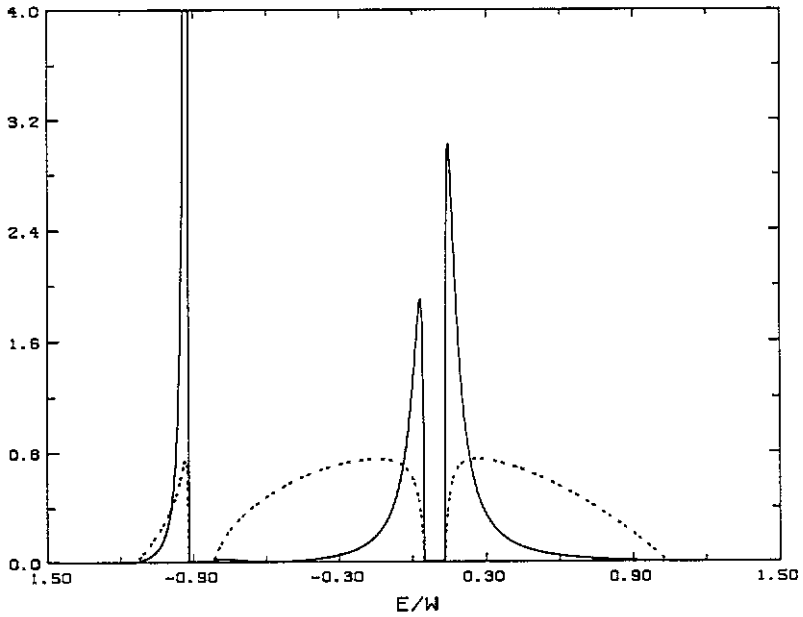**Figure 3.** Same as in figure 1, with $V/W = 0.3$.

Figure 4. Same as in figure 2, with $V/W = 0.3$ (the peak near $\epsilon_f + U$ is not shown).
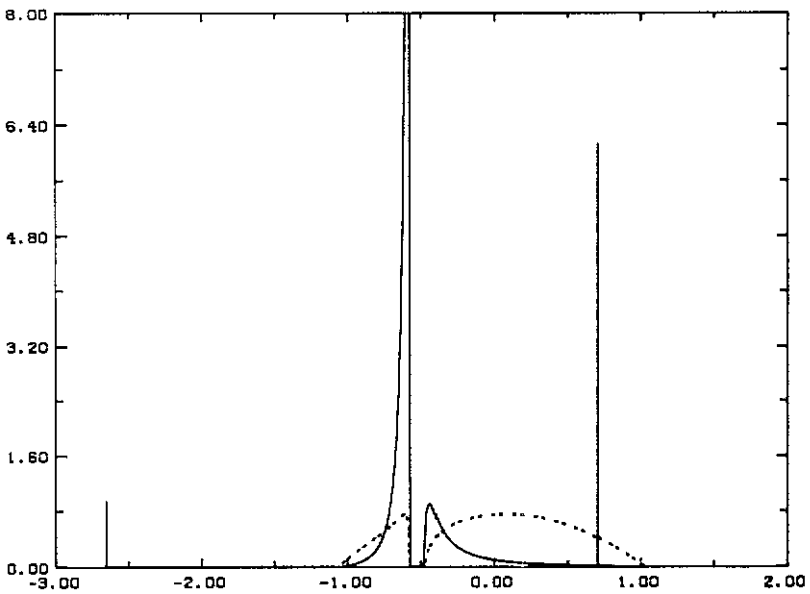

Figure 5. Same as in figure 1, with $U/W = 1.5$.

Figure 5 shows the DOSs for the same choice of parameters as in figure 1, the only difference being a lower value for the correlation energy ($U/W = 1.5$). We see that for $\epsilon_f = -2$ a decrease in U leads on one hand to a strong reduction in the f-peaks at ϵ_f and $\epsilon_f + U$; and on the other hand to a broadening of the double peak structure

around the chemical potential. The low values of both U and $\epsilon_f + U$ make it easier for an electron to go into an f-state already occupied, so that the site occupation is almost completely distributed over the high and wide f-peak on the left of the hybridization gap (we obtain in this case $\langle n_f \rangle = 1.610$).

This trend is enhanced when we lower U further. At $U/W = 1.1$ (we have not given the diagram for brevity) the side f-peaks completely disappear whereas the central ones become very wide with an f-occupation equal to 1.803.

In contrast, values of U/W higher than three do not substantially modify the DOSs, the main effect being only a narrowing of the f-peaks. This is easily explained, because high values of U tend to forbid the multi-occupancy of sites, so that the mobility of the f-electrons is strongly reduced.

We have performed a similar analysis of the effect of U with the f-level inside the conduction band. We do not give the diagrams here because the DOS structure shown in figure 2 is not qualitatively altered by physically significant variations of U. We only find, as before, that the f-peaks are broadened by a decrease in U (and *vice-versa*), the f-occupation always remaining nearly equal to one.

We have also studied the dependence of the hybridization gap width on the parameters ϵ_f, V and U. From figures 1–5 and the data reported in table 1, we see that the gap becomes broader with increasing V and decreasing U. As far as the dependence on ϵ_f is concerned, we find that the gap is an increasing function of ϵ_f as long as U/W is greater than a certain value that we estimate to be about three. For smaller U the behaviour is no longer monotonic, as can be seen from the last set of data reported. Apart from this latter result, the general trend that can be inferred from table 1 is in good agreement with the zero-temperature results shown in [14]. Considering that our data are expressed in bandwidth units, some of the values obtained are consistent with the measured ones, which are of the order of meV [15].

Table 1. (*a*) The other parameters are: $\epsilon_f/W = -0.5$, $U/W = 3$, $k_B T/W = 0.00086$. (*b*) The other parameters are: $\epsilon_f/W = -2$, $V/W = 0.2$, $k_B T/W = 0.00086$. (*c*) The other parameters are: $V/W = 0.2$, $U/W = 3$, $k_B T/W = 0.00086$. (*d*) The other parameters are: $V/W = 0.2$, $U/W = 2$, $k_B T/W = 0.00086$

(*a*)		(*b*)		(*c*)		(*d*)	
V	Gap	U	Gap	ϵ_f	Gap	ϵ_f	Gap
0.1	0.000	1.5	0.099	−2.0	0.014	−2.0	0.060
0.2	0.014	2.0	0.060	−1.3	0.015	−1.3	0.025
0.3	0.025	3.0	0.014	−0.8	0.017	−0.8	0.023
0.4	0.170	5.0	0.005	−0.5	0.025	−0.5	0.030

Finally, in figure 6 we show the DOSs with the same parameters as in figure 2, but at a higher temperature ($k_B T/W = 0.02583$; for $W = 1$ eV this gives $T = 300$ K). We note that the location of the hybridization gap (and the chemical potential inside it) is only very slightly affected by an increase in the temperature (in figures 2 and 6 E_F/W is equal to 0.056 and 0.041, respectively). The main temperature effect consists in an increase in the number of the f-peaks, leaving the site occupation substantially unaltered. The inset in the figure shows that the f-DOS structure in the region around the chemical potential is much more complex than that reported in [11]. This is an important result, because of the fundamental role played by the DOS structure in the
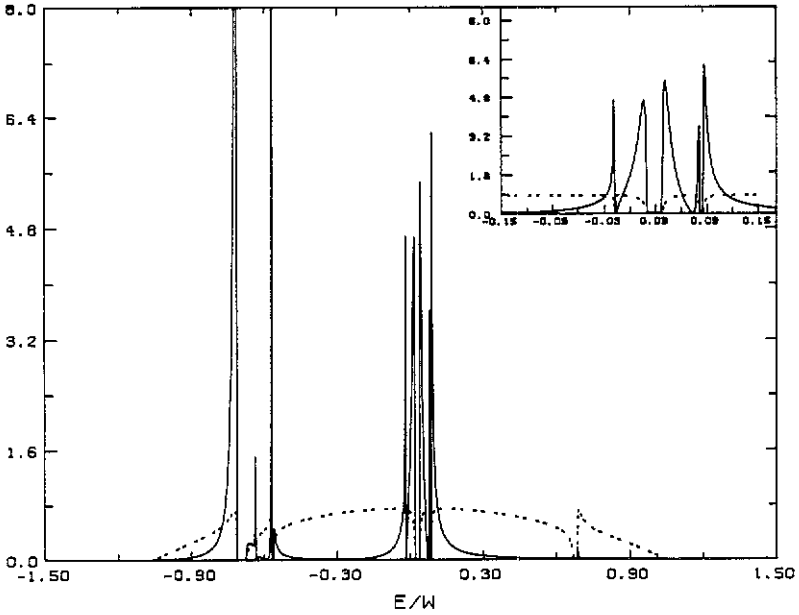
Figure 6. Same as in figure 1, with $k_B T/W = 0.02583$ (the inset shows an enlargement of the region around the chemical potential; the peak near $\epsilon_f + U$ is not shown).

proximity of the chemical potential in the determination of the physical properties of the system.

We conclude the discussion of the results by pointing out that these calculations were also performed by fixing the total number of particles per site equal to three. We always found the chemical potentials lie within the conduction band, to the right of the hybridization gap.

Acknowledgments

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