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Thermodynamics of the n -channel Kondo model for general n and impurity spin S in a magnetic field

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Abstract. The numerical solution of the Bethe *ansatz* equations of the n -channel Kondo problem is presented. The thermodynamics of the impurity is obtained as a function of temperature, external field, impurity spin S and the number of channels. Three situations have to be distinguished: (i) If $n = 2S$ the conduction electrons exactly compensate the impurity spin into a singlet at low temperatures, (ii) if $n < 2S$ the impurity spin is only partially compensated (undercompensated), and (iii) if $n > 2S$ the impurity spin is said to be overcompensated giving rise to critical behaviour. The results are briefly discussed in the context of magnetic impurities, the quadrupolar Kondo effect, an impurity spin embedded in the Takhtajan-Babujian model and a two-level system interacting with conduction electrons.

1. Introduction

Probably the most exciting model of a magnetic impurity embedded in a lattice is the n -channel Kondo problem. The first exhaustive analysis of the model is due to Nozières and Blandin [1] within a renormalization group approach. The Hamiltonian was then later diagonalized by means of Bethe's *ansatz* by Andrei and Destri [2] and Wiegmann and Tsel'ick [3]. Three situations have to be distinguished (n is the number of orbital conduction electron channels and S is the impurity spin).

(i) If $n = 2S$ the number of conduction electron channels is exactly sufficient to compensate the impurity spin into a singlet, giving rise to Fermi-liquid behaviour. This situation is believed to be realized for Fe and Cr impurities in simple metals [4], like Cu and Ag.

(ii) If $n < 2S$ the impurity spin is only partially compensated (undercompensated spin), since there are not enough conduction electron channels to yield a singlet ground state. This leaves an effective degeneracy (in zero field) at low temperatures of $(2S + 1 - n)$. The integer-valent limit of impurities with two magnetic configurations like Tm [5] could be related to this situation.

(iii) If $n > 2S$ the number of conduction-electron channels is larger than required to compensate the impurity spin. The impurity is said to be overcompensated and critical behaviour is obtained [6]. Applications for this case are the quadrupolar Kondo effect

[7, 8] and a two-level system interacting with several conduction electron channels close to the strong coupling fixed point [9, 10].

A magnetic impurity embedded in the Takhtajan–Babujian generalization of the Heisenberg chain has thermodynamic properties which are closely related to the three situations described above [11, 12].

In this paper we present the numerical solution of the thermodynamic Bethe *ansatz* equations of the n -channel Kondo problem for $S \leq 5/2$ and $n \leq 5$. In particular, the magnetic field and temperature dependence of the entropy, the specific heat and the susceptibility is discussed. This extends our previous results [4, 8, 10, 13] which are limited to the situations (i) $n = 1$ and arbitrary S , (ii) $n = 2S$ and (iii) $S = \frac{1}{2}$ and arbitrary n . The zero-field thermodynamics for $n, 2S \leq 5$ was previously obtained by Desgranges [14].

The rest of the paper is organized as follows. In section 2 we summarize the thermodynamic Bethe *ansatz* equations for the model (previously derived by Andrei and Destri [2] and Tsvetick [6]) and sketch the numerical procedure used to solve these equations. The results are presented in section 3 and are discussed in the context of possible applications and related models. Some concluding remarks follow in section 4.

2. Bethe *ansatz* equations and numerical procedure

The n -channel Kondo model for an impurity spin S and an arbitrary number of orbital conduction electron channels is given by

$$H_K = \sum_{k,m,\sigma} \varepsilon_k a_{km\sigma}^\dagger a_{km\sigma} + J \sum_{\substack{k,k',m \\ \sigma,\sigma'}} S \cdot a_{km\sigma}^\dagger \sigma_{\sigma\sigma'} a_{k'm\sigma'} \quad (1)$$

where S are the spin operators describing the magnetic impurity, J is the anti-ferromagnetic coupling constant and m labels the orbital channels. Although the Hamiltonian is diagonal in m the different orbital channels are not independent of each other. On the contrary, the exact solution shows that they are strongly coupled and form an orbital singlet, i.e. the spins of the conduction electrons at the impurity site are glued together to form a total spin $s_e = n/2$, which compensates the impurity degrees of freedom partially or totally.

The n -channel Kondo problem has been exactly diagonalized by means of Bethe's *ansatz* [2, 3] for a contact interaction at the impurity site and a linearized energy dispersion about the Fermi level with a built-in cutoff. This cutoff is necessary to correctly obtain the interaction between different orbital channels. The charge excitations completely decouple from the orbital and spin degrees of freedom. The effective attraction in orbital space leads to an orbital singlet and maximization of the spin as required by Hund's first rule. Within the Bethe *ansatz* many-particle spin wavefunctions are constructed from the ferromagnetic state by gradually flipping spins. Each flipped spin gives rise to a spin wave, characterized by a rapidity, which parametrizes its energy and momentum. The spin waves may form bound states; in this case the motion of the centre of mass is characterized by a common rapidity Λ . In the thermodynamic limit and in thermal equilibrium the thermal population of a bound state of k spin waves is determined by the function $\eta_k(\Lambda) = \exp(\varepsilon_k(\Lambda)/T)$, where ε_k is the thermodynamic energy of the bound state. Here $k = 1$ corresponds to a free unbound spin wave. The functions

η_k are self-consistently obtained as a solution of an infinite recursion sequence, known as the thermodynamic Bethe *ansatz* equations [2, 6, 14],

$$\ln[\eta_k(\Lambda)] = G * \ln[(1 + \eta_{k-1})(1 + \eta_{k+1})] - \delta_{k,n} \exp(\pi\Lambda/2) \quad k = 1, 2, 3, \dots \quad (2)$$

with the integration kernel given by

$$G(\Lambda) = [4 \cosh(\pi\Lambda/2)]^{-1} \quad (3)$$

where the asterisk denotes convolution and $\eta_0 \equiv 0$. These equations are completed by the asymptotic condition

$$\lim_{k \rightarrow \infty} (1/k) \ln[\eta_k(\Lambda)] = H/T = 2x_0 \quad (4)$$

where H is the field and the impurity free energy is given by

$$F_{\text{imp}} = -T \int_{-\infty}^{\infty} d\Lambda G[\Lambda - (2/\pi) \ln(T_K/T)] \ln[1 + \eta_{2S}(\Lambda)]. \quad (5)$$

Note that the field and temperature dependence of the equations only enters via the asymptotic condition, equation (4).

In the limits $\Lambda \rightarrow \pm\infty$ the Λ -dependence in (2) becomes irrelevant and the equations can be solved analytically. The asymptotic solutions are [14]

$$\ln[1 + \eta_k(+\infty)] = \begin{cases} 2 \ln\{\sin[\pi(k+1)/(n+2)]/\sin[\pi/(n+2)]\} & k < n \\ 2 \ln\{\sinh[(k+1-n)x_0]/\sinh[x_0]\} & k \geq n \end{cases} \quad (6a)$$

$$\ln[1 + \eta_k(-\infty)] = 2 \ln\{\sinh[(k+1)x_0]/\sinh[x_0]\} \quad \forall k. \quad (6b)$$

The functions $\eta_k(\Lambda)$ are monotonically decreasing functions of Λ and interpolate smoothly between the asymptotic values at $\Lambda \rightarrow \pm\infty$. From (6a) it is clear that the $\eta_k(\Lambda)$ are finite everywhere, except for $k = n$ as Λ tends to $+\infty$, implying that $\epsilon_n(\infty) = -\infty$. Hence, the conduction electron states coupling to the impurity at low T consist of bound states of n spin waves, i.e. they are strongly coupled in orbital singlet states of effective spin $s_e = n/2$. All other states are frozen out or decoupled from the impurity at low T .

For intermediate values of Λ the recursion sequence (2) has to be solved numerically. To implement this solution the infinite sequence (2) is truncated at an index k_c and the functions $\ln[1 + \eta_k]$ for $k > k_c$ are replaced by an appropriate interpolating asymptotical form. The numerical problem then reduces to the simultaneous solution of k_c coupled integral equations. Also the range of values of Λ is truncated at $\pm\Lambda_c$, where Λ_c is a value of the rapidity so that all the functions $\eta_k(\Lambda)$ have reached their asymptotic values, (6). The errors in the free-energy derivatives (obtained numerically) are controlled by varying k_c and Λ_c . Satisfactory results for $x_0 = H/T < 10$ were obtained for $k_c = 50$ and $\Lambda_c = 56$. This method is similar to the ones employed previously [4, 5, 8, 10, 13, 14], except that a higher numerical precision is required if $n \neq 2S$, in particular if $n > 2S$.

This numerical procedure is not accurate enough at low temperatures for $H/T > 10$ and the numerical derivatives turn out to be unreliable. This is in part due to the exponential behaviour with x_0 of the asymptotic expressions (6), but arises mainly from the exponential dependence on Λ of the integration kernel and the asymptotic of the functions η_k for $k \leq n$. The low- T properties of the impurity are determined by the $\Lambda \rightarrow +\infty$ asymptotic of η_{2S} . This low- T behaviour is particularly difficult to obtain in the

overcompensated case. A brief description of the procedure employed for $H/T > 10$ can be found in [10] (a detailed outline is given in [14]).

In summary, we solve the thermodynamic Bethe *ansatz* equations using two different numerical procedures: a standard one giving good results for $H/T < 10$ and a second one suitable for $H/T > 10$. The results for C/T (second temperature derivative of the free energy) match at $H/T = 10$ within a few percent.

3. Results

As already discussed in the introduction at low temperatures we have to distinguish three qualitatively different situations: (i) the undercompensated impurity, $S > n/2$; (ii) the totally compensated impurity spin, $S = n/2$; and (iii) the overcompensated case, $S < n/2$.

Some of the low- T properties can be understood in terms of the zero-temperature magnetization, which has been obtained analytically [3, 15, 16]

$$M^{2S \geq n} = \frac{1}{2}(2S - n) - \frac{in}{4\pi^{3/2}} \int_{-\infty}^{\infty} d\omega \frac{\exp(i\omega(2/\pi) \ln(H/T_H))}{\omega - i\delta} \left(\frac{i\omega n + \delta}{e\pi} \right)^{i\omega n/\pi} \\ \times \exp(-(2S - n)|\omega|) \Gamma(1 + i(\omega/\pi)) \Gamma(\frac{1}{2} - i(\omega/\pi)) / \Gamma(1 + in(\omega/\pi)) \quad (7a)$$

and

$$M^{2S \leq n} = -\frac{in}{4\pi^{3/2}} \int_{-\infty}^{\infty} d\omega \frac{\exp(i\omega(2/\pi) \ln(H/T_H))}{\omega - i\delta} \left(\frac{i\omega n + \delta}{e\pi} \right)^{i\omega n/\pi} \\ \times (\sinh 2S\omega / \sinh n\omega) [\Gamma(1 + i(\omega/\pi)) \Gamma(\frac{1}{2} - i(\omega/\pi)) / \Gamma(1 + in(\omega/\pi))] \quad (7b)$$

where T_H is given by

$$T_H = (2\pi/n) [(n/2e)^{n/2} / \Gamma(n/2)] T_K. \quad (8)$$

In order to extract the small-field behaviour ($H \ll T_K$) the contour of the integrals in (7) has to be closed through the lower half-plane. For the case $2S > n$ the dominating singularity is the cut along the imaginary axis, which gives rise to logarithmic singularities [16]

$$M^{2S > n} = (S - \frac{1}{2}n) \{ 1 + (\frac{1}{2}n) / \ln(H/T_K) \\ + (\frac{1}{2}n)^2 (\ln |\ln(H/T_K)|) / (\ln(H/T_K)^2 + \dots) \}. \quad (9a)$$

Hence, even a small magnetic field aligns the remaining spin of magnitude $(S - \frac{1}{2}n)$ and this remaining spin is only weakly coupled to the electron gas (logarithmic singularities). In the case $2S = n$ the impurity is completely compensated and the cut along the imaginary axis does no longer contribute. The leading singularity is due to the pole at $\omega = -i\pi/2$, which gives rise to a magnetization proportional to the field. The susceptibility for $S = \frac{1}{2}n$ is given by [1, 4, 5, 14, 15]

$$\chi^{2S=n} = S / (\pi T_K) \quad (9b)$$

i.e. finite, as expected for a system with Fermi-liquid-like properties. The low- T fixed

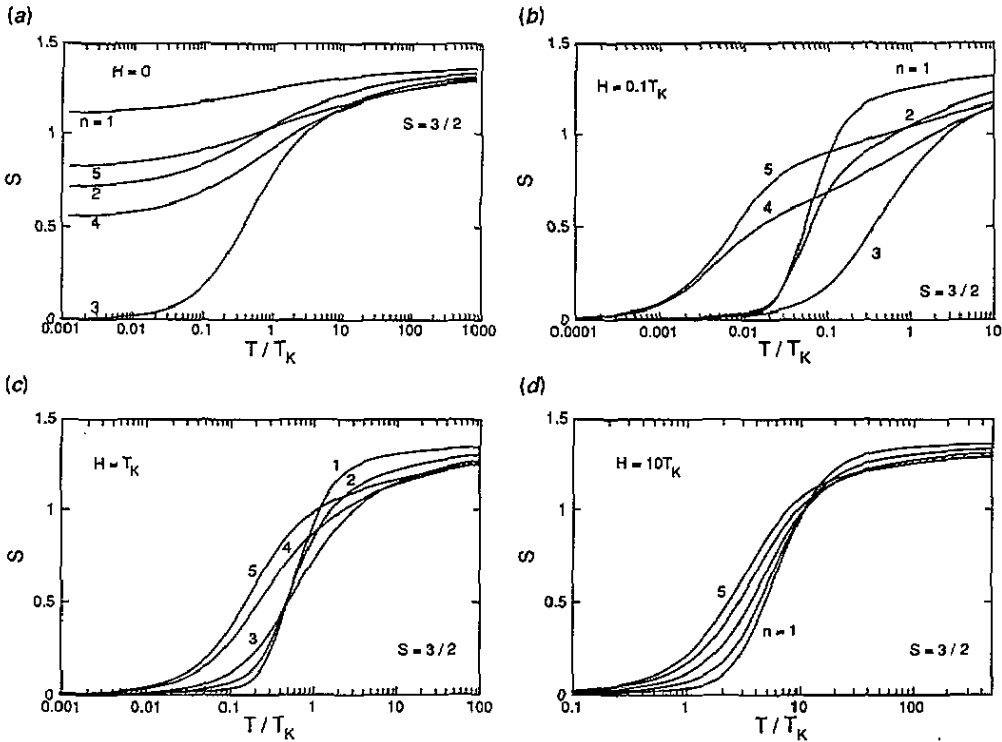


Figure 1. Entropy as a function of T/T_K for $S = \frac{3}{2}$, $n = 1, \dots, 5$ and four values of the field: (a) $H = 0$, (b) $H = 0.1 T_K$, (c) $H = T_K$ and (d) $H = 10 T_K$. The entropy vanishes as $T \rightarrow 0$ if $H \neq 0$, but remains finite if $H = 0$ unless $n = 2S$.

point in this case is a strong coupling one with $J \rightarrow \infty$. In contrast, the situation $2S < n$ has a strong coupling fixed point with finite coupling strength J . The leading singularity in (7b) is due to the pole arising from the zero of $\sinh(n\omega)$ closest to the real axis (but $\omega \neq 0$). The susceptibility diverges with a power law given by [3, 10]

$$\chi^{2S < n} \sim H^{(-1+2/n)} \quad n > 2. \quad (9c)$$

The exponent vanishes if $n = 2$ and $S = \frac{1}{2}$ and a logarithmic dependence on the field [3, 8, 12, 14, 16] is obtained as a consequence of a double pole at $\omega = -i\pi/2$. Note that the critical exponent in (9c) only depends on the number of channels.

Another quantity of interest is the zero-temperature zero-field entropy of the impurity, which can be obtained from (5) and (6a) (using $k = 2S$) [6, 8, 10, 12, 14]

$$S(T = 0, H = 0) = \begin{cases} \ln[|2S - n| + 1] & 2S \geq n \\ \ln\{\sin[\pi(2S + 1)/(n + 2)]/\sin[\pi/(n + 2)]\} & 2S \leq n \end{cases} \quad (10a)$$

$$(10b)$$

Hence only for $S = \frac{1}{2}n$ the ground state is a singlet in the absence of a magnetic field. For $S < n/2$ the ground-state entropy corresponds to a fractional spin. It can be shown that in the presence of a field the ground state is always a singlet [6, 15]. At high temperatures, on the other hand, the impurity free energy is obtained using (6b)

$$F_{\text{imp}} = -T \ln\{\sinh[(2S + 1)H/2T]/\sinh(H/2T)\}. \quad (11)$$

This is the free energy of a free spin S in a magnetic field.

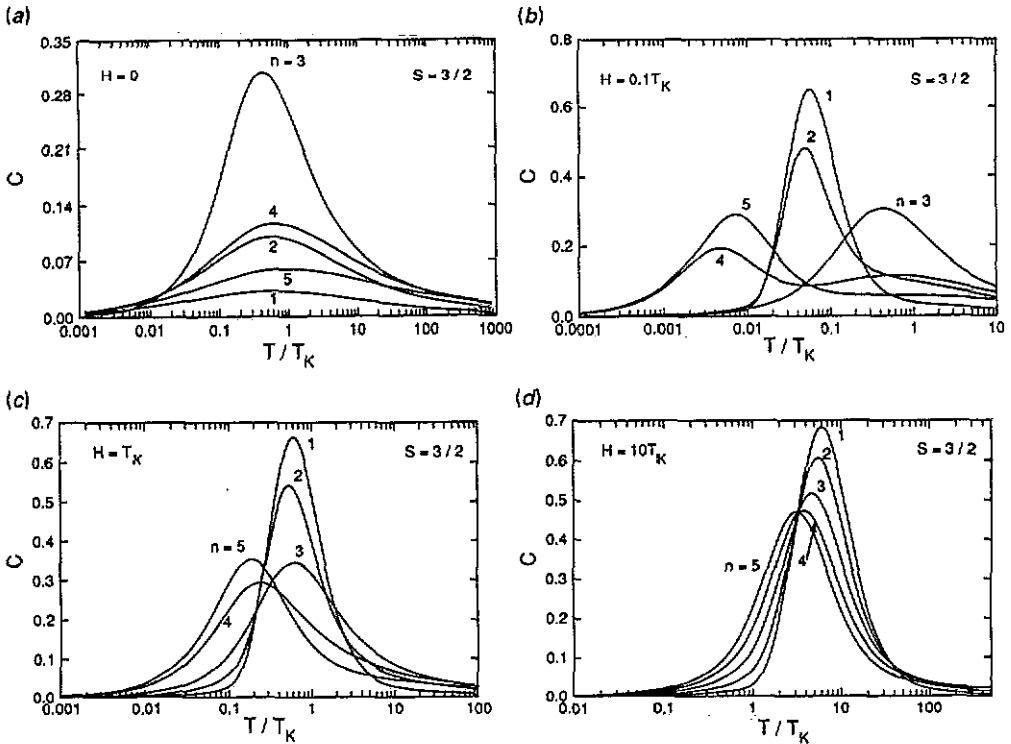


Figure 2. Specific heat as a function of T/T_K for $S = \frac{3}{2}$, $n = 1, \dots, 5$ and four values of the field: (a) $H = 0$, (b) $H = 0.1T_K$, (c) $H = T_K$ and (d) $H = 10T_K$. Note the double-peak structure for the overcompensated cases in (b).

The low- T (zero-field) susceptibility is also qualitatively different in the three cases. For an undercompensated spin χ diverges as T^{-1} (with logarithmic corrections) corresponding to the Curie law for an effective spin $(S - n/2)$. In a small field the specific heat shows the expected Schottky anomaly [5]. For a completely compensated impurity the susceptibility decreases with T^2 and the low- T specific heat is proportional to T , with the proportionality constant being [6]

$$\gamma = (\pi/T_K)[S/(S + 1)]. \tag{12}$$

All properties are Fermi-liquid-like and the Wilson ratio is $\chi/\gamma = (S + 1)/\pi^2$. Critical behaviour is again obtained in the over-compensated situation [6, 10, 12, 14]

$$\chi_{\text{imp}} \propto (T/T_K)^{\tau-1} \quad C_{\text{imp}}/T \propto (T/T_K)^{\tau-1} \tag{13}$$

where $\tau = 4/(n + 2)$. Note that the scaling dimensions of the temperature and the field are different. For $n = 2$ the critical exponents vanish and a logarithmic dependence on the temperature arises [6, 8, 10, 14].

Properties at intermediate temperatures and the simultaneous effects of temperature and field can only be obtained numerically. The results are shown in the figures. We first focus on $S = \frac{3}{2}$ and study the entropy, the specific heat and the susceptibility as a function of n , T and H .

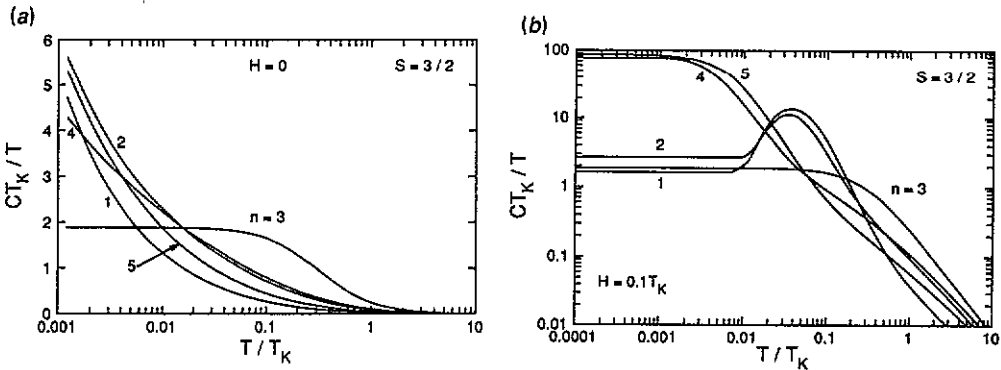


Figure 3. Specific heat over temperature as a function of T/T_K for $S = \frac{3}{2}$, $n = 1, \dots, 5$ in (a) zero-field and (b) $H = 0.1T_K$. Note that for $H = 0$ γ is only defined for $n = 2S$.

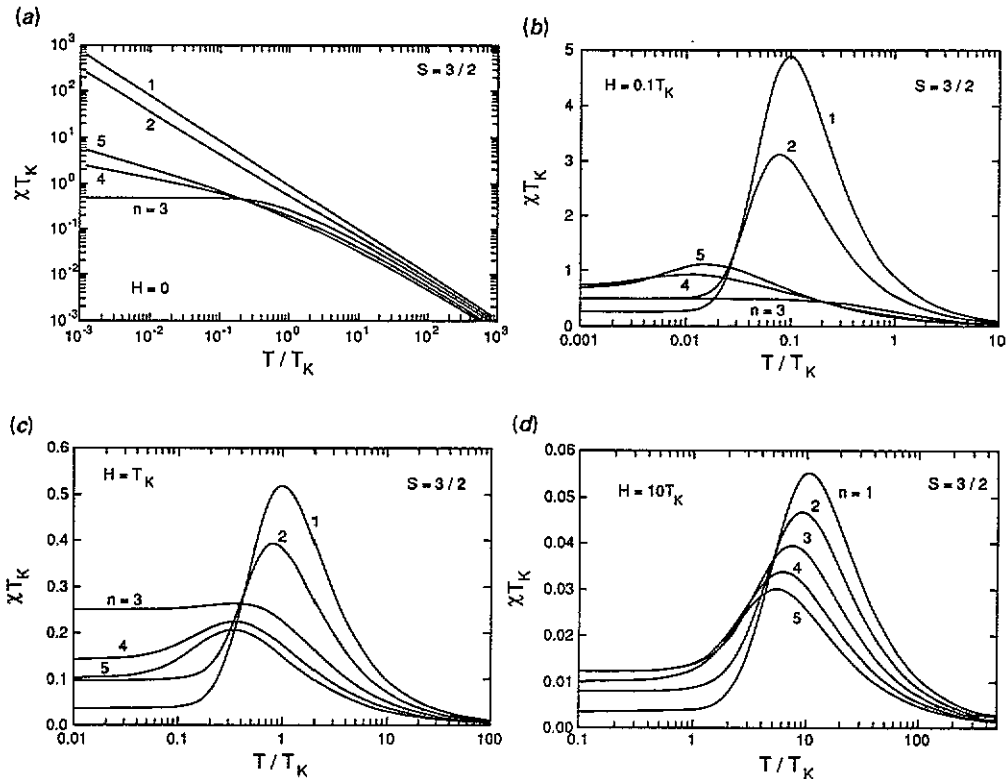


Figure 4. Susceptibility as a function of T/T_K for $S = \frac{3}{2}$, $n = 1, \dots, 5$ and four values of the field: (a) $H = 0$, (b) $H = 0.1T_K$, (c) $H = T_K$ and (d) $H = 10T_K$. Note that if $H = 0$ χ diverges as $T \rightarrow 0$ unless $n = 2S$.

The entropy for $S = \frac{3}{2}$ as a function of T is displayed in figure 1. In zero-field the entropy (figure 1(a)) interpolates between its $T = 0$ value, (10a) and (10b), and the high- T asymptotic, $S = \ln(2S + 1)$. Only if $n = 2S$ the ground state is a singlet and Fermi-liquid properties are obtained. This situation is realized for magnetic impurities like Fe

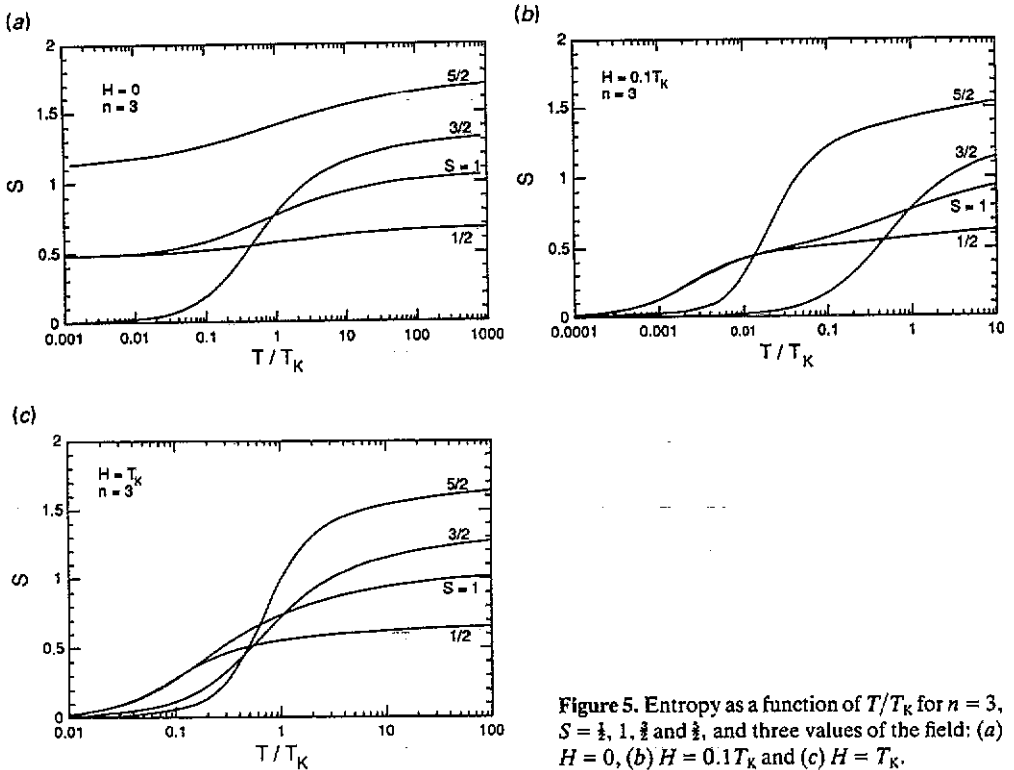


Figure 5. Entropy as a function of T/T_K for $n=3$, $S = \frac{1}{2}, 1, \frac{3}{2}$ and $\frac{5}{2}$, and three values of the field: (a) $H=0$, (b) $H=0.1T_K$ and (c) $H=T_K$.

($n = 2S = 4$) and Cr ($n = 2S = 5$) in simple metals [4], e.g. Cu and Ag. In the presence of a magnetic field (figures 1(b)–(1d)) the entropy always tends to zero as $T \rightarrow 0$, since the Zeeman splitting removes the remaining groundstate degeneracy. Hence, if $H \neq 0$ the ground state is a singlet. For large fields, e.g. $H = 10T_K$ (figure 1(d)), all curves are similar, but for fields small compared with the Kondo temperature (figure 1(b)) a qualitatively distinct behaviour is found for the three cases. For $n = 2S$ the singlet binding is strong and a heat bath of the order of T_K is needed to free the impurity spin. For $n < 2S$ the entropy has a strong variation in the temperature range $T \sim H$; the large slope gives rise to the Schottky anomaly. In the over-compensated situation a shoulder appears, which is indicative of a double-peak structure in the specific heat [8]. The high- T structure is caused by the Kondo resonance and is a consequence of the Kondo screening. The low- T structure is very field-dependent and can be associated with the removal of the zero-field, zero-temperature entropy (figure 1(a)) by the Zeeman splitting.

The specific heat as a function of T for an impurity of spin $S = \frac{3}{2}$ is displayed in figures 2(a)–(2d) for the same values of n and H as in figures 1. The specific heat is just T times the slope of the curves shown in figures 1. In zero-field (figure 2(a)) the height of the peak is maximum for the $n = 2S$ curve, since the entropy removal is maximum in this case. The peaks shown in figure 2(a) are the consequence of the Kondo resonance and appear at $T \sim T_K$. The two-peak structure mentioned above [8, 10] is explicitly seen in figure 2(b) for $n = 4$ and 5. The smaller peak (at the higher temperature) is again the Kondo resonance, while the low- T peak is strongly field-dependent and is caused by the

entropy drop from its $H = 0$ value (equation (10b)) to zero. The field dependence of this peak follows from the scaling dimensions of the field and the temperature to be on an energy scale proportional to $H^{(n+2)/n}$. For $n = 1$ and 2 (under-compensated impurity) the large peak essentially corresponds to a Schottky anomaly of an effective spin ($S - n/2$). At higher temperatures the shoulder arising from partial Kondo screening is seen. The two peaks for $n \neq 2S$ merge at higher fields ($H \sim T_K$) and asymptotically approach a free spin S Schottky anomaly at very large fields (on a logarithmic scale as expected for asymptotic freedom).

In figure 3 C_{imp}/T is shown to highlight the low- T behaviour. If $H = 0$ C_{imp}/T diverges for all $n \neq 2S$; for $n > 2S$ it diverges according to (13) and for $n < 2S$ as T^{-1} with logarithmic corrections (the $T \rightarrow 0$ entropy is only properly defined with these logarithms). For $n = 2S$, on the other hand, C_{imp}/T saturates at the value given by (12). A small field dramatically changes the behaviour (see figure 3(b)) and gives rise to a finite γ in agreement with the expected Fermi-liquid properties. In the over-compensated case it follows from the scaling dimensions that for small fields $\gamma \sim H^{-(n+2)/n}$ [17]. In all cases γ decreases with field.

The susceptibility for an impurity spin $S = \frac{3}{2}$ and for several fields is shown in figure 4. The Curie-like behaviour for a spin S is approached at high temperatures. Figure 4(a) displays the zero-field susceptibility, which is finite at $T = 0$ only if $n = 2S$ (see (9b)). If $n > 2S$ (over-compensated spin) χ diverges as $T \rightarrow 0$ according to (13) and for $n < 2S$ with a Curie law corresponding to an effective spin ($S - n/2$). Since the ground-state degeneracy is lifted by a Zeeman energy, χ is always finite if $H \neq 0$ (Fermi-liquid behaviour). The peaks of $\chi(H, T)$ correlate with those of the specific heat. In large fields the susceptibilities for the various n merge into the $\chi(H, T)$ for a free spin S .

The entropy for $n = 3$ as a function of T/T_K for various spins and three fields is displayed in figure 5.

4. Concluding remarks

We have discussed the numerical solution of the Bethe *ansatz* equations for the n -channel Kondo model as a function of field, temperature, the impurity spin and the number of channels. Three situations have to be distinguished: (i) the undercompensated impurity, (ii) the totally compensated spin and (iii) the over-compensated impurity spin. The physical properties are qualitatively different for the three cases. Only the $n = 2S$ situation exhibits Fermi-liquid behaviour, i.e. the ground state of the system is a singlet for all fields. This situation is realized for isolated magnetic impurities (e.g. Fe and Cr, described by a Hund's rule ground multiplet of spin S) in simple metals (e.g. Cu and Ag) and very good agreement with experiment can be obtained [4] with only one fitting parameter (T_K). In the under-compensated case, $S > n/2$, the low- T fixed point corresponds to an effective spin ($S - n/2$), which is weakly coupled to the electron gas. The impurity is then magnetic at low T , and probably suitable to describe some of the properties of nearly integer-valent Tm-impurities in a metallic environment [5].

The most exciting case is the over-compensated Kondo impurity. Here the strong coupling fixed point is not the usual $J \rightarrow \infty$ fixed point, but one with finite coupling strength [1]. This unusual fixed point has properties reminiscent of critical behaviour. The entropy is essentially singular as H and T tends to zero. The susceptibility diverges with a power of the field and temperature. Fingerprints of the overcompensated system are the two-peak structure in the specific heat at low fields and extremely large γ -values

as $H \rightarrow 0$. Two possible applications of this situation (for $S = \frac{1}{2}$) are the quadrupolar Kondo effect ($n = 2$) [7, 8] and the low- T fixed point of a two-level system interacting with conduction electrons (an atom in a double-well potential with electron-assisted tunnelling) [9, 10]. In both cases the magnetic field in the Kondo problem corresponds to a lattice distortion. Due to the divergent 'quadrupolar' susceptibility a tetragonal lattice distortion is induced by the quadrupolar Kondo impurity below a critical temperature T_c . For the same reason the symmetric double-well configuration is not stable for a tunnelling atom at very low T .

The same properties as for the n -channel Kondo impurity hold for a magnetic impurity of spin S' embedded in the antiferromagnetic Babujian-Takhtajan Heisenberg chain of spin S [12]. Again, if $S' > S$ the impurity is undercompensated, if $S' = S$ the impurity is just one more link in the chain and if $S' < S$ the over-compensated situation is realized. At low T and for small H the Bethe *ansatz* equations are identical to those of the Kondo problem.

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