# Magnetic-field dependence of the specific heat of a heavy-fermion system

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(Received 22 May 1992)

We use the lattice Anderson model on a small cluster to calculate the effect of an external magnetic field on the specific heat of a heavy-fermion system. The suppression of the specific heat results from the spreading of a manifold that contains states of different spins through the Zeeman effect. Our results are compared qualitatively with experiments on $CeCu_6$.

A defining characteristic of heavy-fermion metals is the extraordinarily large size of the electronic specific heat at low temperatures. If one writes, in a standard way, $C_e \sim \gamma T$, then the specific-heat coefficient $\gamma$ can be as large as 2 J/mol(deg)$^2$. Additionally, it is sometimes found that specific heat can be drastically reduced by an external magnetic field at very low temperatures and enhanced at slightly larger temperatures.[1,2] We will show here that this behavior can be reproduced in a simple calculation for a finite cluster, although the simplicity of the cluster model does not permit quantitative comparison with experiment.

This problem has been discussed from a single-particle viewpoint by Schotte and Schotte[3] and Edelstein[4] in terms of an enhanced density of states around the Fermi energy. Because we consider a small system, we can work with many-body states. Our calculation is essentially exact for a given model cluster, the only caveat being that we ignore the effect of a field on the single-particle hopping.

The physical picture which emerges from our calculations is simple. The system is characterized at low energies by a narrow, dense manifold of states which are mostly spin rearrangements of the $f$ electrons. These states are responsible for the high specific heat. We believe this is also true for large (bulk) systems, whether or not the material is ordered magnetically. Although the ground state is a singlet, the manifold contains states with differing values of the total spin quantum number. Application of a magnetic field separates the Zeeman components and broadens the energy distribution. The specific heat will be decreased at some temperatures, generally the lowest, and increased at higher temperature. For temperatures large compared to the width of the manifold, the entropy and specific heat are unaffected by the field.

The model is one we have considered previously:[5] a four-site Anderson lattice, with two nondegenerate orbitals ($c$ and $f$) on each site. The four sites are arranged to form a tetrahedron. We believe this geometry is more appropriate for application to three-dimensional systems than other simple four-site arrangements such as the square or rhombus. Crystal fields and spin-orbit coupling are ignored. These restrictions, which are necessary for our computations, inhibit us from trying to fit experiment data numerically. We are content to demonstrate here that the same qualitative behavior is exhibited by our model and a real physical system for reasonable values of the parameters. Preliminary results were reported in Ref. 6.

The Hamiltonian considered is, in a standard notation,

$$H = t\sum_{ij\sigma} c_{i\sigma}^{\dagger}c_{j\sigma} + V\sum_{i,j,\sigma}(c_{i\sigma}^{\dagger}f_{j\sigma} + f_{i\sigma}^{\dagger}c_{i\sigma}) + \varepsilon_f\sum_{i\sigma} n_{fi\sigma} + U\sum n_{fi\uparrow}n_{fi\downarrow} + g\mu_B B\sum_i s_{iz} \,. \quad (1)$$

The last term describes the interaction with an external magnetic field. Let

$$S_z = \sum_i S_{iz} \,, \quad (2)$$

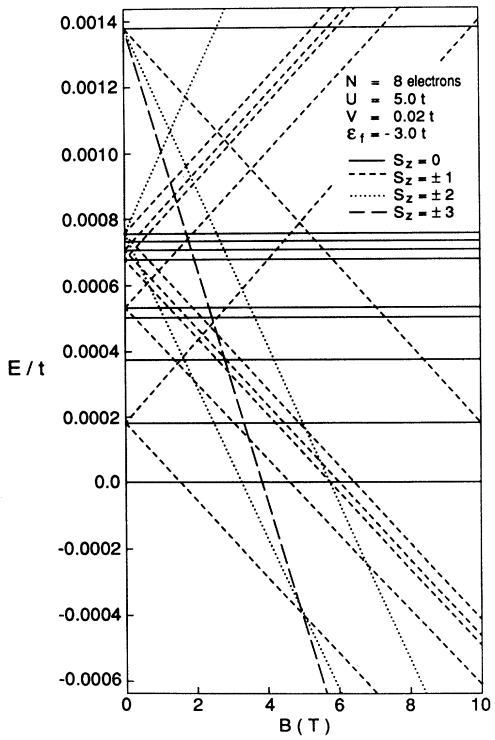


FIG. 1. Zeeman effect on the low-lying states of the lowest manifold. Parameters $t=1$ eV, $U/t=5$, $V/t=0.02$, and $\varepsilon_f/t=-3.0$. Not all states are shown.

 

so that $S_z$ is the total-spin operator for the cluster. $S_z$ commutes with the remainder of the Hamiltonian, so that the eigenstates of the system are characterized in part by the eigenvalues $M$ of $S_z$. Hence the energy of a state $|\alpha,M\rangle$ ($\alpha$ represents all other quantum numbers), $E_{\alpha,M}(B)$, in the presence of a field is

$$E_{\alpha,M}(B)=E_{\alpha}^{(0)}+g\mu_B BM \ , \tag{3}$$

in which $E_{\alpha}^{(0)}$ is the energy for zero $B$.

We consider here parameters such that the system is in the Kondo regime, such that the number of $f$ and $c$ electrons is close to 1 per site. Then, for $V \ll t \ll U$, which we believe to be the physically appropriate situation, the spectrum of the Hamiltonian consists of well-separated manifolds which are characterized by nearly integral numbers of $f$ electrons. For example, for $U/t=5$, $V/t=0.1$, $E_f/t=-3.0$, the lowest manifold for a system with the tetrahedral geometry considered here and two electrons per site contains states with essentially one $f$ electron and one $c$ electron has a width of about $0.03t$, and is separated from the next higher manifold by about $2t$. The low-temperature specific heat is governed by the excitation of states in this manifold. There are (again for the specific geometry) 240 states in the lowest manifold, of which 3 are spin septets, 18 quintets, 36 triplets, and 21 singlets. The ground state is a singlet; the first excited state is a triplet.

Our procedure is to diagonalize the Hamiltonian with $B=0$ and then add the $B$ dependence in accord with Eq. (3) when the partition function is calculated. The dependence of the energies of some states in the lowest manifold for a particular set of parameters is shown in Fig. 1. A complicated pattern of Zeeman splitting emerges.

The thermodynamic calculations are made using the cannonical ensemble. The variation of the lowest-energy levels with field shown in Fig. 1 leads to the dependence of the specific heat on field. For some fields below about 6 T and for the parameters of Fig. 1, there are double low-temperature peaks. As the field is increased, the Zee-

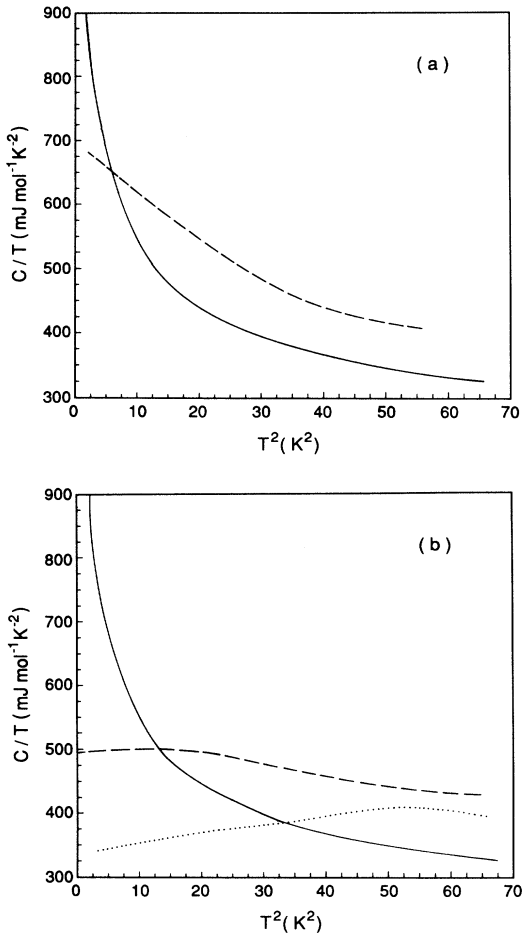


FIG. 2. Suppression of the specific heat of $CeCu_6$ by an external field (redrawn from the results of Ref. 1): (a) fields of 0 (solid line) and 11 T (dashed line); (b) fields of 0 (solid line), 14.5 T (dashed line), and 24 T (dotted line).

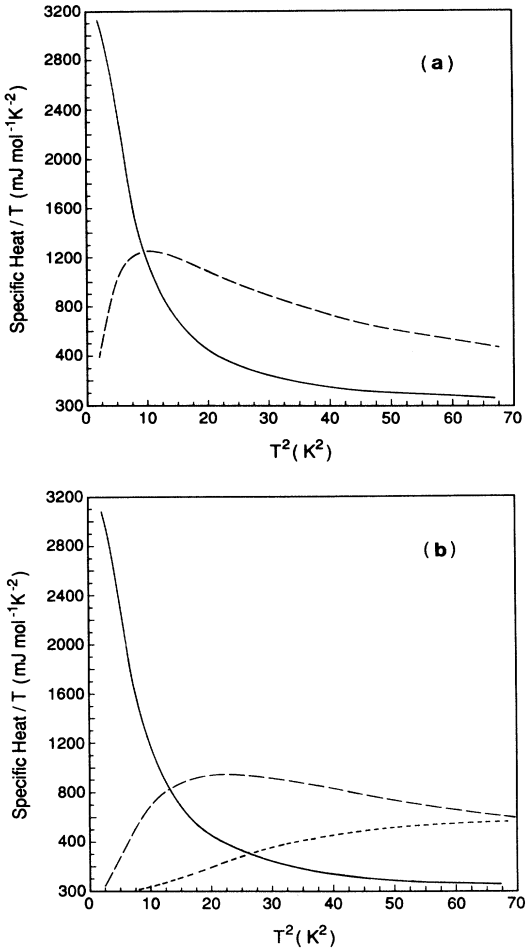


FIG. 3. Specific heat determined from the model cluster calculations: Parameters $t=1$ eV, $U/t=5$, $V/t=0.02$, and $E_f/t=-3.0$. (a) fields of 0 (solid line) and 11 T (dashed line); (b) fields of 0 (solid line), 14.5 T (dashed line), and 24 T (short-dashed line).

man splitting ultimately resolves itself so that the states are ordered according to $S_z$, and the specific-heat peak simply decreases in magnitude and broadens.

We will focus on $CeCu_6$, a system for which there are experimental results covering a wide range of fields (shown in Fig. 2). We cannot simulate this material in any detailed way for reasons associated with the small size of the system that we consider (neglect of orbital degeneracy of $f$ states, inadequate representation of the continuous distribution of $c$ states, etc., but the calculated specific heat shown in Fig. 3, though larger, is qualitatively sufficiently similar, so that we believe the essential physics has been identified.

As long as the parameters of the system are such that the system is in the Kondo regime, the on-site interaction parameter $U$ has little influence on the results. The system avoids having any doubly occupied $f$ orbitals. The parameter $t$ is important insofar as it sets the energy scale. We have simply set $t=1$ eV, a reasonable value which places the temperatures and magnetic-field strengths for which the specific heat is studied in the experimental range. The critical dimensionless parameter is the combination $V^2/t\varepsilon_f$, which controls the hybridization and thereby both the width of the lowest manifold and the position of states within that manifold. This quantity corresponds approximately to the resonance width in the resonant-level mode.[3,4] Since $t$ cancels out from comparison of dimensionless ratios, we see that we have, as a condition for an appreciable effect,

$$g\mu B \sim V^2/\varepsilon_f \ .$$

We have relied principally on the crossing of curves representing the specific heat as a function of temperature in differing magnetic fields in comparison with the experimental data in Fig. 2 to determine reasonable values for $V^2/t\varepsilon_f$, which we think are in the range of $1-3\times10^{-4}$ for $CeCu_6$. Systems with larger hybridization would require stronger fields to show magnetic-field dependence and conversely for those with smaller hybridization.

In conclusion, we have shown that an external magnetic field will alter the specific heat of a heavy-fermion system described by an Anderson-lattice model if the magnetic-field energy $g\mu B$ is comparable to the ratio of the square of the hybridization energy to the $f$-electron energy. A small-cluster calculation has given results for the specific heat similar to those observed for $CeCu_6$.

This Brief Report emphasized the view that small-cluster calculations an capture some of the essential physics of heavy-fermion systems, although many characteristics of real materials are omitted. Further confrontation with experiments is obviously required. The most straightforward test would be to determine whether calculations of the sort reported here are able to account for the field dependence of the specific heat of other heavy-fermion systems, using parameters (particularly $V$) which vary between materials in a manner consistent with other experimental determinations or theoretical estimates of these quantities. On the theoretical side, the effects of the choice of cluster geometry need to be determined. Calculations of the spectral-weight function for model clusters would help in understanding the relation between studies such as the present one and the more conventional view of Ref. 4.

The research was supported in part by the National Science Foundation under Grant No. 91-20166.

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