# Specific heat of the periodic Anderson model: From weak to strong coupling

N. M. R. Peres
*Departamento de Física, Universidade de Évora, Rua Romão Ramalho, 59, P-7000-671 Évora, Portugal and Centro de Física da Universidade do Minho, Campus Gualtar, P-4700-320 Braga, Portugal*

P. D. Sacramento
*Departamento de Física and CFIF, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal*

M. A. N. Araújo
*Departamento de Física, Universidade de Évora, Rua Romão Ramalho, 59, P-7000-671 Évora, Portugal and Centro de Física da Universidade do Minho, Campus Gualtar, P-4700-320 Braga, Portugal*

(Received 16 February 2001; revised manuscript received 17 April 2001; published 29 August 2001)

We study the temperature dependence of the specific heat in the periodic Anderson model as function of the on-site Coulomb interaction, hybridization, and position of the $f$ electrons energy level. At strong coupling ($U=\infty$) we use slave bosons, whereas at weak coupling we use a simple Hartree-Fock decomposition. We find that both in the strong and weak coupling limits the specific heat of the system presents a multiple peak structure in a mean field treatment. We believe these features to be related to band-shape effects. The temperature evolution of the low-temperature peak position on the model parameters for the non-half-filled nonsymmetric case is discussed.

DOI: 10.1103/PhysRevB.64.113104 PACS number(s): 75.20.Hr, 71.27.+a, 71.28.+d, 65.40.−b

Heavy-fermion materials are compounds containing rare earth and actinide atoms that exhibit high specific heats and spin susceptibilities at low temperature. This feature is associated with high effective masses of quasi-particles due to strong Coulomb interactions among the $4f$ or $5f$ electrons.[1] The behavior of these materials is controlled by three parameters: the hybridization $V$ between $f$ and $d$ orbitals, which confers the $f$ electrons an itinerant character, the value of the $f$ level $\epsilon_0$ energy relatively to the chemical potential, and the value of the Coulomb energy $U$.[2]

The strong Coulomb interaction together with the small values of the hybridization matrix allow for formation of local moments leading to magnetic behavior in these systems. The Kondo effect and the magnetic order due to the RKKY (Ruderman-Kittel-Kasuya-Yosida) interaction are consequences of the interplay between Coulomb interaction and hybridization.[3,4] Together with magnetism, heavy-fermion materials may present superconducting ground states, whose origin and nature are far from being fully understood.[5–7]

The periodic Anderson model (PAM) is considered a good candidate for describing heavy-fermion systems. It is generally accepted that a complete understanding of heavy-fermion system properties requires going beyond mean field theory. Nevertheless, mean field theory still gives qualitatively correct information about some properties of heavy-fermion systems.[2]

Recently, the temperature dependence of the specific heat of the PAM, at half filling, was studied using the equation of motion method, both in the symmetric and nonsymmetric cases,[8,9] and a multiple peak structure was found. This multiple peak structure was first obtained by Zieliński and Matlak in the half filled symmetric ($2\epsilon_0+U=0$) case.[10] However, it is believed that mean field theory is not able to capture this multiple peak structure in the specific heat.

This belief contrasts with Monte Carlo results showing that the magnetic Hartree-Fock approximation reproduces well the free energy of the PAM at low temperatures when $V \ll U$,[11] implying that the thermodynamics must be well described by the Hartree-Fock approximation in this limit.

In this study we report results for the PAM's specific heat both in the weak and infinite coupling limits. Our study is done away from half filling and in the non-symmetric case. The strong-coupling limit $U=\infty$ is studied using slave bosons, whereas the weak coupling limit is treated within Hartree-Fock approximation. We find that in both limits the specific heat presents a multiple peak structure and that its dependence on the model parameters is in qualitative agreement with what is physically expected.

The standard periodic Anderson model model for spin 1/2 electrons is written as

$$H=H_d^0+H_f^0+H_{df}+H_U, \tag{1}$$

where

$$H_d^0=\sum_{\vec{k},\sigma}(\epsilon_{\vec{k}}-\mu)d_{\vec{k},\sigma}^{\dagger}d_{\vec{k},\sigma}, \tag{2}$$

$$H_f^0=\sum_{i,\sigma}(\epsilon_0-\mu)f_{i,\sigma}^{\dagger}f_{i,\sigma}, \tag{3}$$

$$H_{cf}=V\sum_{i,\sigma}(d_{i,\sigma}^{\dagger}f_{i,\sigma}+f_{i,\sigma}^{\dagger}d_{i,\sigma}), \tag{4}$$

$$H_U=U\sum_i n_{i,\uparrow}^f n_{i,\downarrow}^f, \tag{5}$$

and $\epsilon_{\vec{k}}$ is the dispersion of the $d$ electrons, $\epsilon_0$ is the bare energy of the localized $f$ states, $\mu$ is the chemical potential, $V$ is the hybridization matrix element (assumed $\vec{k}$ independent), $U$ is the on-site Coulomb interaction, and $n_{i,\sigma}^f=f_{i,\sigma}^{\dagger}f_{i,\sigma}$.

 

This model describes two electronic subsystems, the *d* and *f* electron systems, which are coupled by the hybridization matrix. Since the *f* states form very narrow bands, the Coulomb interaction has a strong effect on the *f* states.

It is well known that, at the mean field level, the PAM presents a two-band structure, separated by a gap. Therefore, the model describes a Kondo-insulator for $n=2$, describing a metal for other values of *n*. The full density of states shows a sharp peak of width $V^2\rho_0$ (with $\rho_0$ the *d*-electron density of states) close to the renormalized *f* level energy, which is responsible for the quasiparticle heavy-masses when the chemical potential lies within this peak.

In our study we consider the non-magnetic phase such that $\langle n^f_\uparrow\rangle=\langle n^f_\downarrow\rangle$. In the strong coupling limit ($U=\infty$), double occupancy of the *f* sites is forbidden. The simplest implementation of the $U=\infty$ condition is due to Coleman,[12] in which the empty *f* site is represented by a slave boson $b_i$ and the physical operator $f_i$ in Eq. (4) is replaced with $b^\dagger{}_i f_i$. Condensation of the slave-bosons can be described by the replacement $b_i\to\langle b_i\rangle=\langle b^\dagger{}_i\rangle=\sqrt{z}$.

The density of the boson condensate *z* minimizes the free energy of the system and the renormalized $\epsilon_f$ energy level is obtained after imposing local particle (boson+fermion) conservation at the *f* sites. Using the results of Ref. 13 for the nonsuperconducting case, the mean field equations can be written in terms of the Fourier transform of the Green's functions

$$\mathcal{G}_{f,\sigma}(\vec{k},\tau-\tau')=-\langle T_\tau f_{\vec{k},\sigma}(\tau)f^\dagger_{\vec{k},\sigma}(\tau')\rangle, \tag{6}$$

$$\mathcal{G}_{d,\sigma}(\vec{k},\tau-\tau')=-\langle T_\tau d_{\vec{k},\sigma}(\tau)d^\dagger_{\vec{k},\sigma}(\tau')\rangle, \tag{7}$$

$$\mathcal{G}_{df,\sigma}(\vec{k},\tau-\tau')=-\langle T_\tau d_{\vec{k},\sigma}(\tau)f^\dagger_{\vec{k},\sigma}(\tau')\rangle, \tag{8}$$

as

$$\begin{aligned} z&=1-\frac{T}{N_s}\sum_{\vec{k},\sigma}\sum_{i\omega_n}\mathcal{G}_{f,\sigma}(\vec{k},i\omega_n)\\ &=1-2\int_{-D}^{D}d\epsilon\rho_0(\epsilon)[u^2_+(\epsilon)f(E_+)+u^2_-(\epsilon)f(E_-)], \end{aligned} \tag{9}$$

and

$$\begin{aligned} \epsilon_f&=\epsilon_0-\frac{VT}{\sqrt{z}N_s}\sum_{\vec{k},\sigma}\sum_{i\omega_n}\mathcal{G}_{df,\sigma}(\vec{k},i\omega_n)\\ &=\epsilon_0-\frac{2V}{\sqrt{z}}\int_{-D}^{D}d\epsilon\rho_0(\epsilon)\sqrt{u^2(\epsilon)_+u^2_-(\epsilon)}\\ &\quad\times[f(E_+)-f(E_-)], \end{aligned} \tag{10}$$

where $N_s$ denotes the number of lattice sites, $\epsilon_f$ is the renormalized energy of the *f* orbitals due to the on-site repulsion and $f(E)$ is the Fermi function. Equation (9) states that the mean number of electrons at an *f*-site is $1-z$. For a given number of particles per site *n*, these equations must be supplemented with the particle conservation condition which yields the chemical potential $\mu$ for any temperature:

$$\begin{aligned} n&=1-z+\frac{T}{N_s}\sum_{\vec{k},\sigma}\sum_{i\omega_n}\mathcal{G}_{d,\sigma}(\vec{k},i\omega_n)\\ &=2\int_{-D}^{D}d\epsilon\rho_0(\epsilon)[f(E_+)+f(E_-)]. \end{aligned} \tag{11}$$

In the above equations the energies $E_\pm$ and the coherence factors $u^2_\pm(\epsilon)$ are given by

$$\begin{aligned} E_\pm&=\tfrac{1}{2}(\epsilon_{\vec{k}}+\epsilon_f)\pm\tfrac{1}{2}E(\epsilon_{\vec{k}}),\\ E(\epsilon_{\vec{k}})&=\sqrt{(\epsilon_{\vec{k}}-\epsilon_f)^2+4zV^2},\\ u^2_\pm(\epsilon)&=\frac{1}{2}\left[1\mp\frac{\epsilon_{\vec{k}}-\epsilon_f}{E(\epsilon_{\vec{k}})}\right] \end{aligned} \tag{12}$$

and $\rho_0(\epsilon)$ represents the density of states of the free *d* electrons, which we choose of the form

$$\rho_0(\epsilon)=\frac{2}{\pi D^2}\sqrt{D^2-\epsilon^2},\quad -D\leqslant\epsilon\leqslant D, \tag{13}$$

where *D* is half the *d*-electrons bandwidth.

At weak coupling the on-site Coulomb repulsion term $H_U$ is treated using the usual Hartree-Fock decomposition $H_U\to U\langle n^f\rangle/2\Sigma_{i,\sigma}n^f_{i,\sigma}$. Since the total number of electrons $n_d+n_f$, is fixed, we obtain a mean field equation for $n_f$, which is solved together with the equation for the chemical potential $\mu$. The Coulomb interaction contributes to the renormalization of $\epsilon_0$, leading to a renormalized *f* energy given by $\epsilon_f=\epsilon_0+U\langle n^f\rangle/2$.

Once the mean field equations are solved, the specific heat is computed as

$$C=\frac{1}{N_s}\frac{d\langle H\rangle}{dT}. \tag{14}$$

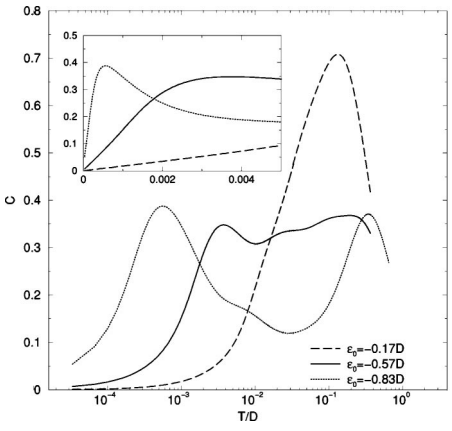


FIG. 1. Specific heat of the PAM in the $U=\infty$ limit as function of $T/D$ for different values of $\epsilon_0$. The inset shows a linear low-temperature behavior of $C(T)$, as it should be for a metal. The parameters are $V=0.17D$, $n=1.1$.

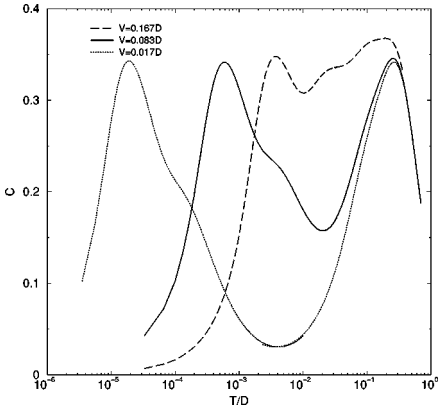


FIG. 2. Specific heat as function of $T/D$ for different values of $V$, in the $U=\infty$ regime. The parameters are $\epsilon_0=-0.57D$ and $n=1.1$.

At weak coupling, the mean field parameters are $n_f$ and $\mu$, whereas at $U=\infty$ these are $n_f$, $\epsilon_f$, and $\mu$. In what follows we take $D=6$ and $U$, $\epsilon_0$, $V$, and $T$ are measured in units of $D$.

In Figs. 1 and 2 we show the specific heat of the PAM in the $U=\infty$ limit for several values of $\epsilon_0$ and $V$, respectively. Since we are in the metallic regime the specific heat is linear at low temperatures (check inset in Fig. 1). Both the $\gamma$ coefficient and the zero-temperature spin susceptibility are much higher than the corrresponding values for nonhybridized $d$-electrons, signaling the presence of heavy quasiparticles. We see that as $V$ or $\epsilon_0$ decrease (with $\epsilon_0<0$) the low temperature peak is shifted to lower and lower temperatures, whereas the temperature position of the high temperature peak remains essentially constant. Let us define a characteristic temperature $T^*$ as the temperature value where $d\langle d^\dagger_{i,\sigma} f_{i,\sigma}\rangle/dT$ has its first local maximum, as can be seen in Fig. 3 for two values of $V$. A similar definition has been adopted for the Kondo temperature $T_K$ (on the lattice) in Ref. 8. Comparing the results for $T^*$ in Fig. 4 with those in Figs. 1 and 2 for $C(T)$, we see that the temperature position of the low-temperature peak coincides with $T^*$. The dependence of $T^*$ on $V$ and $\epsilon_0$ follows the same trends as those found for $T_K$ in Ref. 8, for the half-filled symmetric case, where a Kondo intrasite interaction of the form $J_K \sim V^2 U/[\epsilon_0(\epsilon_0+U)]$, was assumed to be present. Since we have not included the fluctuations of the boson fields, it is remarkable that mean field theory (in the boson fields) can capture this effect since the Kondo interactions are not generated at mean field level. We interpret the appearence of a specific heat peak at temperature $T^*$ as being associated with the existence of a peak in the density of states.

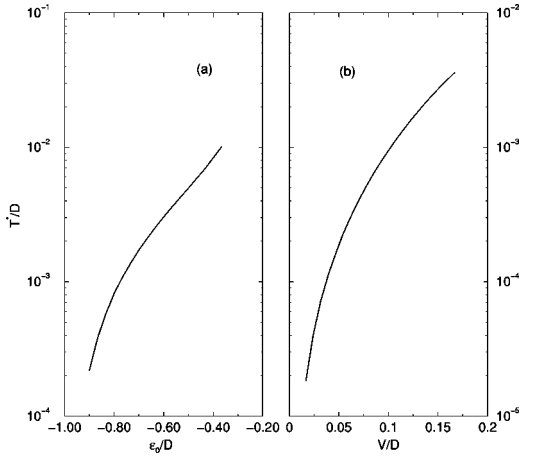


FIG. 4. Dependence of the correlation temperature $T^*$ as a function of: (a) $\epsilon_0$ and (b) $V$ in the $U=\infty$ regime and for $n=1.1$.

As we have seen, in the strong coupling limit $U=\infty$ the constraint $n_f \leqslant 1$ introduces boson fields. At the mean field level, the effect of these fields is to renormalize the hybridization matrix $V$ to $V_z=\sqrt{z}V$. This implies that for the same parameters as in the weak coupling (Hartree-Fock) regime the low temperature peak in $C(T)$ shifts to lower temperatures. This can be clearly seen comparing Fig. 1 with Fig. 5, and Fig. 2 with Fig. 6. We have also checked that the low-temperature peaks for different $V$ or $\epsilon_0$ tend to collapse into a single peak if $T$ is scaled by $T^*$, as observed for the sym-

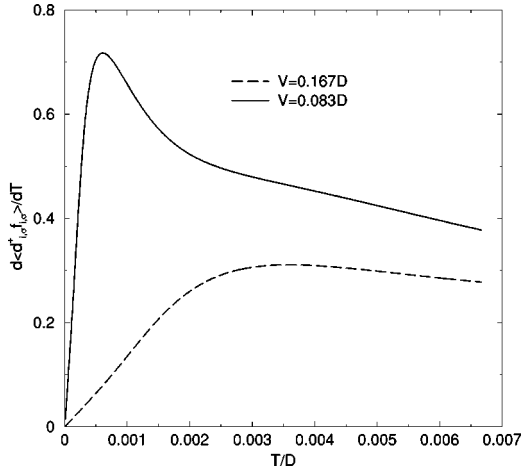


FIG. 3. Temperature dependence of the temperature derivative of matrix element $\langle d^\dagger_{i,\sigma} f_{i,\sigma}$ for two different values of $V$, in the $U=\infty$ regime, for $\epsilon_0=-0.57D$ and $n=1.1$.

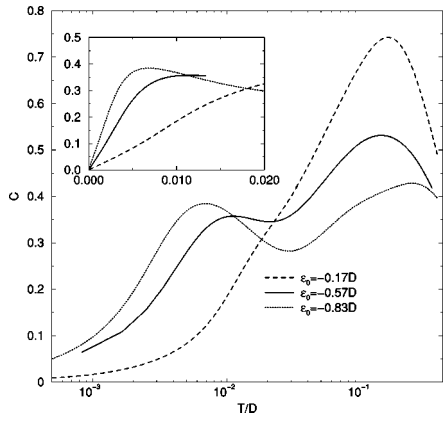


FIG. 5. Specific heat of the PAM in the Hartree Fock approximation as function of $T/D$ for different values of $\epsilon_0$. The inset shows a linear low-temperature behavior of $C(T)$, as it should be for a metal. The parameters are $U=0.47D$, $V=0.17D$, $n=1.1$.

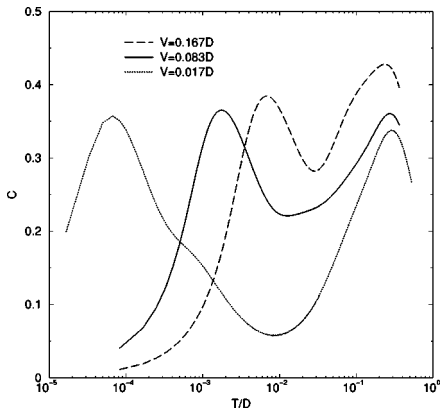


FIG. 6. Specific heat of the PAM in the Hartree Fock approximation as function of $T/D$ for different values of $V$. The parameters are $U=0.47D$, $\epsilon_0=-0.83D$, $n=1.1$.

metric case in Ref. 8. It is also clear from Figs. 1 and 2 that as we move the system towards $n_f \rightarrow 1$, which in a more elaborated description would correspond to the Kondo limit, the single peak structure separates into two peaks. It is also clear that the low-temperature peak is in fact a superposition of two peaks not completely separated. In Ref. 8 the complete separation of these two peaks took place only at very negative values of $\epsilon_0$.

In the single impurity case the model has been solved by the Bethe ansatz.[14] In that case, $C(T)$ also presents a double peak structure. In that solution the charge and spin excitations are described by different rapidities becoming clear that the low-temperature peak in $C(T)$ is associated with the spin excitations whereas the high-temperature peak is due to the charge excitations. An exact solution is not available for the lattice problem, however.

In more sophisticated treatments of the PAM (Refs. 8,9) a lattice Kondo temperature $T_K$ has been identified with the first maximum in the specific heat leading the authors to conclude that the first peak is associated with the Kondo shielding (spin excitations) whereas the second peak is associated with the charge transport (at an energy of the order of the hopping taken as unity in this paper). But the calculation we just presented shows that both the slave-boson mean field theory and the most simple Hartree Fock approximation lead to a multiple peak structure in the specific heat. These approximations do not describe the dynamics or screening of local moments. We therefore conclude that the double peak structure in the specific heat is simply a band-shape effect, namely, the appearence of a peak in the density of states. Indeed, such a feature is also present in more sophisticated treatments of the PAM.[8,9]

If the system undergoes a magnetic or superconducting transition, the peak structure is replaced, in general, by a lambda-shaped peak signaling the transition to the ordered phase or phases if they coexist. In the particular case of a superconducting ground state[13] and zero magnetization we have observed that in some cases the low-temperature peak is still present. A study of the ordered phases will be presented elsewhere.[15]

In many heavy-fermion materials the $f$ electrons have large total angular momentum. At mean field level and for $N>2$ the $z$ parameter has a critical temperature given by $T_z=(\epsilon_f-\mu)/\ln(N-1)$. In the ''Kondo regime'' $\epsilon_f-\mu$ is a very small quantity.[3,12] As the temperature rises $V_z$ vanishes. Therefore, we expect for $C(T)$, and within mean field theory, a different temperature behavior from that reported here.

In summary, we have found that $C(T)$ for the PAM presents a double peak structure both in the strong coupling limit and in the Hartree-Fock approach. This multiple peak structure in $C(T)$ is associated with a peak in the density of states of the system, due to hibridization between delocalized $d$ and localized $f$ states. The temperature $T^*$ of the first peak corresponds to a maximum in the derivative of $\langle d^{\dagger}_{i,\sigma} f_{i,\sigma}\rangle$ with respect to temperature. $T^*$ decreases as both $V$ and $\epsilon_0$ decrease. This effect is much more pronounced in the strong coupling regime, since $V$ is renormalized to smaller values due to the factor $\sqrt{z}$.

This research was supported by the Portuguese Program PRAXIS XXI under Grant No. 2/2.1/FIS/302/94.

[1] A. C. Hewson, *The Kondo Problem to Heavy-Fermions* (Cambridge University Press, Cambridge, 1997), and references therein.
[2] D. M. Newns and N. Read, Adv. Phys. **36**, 799 (1987).
[3] A. J. Millis and P. A. Lee, Phys. Rev. B **35**, 3394 (1987).
[4] A. Houghton, N. Read, and H. Won, Phys. Rev. B **37**, 3782 (1988).
[5] N. Bernhoeft, N. Sato, B. Roessli, N. Also, A. Hiess, G. H. Lander, Y. Endoh, and T. Komatsubara, Phys. Rev. Lett. **81**, 4244 (1998).
[6] N. Also, B. Roessli, N. Bernhoeft, R. Calemczac, N. K. Sato, Y. Endoh, T. Komatsubara, A. Hien, G. H. Lander, and H. Kadowaki, Phys. Rev. B **61**, R11 867 (2000).
[7] Ronald J. Keizer, Ph.D. thesis, University of Amsterdam, Van der Waals-Zeeman Intitute, 1999; Pedro Estrela, Ph.D. thesis, University of Amsterdam, Van der Waals-Zeeman Intitute, 2000.
[8] Ben Hur Bernhard and Claudine Lacroix, Phys. Rev. B **60**, 12149 (1999); H. B. Bernhard, C. Lacroix, J. R. Iglesias, and B. Coqblin, Physica B **259-261**, 227 (1999); Phys. Rev. B **61**, 441 (2000).
[9] Hong-Gang Luo and Shun-Jin Wang, Phys. Rev. B **62**, 1485 (2000).
[10] J. Zieliński and M. Matlak, Physica A **110**, 624 (1982).
[11] Carey Hurscroft, A. K. McMahan, and R. T. Scalettar, Phys. Rev. Lett. **82**, 2342 (1999).
[12] P. Coleman, Phys. Rev. B **29**, 3035 (1984); **35**, 5072 (1987).
[13] M. A. N. Araújo, N. M. R. Peres, P. D. Sacramento, and V. R. Vieira, Phys. Rev. B **62**, 9800 (2000).
[14] A. Okiji and N. Kawakami, Phys. Rev. Lett. **50**, 1157 (1983).
[15] N. M. R. Peres, P. D. Sacramento, and M. A. N. Araújo (unpublished).