Thermodynamics of the single-channel Kondo impurity of spin $S\,(\leq \frac{7}{2})$ in a magnetic field

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The thermodynamic Bethe-ansatz equations of the *s-d* exchange model of arbitrary spin S (derived by Fateev and Wiegmann) are solved numerically. We present the magnetic field and temperature dependence of the specific heat, the entropy, the magnetization, and the susceptibility for $S\leq\frac{7}{2}$.

I. INTRODUCTION

The diagonalization of the $S=\frac{1}{2}$ Kondo model by Andrei[1] and Wiegmann[2] by means of Bethe's ansatz was followed by numerous extensions of these results. The thermodynamic equations of the *s-d* model were derived by Andrei and Lowenstein[3] and Tsvelick and Wiegmann[4] and then solved numerically by several groups.[5-7] Generalizations of the model to spins larger[8] than $\frac{1}{2}$ and to include orbital degrees of freedom (the Coqblin-Schrieffer and the n-channel Kondo models) were also found to be integrable[9-13] (for a review see Ref. 14).

The purpose of this paper is to present the numerical solution of the thermodynamic Bethe-ansatz equations of the *s-d* exchange model for spins S up to $\frac{7}{2}$ in a magnetic field. This model is the most straightforward generalization of the spin-$\frac{1}{2}$ Kondo problem, with the impurity spin-$\frac{1}{2}$ operators being replaced by those of a spin S, i.e.,

$$\mathcal{H}=\sum_{\mathbf{k},\sigma}\epsilon_k c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}-HS_z +J\sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'}\mathbf{S}\cdot c^\dagger_{\mathbf{k}\sigma}\mathbf{s}_{\sigma\sigma'}c_{\mathbf{k}'\sigma'}\ . \quad (1)$$

Here $c^\dagger_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}\sigma}$ are the usual creation and annihilation operators and $2\mathbf{s}_{\sigma\sigma'}$ is the vector of Pauli matrices. Considering only s-wave scattering and with a linearized dispersion relation, this model was found integrable by Fateev and Wiegmann[8] and Andrei, Furuya, and Lowenstein.[11] The thermodynamic Bethe-ansatz equations were derived by Fateev and Wiegmann[15] (see also Ref. 11). In the absence of a magnetic field the thermodynamic equations were numerically solved by Rajan *et al.*[5] and Desgranges *et al.*[7] Rajan *et al.*[5] also solved the $S=\frac{1}{2}$ case in the presence of a magnetic field. Some results for the case $S=1$ in a magnetic field have been published by Aligia *et al.*[16] This paper represents a more complete study of the thermodynamics in $H\neq 0$ including spins up to $S=\frac{7}{2}$.

The rest of the paper is organized as follows. In Sec. II the nonlinear integral equations are restated and the numerical method is briefly discussed. The results are presented in Sec. III and are followed by concluding remarks (Sec. IV).

II. THERMODYNAMIC BETHE-ANSATZ EQUATIONS AND NUMERICAL PROCEDURE

The thermodynamic Bethe-ansatz equations[11,15] for the model (1) consist of an infinite set of nonlinearly coupled integral equations for function $\eta_n(\Lambda)$. The function $\eta_n(\Lambda)$ characterizes a string excitation of order n with real rapidity Λ. The Λ rapidities represent the spin degrees of freedom of the model, and a string excitation of order n corresponds to a bound state of n spin-flipped electrons. The functions $\eta_n(\Lambda)$ are interrelated via integral equations, and the most convenient representation for a numerical solution is the recursion sequence

$$\ln\eta_n=G*\ln[(1+\eta_{n-1})(1+\eta_{n+1})]-\delta_{n,1}\exp(\pi\Lambda/2)\ ,\qquad n=1,2,\ldots,\quad \eta_0\equiv 0\ , \quad (2)$$

where the asterisk denotes convolution and

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

These equations are completed by the asymptotic condition

$$\lim_{n\to\infty}\left[\frac{1}{n}\ln\eta_n(\Lambda)\right]=\frac{H}{T}=X_0\ , \quad (4)$$

and the free energy of the impurity is given by

$$F=-T\int_{-\infty}^{\infty}d\Lambda\, G\left[\Lambda-\frac{2}{\pi}\ln(T_K/T)\right]\ln[1+\eta_{2S}(\Lambda)]\ , \quad (5)$$

where S is the impurity spin.

For $\Lambda\to-\infty$ the driving term of the integral equations [the last term of Eqs. (2)] vanishes, so that this situation corresponds to a free spin decoupled from the electron gas (high-temperature or weak-coupling limit). Since the integration kernel falls off exponentially, the functions η_n are constants in this limit and the integral equations reduce to a set of algebraic equations, whose solution is

$$\ln(1+\eta_n)=2\ln\{\sinh[\tfrac{1}{2}(n+1)X_0]/\sinh(\tfrac{1}{2}X_0)\}\ ,\qquad T\gg T_K\ , \quad (6)$$

and the free energy is given by

$$F = -T \ln[2\cosh(H/2T)] \ .$$

For $\Lambda \rightarrow \infty$, on the other hand, the driving term becomes dominant, so that $\eta_1 \rightarrow 0$. This situation corresponds to the strong-coupling limit at low temperatures. The solution of the integral equations for this case yields

$$\ln(1+\eta_n) = 2\ln[\sinh(\tfrac{1}{2}nX_0)/\sinh(\tfrac{1}{2}X_0)] \ , \quad T \ll T_K \ . \qquad (7)$$

Hence, as a function of Λ the functions $\eta_n(\Lambda)$ interpolate monotonically and smoothly between the asymptotic values given by (6) and (7). The variation between these asymptotic values relative to the value of the function decreases as $n \rightarrow \infty$. Hence, to a certain degree of approximation we may truncate the recursion relation by replacing the function η_n for $n = n_c$ by an adequate interpolating expression. We have chosen $n_c = 30$ and the integration interval for Λ to be 32, i.e., for $|\Lambda| > 16$ the functions η_n reached their asymptotic expressions, Eq. (6) and Eq. (7), respectively. By varying n_c and the Λ cutoff we estimate our errors to be smaller than 1% in the second derivatives of the free energy, i.e., the specific heat and the susceptibility. In this way the solution of the infinite set of Eqs. (2) reduces to the simultaneous solution of $n_c - 1$ nonlinearly coupled integral equations with appropriate boundary conditions for large Λ and at $n = n_c$. This method is standard and similar to that employed in other papers.[5–7,16]

Note that the integral equations only depend on $X_0 = H/T$ via the boundary conditions, but neither on the spin S nor on the temperature explicitly. Hence, by solving the equations for one value of X_0, we obtain the free energy for all S and all temperatures. The entropy, the specific heat, the magnetization, and the susceptibility are then obtained by numerical differentiation.

III. RESULTS

Using the procedure described in the preceding section, we obtained the magnetization, the entropy, the specific heat, and the susceptibility as a function of the magnetic field and temperature for spin values S up to $\frac{7}{2}$. The characteristic energy scale of the system is the Kondo temperature T_K, and all energies are measured in units of T_K. At high temperatures, i.e., $T \gg T_K$, the impurity behaves essentially as a free spin S. At low temperatures and in zero field, the conduction electron spin density at the impurity site screens one impurity degree of freedom, reducing the impurity spin to an effective $S - \frac{1}{2}$. The case $S = \frac{1}{2}$ (singlet ground state) is then qualitatively different from other spin values, since at low T even a small magnetic field removes the spin degeneracy if $S \geq 1$. In addition, common to all spin values is the suppression of the Kondo effect by a magnetic field of the order of T_K or larger.

Our results are displayed in the figures. Figures 1(a)–1(c) show the magnetization as a function of H/T in constant field for spins up to $\frac{7}{2}$. As expected, the magnetization increases monotonically with the field. It is also seen that the magnetization for a given field increases as T is reduced. Note that the saturation values of M as $T \rightarrow 0$ depend on the magnetic field, as a consequence of the Kondo effect. The magnetic field quenches the Kondo screening only partially, so that M does not reach the value S, but the saturation value is always larger than $S - \frac{1}{2}$. At high temperatures, i.e., $H \ll T$, on the other hand, $M \sim H/T$ and the susceptibility follows the expected Curie law.

The entropy is a measure of the effective degrees of freedom of the impurity at a given temperature and field. Figures 2(a)–2(d) show the entropy as a function of T in

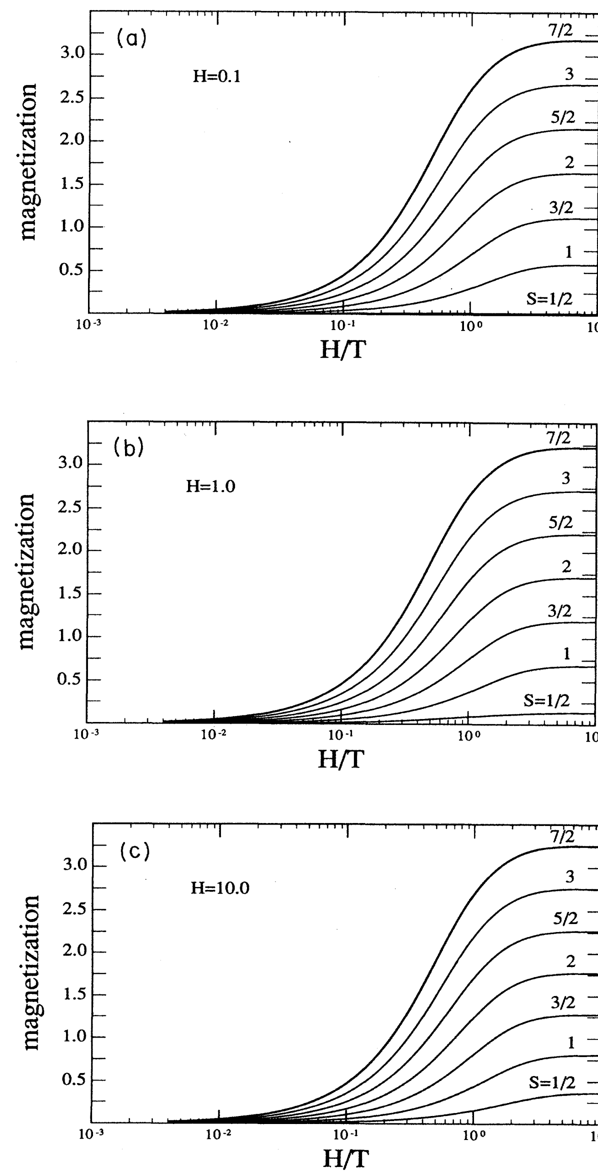

FIG. 1. Magnetization in constant field as a function of H/T for spins up to $\frac{7}{2}$. The values of the magnetic field are (a) $H = 0.1T_K$, (b) $H = T_K$, and (c) $H = 10T_K$.

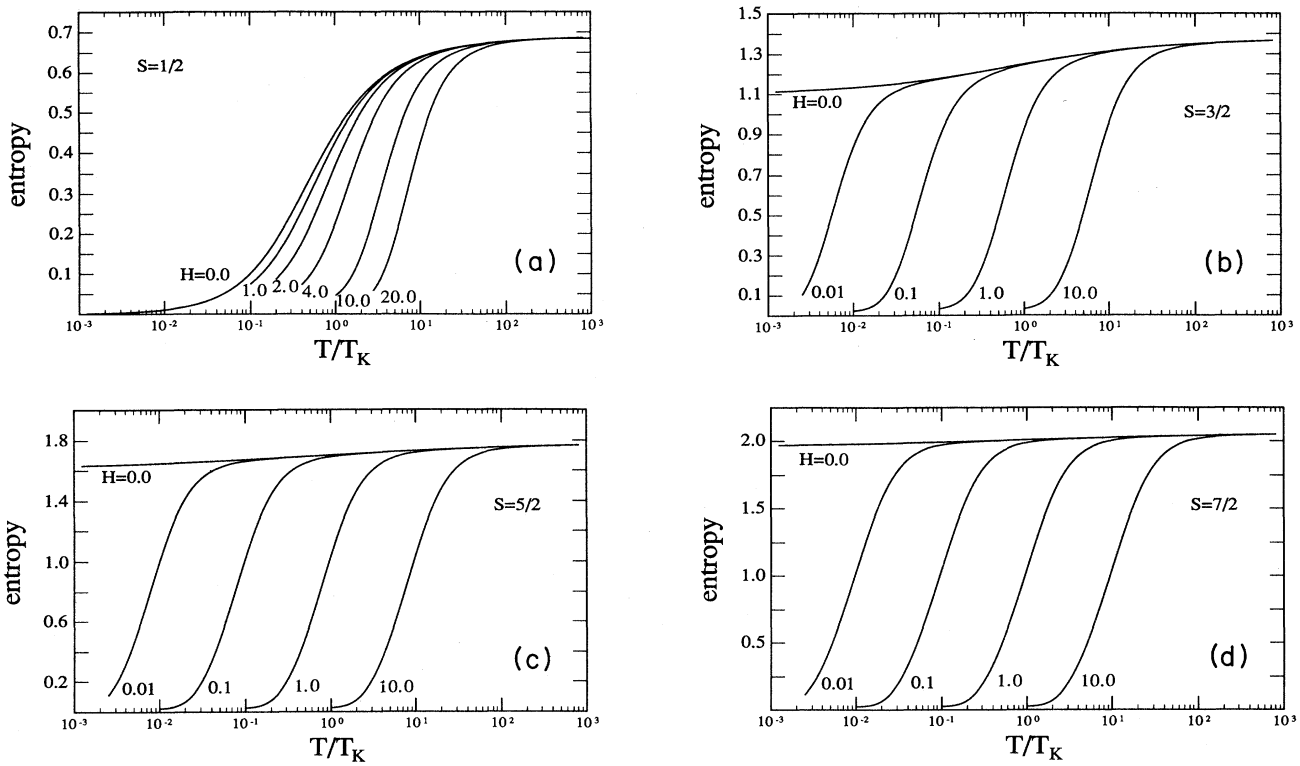

FIG. 2. Entropy as a function of T/T_K in constant magnetic field for the half-integer spins: (a) $S=\frac{1}{2}$, (b) $S=\frac{3}{2}$, (c) $S=\frac{5}{2}$, and (d) $S=\frac{7}{2}$. The field intensity H is given in units of T_K.

constant field for the half-integer spins $S=\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, and $\frac{7}{2}$, respectively. The entropy for $S=\frac{1}{2}$ agrees with the results by Rajan *et al.*[5] and is included for comparison, since the cases $S=\frac{1}{2}$ and $S>\frac{1}{2}$ behave differently. As seen, all cases with $S\neq\frac{1}{2}$ are qualitatively similar. In zero field the entropy varies monotonically between $\ln(2S)$ at low T and $\ln(2S+1)$ for $T \gg T_K$. For $S=\frac{1}{2}$ the crossover between the two asymptotical values is shifted towards higher temperatures, because the magnetic field suppresses the degrees of freedom of the impurity. If $S>\frac{1}{2}$ the degeneracy of the impurity at low T is lifted by the magnetic field and the entropy at $T=0$ ($H\neq 0$) is zero. Hence, in addition to the Kondo crossover, there is a second crossover related to the Zeeman splitting, which occurs approximately at $T\approx H$.

The specific heat is given by the temperature derivative of the entropy at constant field. The specific heat as a function of T is shown in Figs. 3(a)–3(d) for the same set of spin and magnetic field values as in Figs. 2. For spin-$\frac{1}{2}$ the specific heat has a peak which shifts towards higher temperatures as the field is increased (see also Ref. 5). The height of the peak also grows with field and asymptotically (on a logarithmic scale) approaches the value of a free-spin Schottky anomaly. For $S>\frac{1}{2}$ again the zero field and $H\neq 0$ cases are qualitatively different, because the Zeeman splitting lifts the degeneracy of the ground state. The zero-field Kondo specific heat is displayed in Fig. 4(a) as a function of T for several spins. The height of the peak dramatically decreases with the spin (see also Ref. 5) and disappears in the classical spin limit, i.e., as $S\rightarrow\infty$. These curves are shown also in Figs. 3(b)–3(d). The large resonance at about $T\sim H$ in Figs. 3(b)–3(d) refers to the Schottky anomaly due to the Zeeman splitting. For $H \ll T_K$ the Schottky peak is the one of a spin $S-\frac{1}{2}$, while if $H \gg T_K$ it corresponds to a spin S. A smooth crossover between these two regimes is observed. Hence, if $H \ll T_K$ the specific heat has two independent peaks, one corresponding to the Zeeman splitting of the ground multiplet and one to the Kondo screening.

In Figs. 4(a)–4(d) the specific heat for various spins is drawn as a function of T in constant field. While for $H=0$ the spin-$\frac{1}{2}$ resonance is considerably higher than for other spins, this situation is inverted already for a relatively small field, i.e., $H=0.1T_K$. As already discussed, this peak for $S>\frac{1}{2}$ is the consequence of the Zeeman splitting. In Fig. 4(b) the shoulder around $T\approx T_K$ in the $S=1$ curve corresponds to the Kondo resonance. For larger fields [Figs. 4(c) and 4(d)] the expected free-spin hierarchy of the resonances (monotonically increasing with S) is already established.

The magnetic susceptibility as a function of T for the half-integer spins and various magnetic fields is plotted in Figs. 5(a)–5(d). Again $S=\frac{1}{2}$ behaves differently as a consequence of the singlet ground state. For $S=\frac{1}{2}$ the

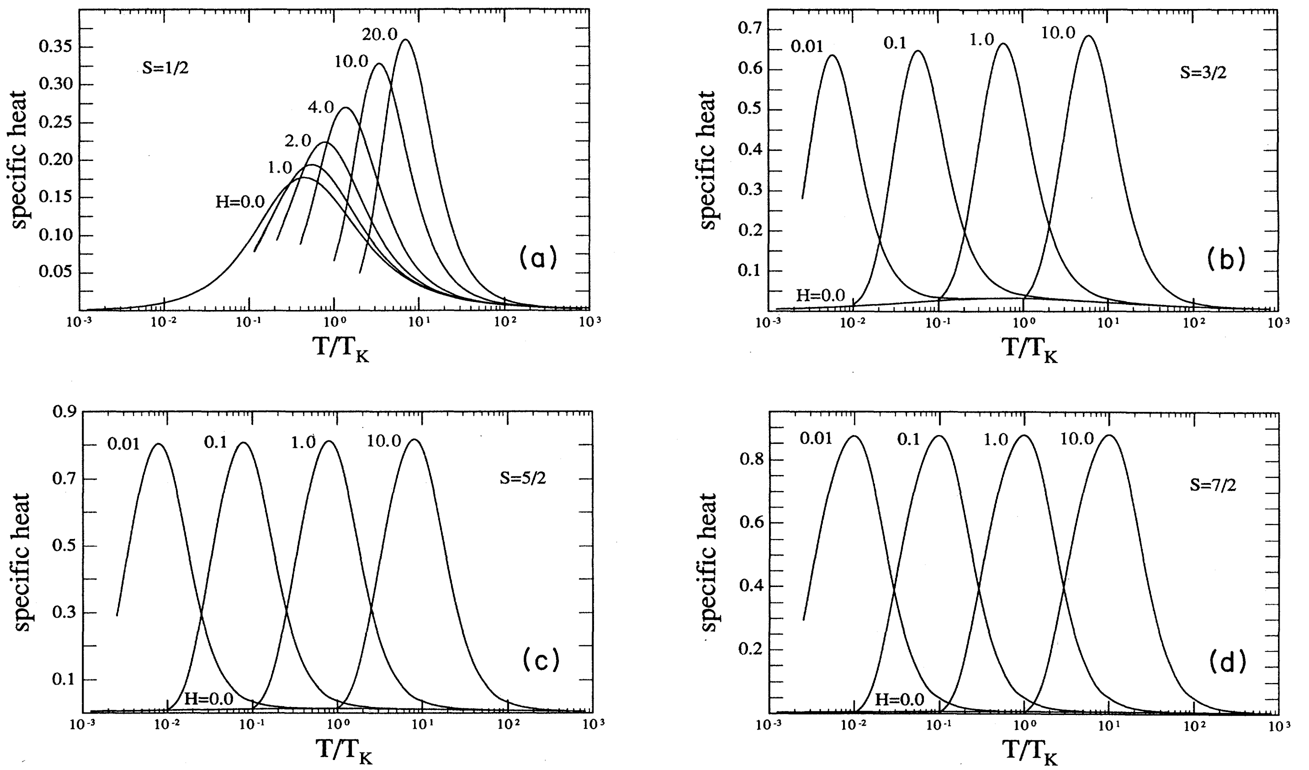

FIG. 3. Specific heat as a function of T/T_K in constant magnetic field for the half-integer spins (a) $S=\frac{1}{2}$, (b) $S=\frac{3}{2}$, (c) $S=\frac{5}{2}$, and (d) $S=\frac{7}{2}$. The field intensity H is given in units of T_K.

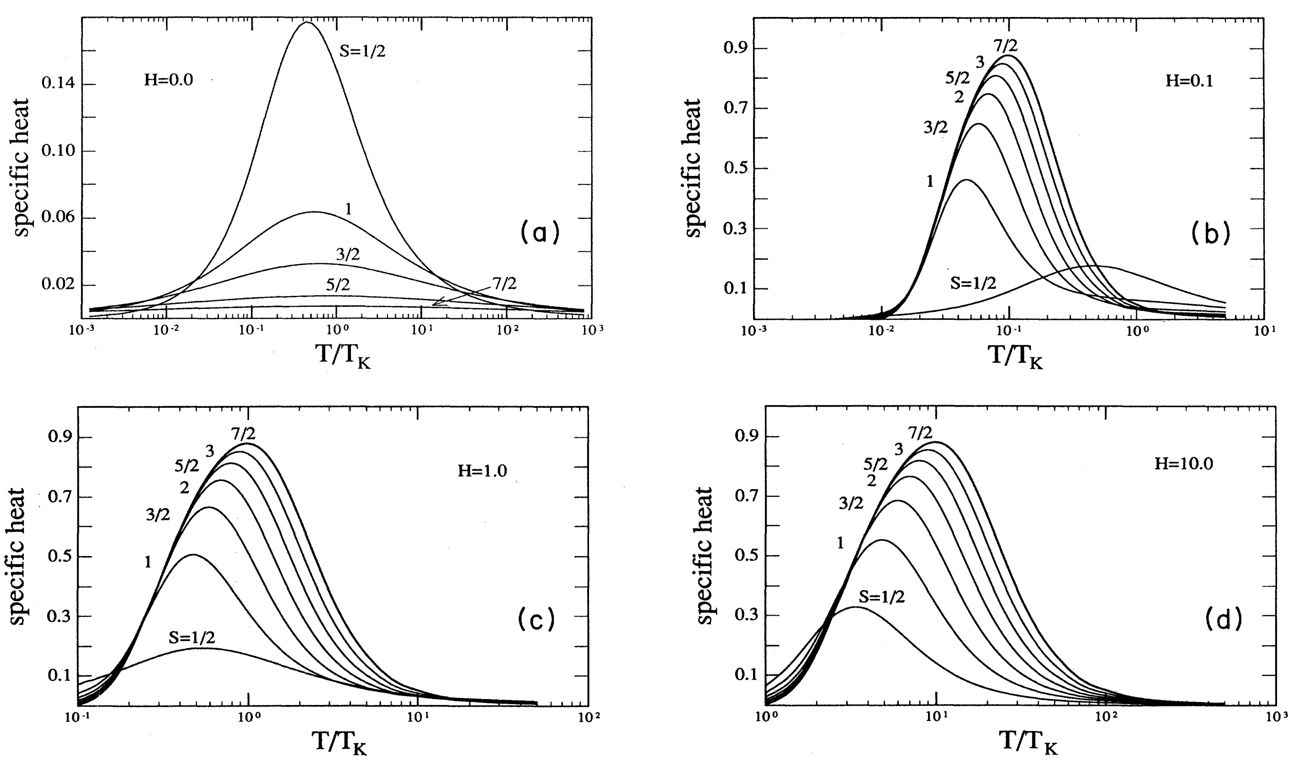

FIG. 4. Specific heat as a function of T/T_K for various spins in a constant magnetic field. The field intensities are (a) $H=0$, (b) $H=0.1T_K$, (c) $H=T_K$, and (d) $H=10T_K$.

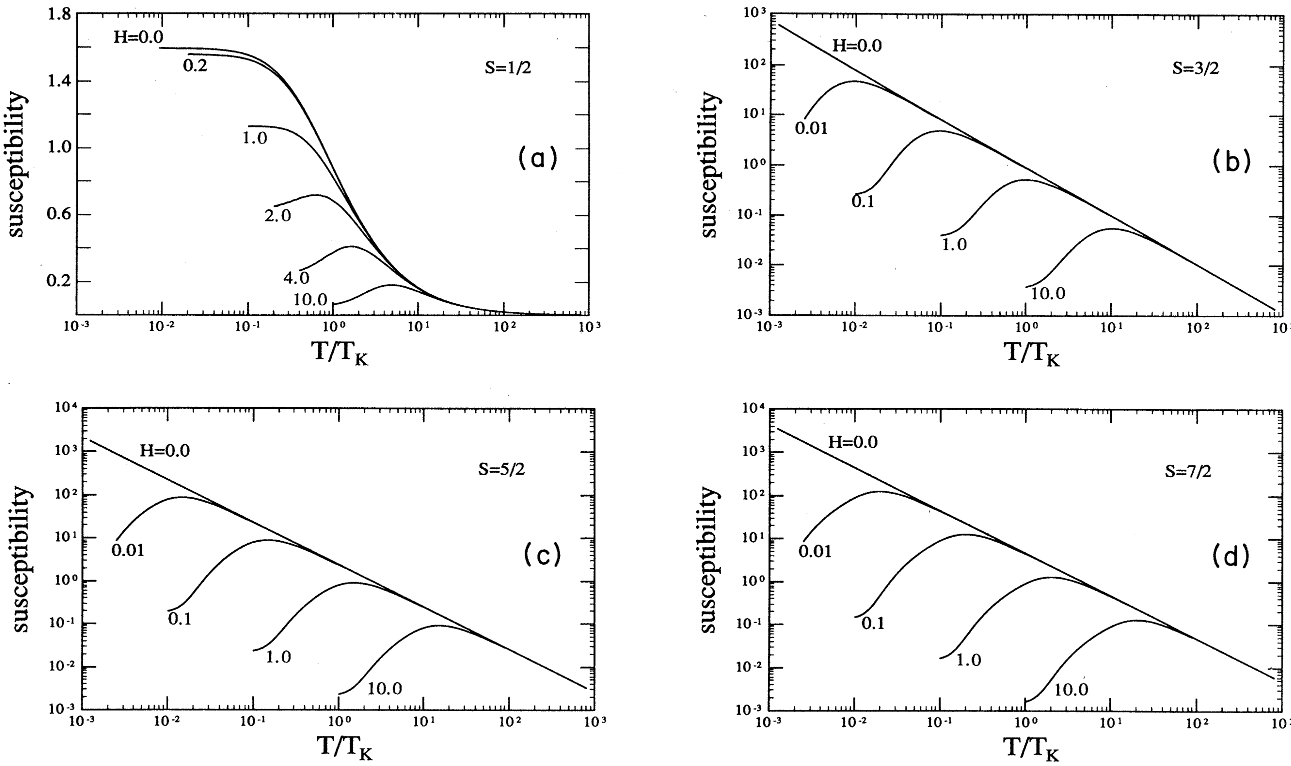

FIG. 5. Susceptibility as a function of T/T_K in constant magnetic field for the half-integer spins: (a) $S=\frac{1}{2}$, (b) $S=\frac{3}{2}$, (c) $S=\frac{5}{2}$, and (d) $S=\frac{7}{2}$.

susceptibility is maximum at low T if H is small, as a consequence of the Kondo resonance. For large fields, on the other hand, χ has its maximum around $T \sim H$, reminiscent of the free-spin behavior. At high temperatures χ follows a Curie law. For $S \neq \frac{1}{2}$, χ is more conveniently presented on a double-log plot. The $H=0$ Curie law appears then as a straight line. There is, however, a smooth change in the Curie constant, since the effective spin is S at high T and $S-\frac{1}{2}$ at low T. The magnetic field lifts the degeneracy at low T and significantly reduces χ, which nevertheless remains finite due to the Kondo-spin-compensated degree of freedom. The maximum of χ at T/H has the same origin as the Schottky anomaly of the specific heat.

IV. SUMMARY AND BRIEF DISCUSSION

Exact results for the magnetization, the entropy, the specific heat, and the susceptibility of an impurity of spin S interacting via an *s-d* exchange with an electron gas have been obtained by solving numerically the thermodynamic Bethe-ansatz equations in a magnetic field. The results extend previous ones by Rajan *et al.*,[5] Desgranges *et al.*,[7] and Aligia *et al.*[16]

At high temperatures the impurity behaves like a free spin S, with some corrections, which vanish asymptotically (on a logarithmic scale) as $T \to \infty$. At low temperatures, one degree of freedom of the impurity is compensated by the conduction electrons, so that the impurity has an effective spin $S-\frac{1}{2}$, i.e., the degeneracy of the ground state is $2S$. A magnetic field lifts the degeneracy of the ground state, giving rise to a Schottky anomaly in the specific heat and a peak in the susceptibility at $T \sim H$. Hence, if $H \ll T_K$ the specific heat shows a two-peak structure, one peak associated with the Zeeman splitting of the ground multiplet and the other peak with a broad Kondo resonance. For intermediate or large fields (compared to T_K) they merge into one peak.

The magnetization increases monotonically with field, as well as if T is lowered in a constant field. In the latter case the saturation value of M as $T \to 0$ lies between S and $S-\frac{1}{2}$. In a finite field the value S is not reached as a consequence of the Kondo effect, which is only partially quenched by the field. The susceptibility ($S \geq 1$) in zero field follows a Curie law, with a Curie constant that is slightly temperature dependent. In a magnetic field, on the other hand, the susceptibility shows a structure (associated with the Schottky anomaly) and reaches a finite value as $T \to 0$.

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