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Low-temperature properties of a two-level system interacting with conduction electrons: An application of the overcompensated multichannel Kondo model

P. D. Sacramento
Department of Physics, Temple University, Philadelphia, Pennsylvania 19122

P. Schlottmann
Department of Physics, Temple University, Philadelphia, Pennsylvania 19122
and Department of Physics, and Center for Materials Research and Technology, Florida State University, Tallahassee, Florida 32306
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We consider an atom in a double-well potential [parametrized by a two-level system (TLS)] interacting with screened conduction electrons. The tunneling of the TLS is assisted by the Fermi gas. Close to the strong-coupling fixed point the renormalization-group equations for the noncommutative model in the case of spinless fermions, but an arbitrary number of relevant orbital channels, lead to the n-channel Kondo problem with $S=\frac{1}{2}$. By solving the thermodynamic Bethe-ansatz equations for the n-channel Kondo problem numerically in the presence of a magnetic field, we discuss the low-temperature properties of the TLS close to the fixed point. The Zeeman splitting corresponds to the energy difference between the two positions of the tunneling atom. The atom is not localized at one of the potential minima. The susceptibility diverges as $H\rightarrow 0$ and $T\rightarrow 0$, indicating that the symmetric TLS is unstable against a local lattice deformation via coupling to phonons. The lattice distortion disappears above a critical temperature T_c. The ground-state equilibrium situation of the TLS corresponds to $H\neq 0$ and a Fermi-liquid picture applies. The values for the specific heat become very large as $H\rightarrow 0$. For small fields the specific heat shows a double-peak structure, which is particularly pronounced for $n=2$.

I. INTRODUCTION

Since the pioneering work of Caldeira and Leggett,[1] the subject of tunneling particles coupled to a heat bath has attracted great interest,[2–4] in particular, also in the context of metallic glasses. In metallic glasses an atom may tunnel between two possible positions possessing levels close in energy, which can be represented as a two-level system (TLS). The tunneling atom is placed in a double-well potential and can then spontaneously hop from one position to the other. These tunneling transitions are rare and a much more efficient mechanism is electron-assisted tunneling, in which the scattering of a conduction electron off the tunneling atom induces the transition. The multiple scattering of electrons with the TLS creates electron-hole excitations of arbitrarily small energy in the electron gas,[5–8] giving rise to logarithmic singularities in the scattering matrix and other physical quantities, in close analogy to the Kondo[9] and x-ray threshold[10] problems. Problems involving logarithmic singularities in all physical properties to all orders in the perturbation expansion are suitable candidates for renormalization-group treatments. In the renormalization-group procedure, high-energy states with energies close to the band edge are gradually eliminated from the system, giving rise to renormalizations of the coupling parameters, vertices, and self-energies. The successive reduction of the band cutoff energy (ultraviolet cutoff) eventually leads to a fixed point, which determines the critical properties of the model. Such a renormalization treatment has been applied to several models involving a TLS interacting with a degenerate Fermi bath.[6–8] For so-called noncommutative models, the relevant fixed point is usually related to a strong-coupling situation. As shown by Muramatsu and Guinea,[8] in some cases the fixed point can be related to a well-known problem, namely the n-channel Kondo model.[11] This model has been solved exactly by means of the Bethe anastz[12,13] and the purpose of this paper is to study the critical properties of the fixed point of the interacting TLS in terms of this solution.

There is experimental evidence for the strong coupling between the TLS and the conduction electrons. In metallic glasses, the tunneling gives rise to an additional contribution to the low-temperature specific heat which is linear in T. The specific-heat contribution linear in T in high-temperature superconductors has also been attributed to TLS tunneling. An anomalously large acoustic saturation intensity as well as a $\log T$ dependence was observed in the acoustic absorption of the metallic glass Pd-Si-Cu.[14,15] The strong coupling of TLS to electrons appears to be responsible for anomalies in the ultrasonic absorption and dispersion in amorphous superconductors.[16,17] The specific heat of superconducting Nb is also strongly affected by the tunneling of H, D and O impurities.[18] Some physical properties of $A15$ compounds have, as well, been attributed to the strong interaction of TLS with electrons.[19]

A general form of the Hamiltonian of a TLS interacting with a degenerate Fermi gas was given by

Zawadowski,[6]

$$H = H_0 + H_{TLS} + H_{int} \ , \quad (1a)$$

where H_0 is the kinetic energy of the conduction electrons, H_{TLS} represents the TLS, and H_{int} describes the scattering of the conduction electrons off the TLS. It is convenient to express the band states in partial waves at the site of the TLS impurity

$$H_0 = \sum_{k,\alpha,s} \varepsilon_k a^\dagger_{k\alpha s} a_{k\alpha s} \ , \quad (1b)$$

where k is the absolute value of the momentum, s is the spin projection, and α is an index labeling both the orbital angular momentum l and its z projection m. The states of the TLS are parameterized in terms of Pauli matrices

$$H_{TLS} = -\tfrac{1}{2}\Delta_0 \sigma^z + \tfrac{1}{2}\Delta_1 \sigma^x \ , \quad (1c)$$

where Δ_0 is the energy splitting between the two states of the double well and Δ_1 is the intrinsic tunneling rate. The interaction of the conduction electrons with the TLS can be written as

$$H_{int} = \sum_{k,k',\alpha,\beta,s,i} a^\dagger_{k\alpha s} V^i_{\alpha\beta} a_{k'\beta s} \sigma^i \ , \quad (1d)$$

where $i = x,y,z$. The k dependence of the potentials $V^i_{\alpha\beta}$ has been neglected, although the important angular dependence (i.e., α,β) is being kept.[7] The k dependence is believed to be irrelevant since the infrared singularities are determined by states close to the Fermi energy. The V^z terms represent the difference of the scattering amplitudes for the two positions of a rigid TLS, while the V^x and V^y terms describe the electron-assisted tunneling, i.e., electron scattering with simultaneous tunneling of the atom. These terms arise from the fluctuations of the potential barrier due to fluctuations in the electron density. Note that the spin of the electrons is not altered in the scattering process. Since atoms are much heavier than electrons, it is expected[7] that, for the bare parameters, $|V^x|, |V^y| \ll |V^z|$. Note that Eq. (1c) can be diagonalized by means of a rotation of the σ matrices to give an effective splitting of $E = (\Delta_0^2 + \Delta_1^2)^{1/2}$; hence, we may choose $\Delta_1 = 0$ without loss of generality.

If we assume that only one partial wave (e.g., s waves) is important, the problem is reduced to a potential scattering one. The renormalized coupling constants do not scale into a strong-coupling regime, resembling in this way the x-ray threshold problem.[10] The tunneling rate decreases with temperature and, at low T the dynamics is frozen into one of the two potential minima. The fermion excitation spectrum can be "bosonized," showing a close analogy with a TLS coupled to a phonon bath.

The physical situation is, in general, very different if two or more partial waves are relevant. It is usual to choose the z axis aligned with the TLS and neglect the extension of the TLS in the x and y directions, so that only $m = 0$ plays a role (m is the z component of the orbital angular momentum of the electron). The special case when

$$V^i_{\alpha\beta} V^j_{\beta\gamma} - V^j_{\alpha\beta} V^i_{\beta\gamma} \quad (1e)$$

is zero for all i and j is called the commutative model.[20] The scaling equations in this case do not renormalize into a strong-coupling fixed point and the situation is similar to the one with only one partial wave. The noncommutative model corresponds to the case where Eq. (1e) is not identically zero.[7] The physical fixed point of the noncommutative model is, in general, a strong-coupling one, i.e., the invariant coupling parameters of the model grow when the electronic band cutoff is lowered. As a consequence, due to the electron-assisted hops, the TLS cannot be localized in one of the states.[21] This situation is mathematically analogous to the Kondo problem where the impurity is spin compensated by the conduction electrons, quenching in this way the magnetic properties at low temperatures.

The analogy between the Kondo problem and the noncommutative model is, of course, only a formal mathematical one. The TLS itself corresponds to the Kondo impurity spin $\frac{1}{2}$, the energy separation Δ of the two positions in the TLS has its analogy in the Zeeman splitting of the Kondo impurity spin, and the partial waves (orbital degrees of freedom) of the conduction electrons interacting with the TLS represent the spin degrees of freedom of the conduction electrons in the Kondo problem. The spin of the conduction electrons interacting with the TLS corresponds to the channel index in the Kondo problem.

Hence, assuming that the interaction of only two partial waves with the TLS is important, we have to further distinguish between models involving spinless fermions and electrons with spin degrees of freedom. In the former case, the fixed point corresponds to the single-channel Kondo problem,[21] while the latter situation reduces to the two-channel Kondo model.[8] The physical properties of the one- and two-channel Kondo models are, however, dramatically different. In Sec. II we argue that, if g partial waves are relevant ($g > 1$), the fixed point in the case of spinless fermions corresponds to the n-channel Kondo problem with impurity spin $\frac{1}{2}$ and $n = g - 1 = 1$. The exact solution of the n-channel Kondo problem was obtained by Andrei and Destri[12] and Tsvelick and Wiegmann[13] in terms of the Bethe ansatz. The thermodynamic Bethe-ansatz equations and the method of solving them numerically are summarized in Sec. III. The thermodynamic properties of the model, obtained numerically, are presented in Sec. IV. We find that the TLS is unstable with respect to an induced asymmetry of the two atomic positions, i.e., the coupling to the phonon bath produces a local distortion. Concluding remarks follow in Sec. V.

II. SCALING OF THE INTERACTING TLS-HAMILTONIAN AND RELATION TO THE n-CHANNEL KONDO PROBLEM

In this section we closely follow arguments given in Refs. 7 and 8. The renormalization of Hamiltonian (1) is simplest within the poor man's scaling approach, in which conduction states with energies close to the band cutoff are successively eliminated from the system. As a consequence, the effective band cutoff D' is gradually reduced and the coupling parameters of the Hamiltonian are renormalized, obeying the following differential equations:[7]

$$\partial V^{s}_{\alpha\beta}(x)/\partial x = -2i\rho \sum_{i,j} \varepsilon^{ijs} \sum_{\gamma} V^{i}_{\alpha\gamma}(x) V^{j}_{\gamma\beta}(x) \ , \tag{2}$$

where $x = \ln(D/D') > 0$, ρ is the density of states, and ε^{ijs} is the Levy-Civita symbol. The logarithmic dependence on the cutoff is due to the electron-hole excitations with arbitrarily small energy, while the ε^{ijs} symbols enter as a consequence of the Pauli matrices describing the TLS and the $V^{i}_{\alpha\beta}$ being noncommutative. Note that the general form of the Hamiltonian remains invariant under the renormalization procedure, except for the change in the coupling amplitudes. The initial conditions for the differential equations (2) are that the $V^{i}_{\alpha\beta}(x=0)$, i.e., for $D'=D$, are equal to the bare coupling parameters.

Equation (2) refers to the renormalization of the model in leading logarithmic order. Renormalization to higher order does not affect the general structure of the differential equations, but generates higher-order terms in V, e.g., V^3, V^4, on the right-hand side of the equations. With minor modifications, the argumentation below remains valid beyond leading-order scaling.

With the repeated application of the renormalization procedure, the system eventually reaches a fixed point. Near the fixed point the vector space on which the matrices operate can be divided into invariant subspaces[7] whose scaling equations can be studied separately. We assume that one subspace is dominant and determines the properties of the system. Consider one subspace labeled with μ. Close to the fixed point it is expected that the matrix character of $[V^{i}_{\alpha\beta}(x)]_{\mu}$ does not change with further scaling and can be factorized[7]

$$[V^{i}_{\alpha\beta}(x)]_{\mu} = V^{*i}_{\alpha\beta}(\mu) v^{i}_{\mu}(x) \ , \tag{3a}$$

where $v^{i}_{\mu}(x)$ is the amplitude that is still renormalized and the $V^{*i}_{\alpha\beta}(\mu)$ are the infinitesimal generators of an irreducible unitary representation of the rotation group satisfying the following equations:

$$iV^{*s}_{\alpha\beta}(\mu) = \sum_{i,j} \varepsilon^{ijs} \sum_{\gamma} V^{*i}_{\alpha\gamma}(\mu) V^{*j}_{\gamma\beta}(\mu) \ . \tag{3b}$$

The different subspaces μ correspond to the different dimensionalities of the generators, i.e., to the different values of an effective "spin" S_{μ} (with dimension $g_{\mu} = 2S_{\mu}+1$).

Assuming that only one subspace μ is relevant at low temperatures and small energies (i.e., it decouples from the rest of the states), the effective Hamiltonian is of the form

$$H_{\text{int}} = V\boldsymbol{\sigma} \cdot \sum_{\alpha,\beta,s,k,k'} A^{\dagger}_{k\alpha s} \mathbf{S}_{\alpha\beta} A_{k'\beta s} \ , \tag{4}$$

where $A^{\dagger}$ and A are fermion operators for conduction states having the symmetry corresponding to the subspace μ. For spinless fermions, and if the subspace is two dimensional, the problem reduces to the single-channel Kondo problem.[7] If the spin of the electrons is not neglected, the two-dimensional case corresponds to the two-channel Kondo model.[8] We now show that if the subspace μ has dimension g, the problem for spinless electrons is equivalent to the n-channel Kondo model with $n = g-1$.

The Hamiltonian of the n-channel Kondo problem[11] is given by

$$H_K = \sum_{k,m,\sigma} \varepsilon_k a^{\dagger}_{km\sigma} a_{km\sigma} + J \sum_{k,k',m,\sigma,\sigma'} \mathbf{S} \cdot a^{\dagger}_{km\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} a_{k'm\sigma'} \ , \tag{5a}$$

where $\mathbf{S}$ are the spin operators describing the magnetic impurity, J is the antiferromagnetic coupling constant, and m labels the orbital channels. Although Eq. (5a) is diagonal in m, the different orbital channels are not independent of each other. On the contrary, the exact solution by means of the Bethe ansatz[12,13] 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 $s_e = n/2$, where n is the number of channels. It has been shown by Tsvelick and Wiegmann[22] that the excitation spectrum of model (5a) is equivalent to that of the following Hamiltonian:

$$H_K = \sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + J \sum_{k,k',\sigma,\sigma'} c^{\dagger}_{k\sigma} P[\mathbf{S} \cdot (\mathbf{s}_e)_{\sigma\sigma'}] c_{k'\sigma'} \ , \tag{5b}$$

where c and $c^{\dagger}$ are new fermion operators with $-n/2 \le \sigma \le n/2$. $P(x)$ is a well-defined special polynomial of order $\min(2s_e, 2S)$ so that the model (5b) is SU(2)-invariant. For the case $S = \frac{1}{2}$, the polynomial is of the fcrm

$$P[\mathbf{S} \cdot \mathbf{s}_e] = a + b(\mathbf{S} \cdot \mathbf{s}_e) \ , \tag{5c}$$

where a and b are constants. Since potential scattering is not relevant in the strong-coupling regime, the Hamiltonian [(5b) and (5c)] is then equivalent to H_{int}, given by Eq. (4), if spinless $A_{k\alpha}$ are considered.

Although we are not able to provide rigorous results for the spin-degenerate case, one may speculate that, due to the strong coupling, the two spin channels in Eq. (4) add together yielding an effective orbital subspace of dimension $g = 4S_{\mu}+1$. Here we invoked the same type of mechanism that led from Hamiltonian (5a) to (5b) and (5c), but without proving it in our case. This result is rigorous if the orbital subspace μ in Eq. (4) is two dimensional. Now that we have established a correspondence between the low-temperature properties of the TLS and the n-channel Kondo model of $S = \frac{1}{2}$ and an appropriately chosen value of n, the exact solution of this model can be used to study the behavior of the TLS close to the fixed point, i.e., for low T and small energies.

III. BETHE-ANSATZ EQUATIONS AND NUMERICAL PROCEDURE

The n-channel Kondo problem has been exactly diagonalized by means of the Bethe ansatz[12,13] for a contact interaction at the impurity state and a linearized energy dispersion around 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 maximization of the spin required by Hund's rules leads to an orbital singlet. Within the Bethe ansatz many-particle spin-wave functions are constructed from the ferromagnetic state by gradually flipping spins. Each flipped spin gives rise to a spin wave, characterized by a rapidity, which parameterizes its energy and momentum. The spin wave may form bound states; in this case the motion of the center 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 the thermodynamic Bethe-ansatz equations[12,23] which consist of an infinite recursion sequence,

$$\ln\eta_k(\Lambda)=G*\ln[(1+\eta_{k-1})(1+\eta_{k+1})] -\delta_{k,n}\exp(\pi\Lambda/2), \quad k=1,2,3,\ldots \tag{6}$$

with the integration kernel given by

$$G(\Lambda)=[4\cosh(\pi\Lambda/2)]^{-1} , \tag{7}$$

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

$$\lim_{k\to\infty}[(1/k)\ln\eta_k(\Lambda)]=H/T=2x_0 , \tag{8}$$

where H is the field (in the case of the TLS H is the asymmetry or level splitting Δ) and the impurity free energy is given by

$$F_{\text{imp}}=-T\int_{-\infty}^{\infty}d\Lambda\, G[\Lambda-(2/\pi)\ln(T_K/T)] \times\ln[1+\eta_{2s}(\Lambda)] . \tag{9}$$

Note that the field and temperature dependence of the equations only enters via the asymptotic condition, Eq. (8).

In the limits $\Lambda\to\pm\infty$, the Λ dependence in Eqs. (6) becomes irrelevant and the equations can be solved analytically. The asymptotic solutions are[24]

$$\ln[1+\eta_k(+\infty)]=2\ln\{\sin[\pi(k+1)/(n+2)]/\sin[\pi/(n+2)]\}, \quad k<n$$
$$=2\ln\{\sinh[(k+1-n)x_0]/\sinh[x_0]\}, \quad k\geq n , \tag{10a}$$
$$\ln[1+\eta_k(-\infty)]=2\ln\{\sinh[(k+1)x_0]/\sinh[x_0]\}, \quad \forall k . \tag{10b}$$

The functions $\eta_k(\Lambda)$ are monotonically decreasing functions of Λ and interpolate smoothly between the asymptotic values at $\Lambda\to\pm\infty$. From Eqs. (10a) we see that the $\eta_k(\Lambda)$ are finite everywhere, except for $k=n$ as Λ tends to $+\infty$. This implies that $\varepsilon_n(\infty)=-\infty$, i.e., the conduction-electron states coupling to the impurity at low T consist of bound states of n spin waves. This corresponds to the notion discussed in Sec. II that the conduction electrons 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 (6) has to be solved numerically. To implement this solution, the infinite sequence (6) is truncated at an index k_c and the functions $\ln[1+\eta_k(\Lambda)]$ for $k>k_c$ are replaced by an appropriate asymptotic interpolating form. The numerical problem then reduces to the simultaneous solution of a finite number, i.e., k_c, of 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 of $\eta_k(\Lambda)$ have reached their asymptotic values, Eqs. (10). The errors in the free-energy derivatives (obtained numerically) are controlled by varying k_c and Λ_c. Satisfactory results were obtained for $k_c=50$ and $\Lambda_c=56$. This method is similar to the ones employed previously,[24-26] except that a higher numerical precision is required if $n\neq 2S$, in particular, if $n>2S$.

The above-described numerical procedure is not accurate enough at low temperatures for large values of H/T and the numerical derivatives become unreliable. This is, in part, the consequence of the exponential behavior with x_0 of the asymptotic expressions (10), but arises mainly from the exponential dependence on Λ of the integration kernel and the asymptotics of the functions η_k for $k\leq n$. The low-T properties of the impurity are determined by the $\Lambda\to+\infty$ asymptotics of η_{2S}. The contributions of $\eta_k(\Lambda\to+\infty)$ for $k>n$ are exponentially large, of the order of $\exp[2x_0(k-n)]$ and corrections due to their Λ dependence can be neglected. Hence, they can be eliminated from the system of integral equations which in this way reduces to a set of n equations. It is convenient to rewrite this set of n integral equations in terms of the energy potentials $\varepsilon_k(\Lambda)$ defined at the beginning of this section. It has been shown by Tsvelick[23] that, for $H\gg T$ and $S<n/2$, the impurity has Fermi-liquid-like properties, i.e., the entropy and the specific heat are proportional to the temperature. The $T=0$ solution of the remaining n integral equations can be obtained analytically. At $T=0$, all ε_k for $k<n$ are nonnegative, while ε_n changes sign at B_n defined by $\varepsilon_n(B_n)=0$. B_n depends logarithmically on the field and it is convenient to shift Λ so that the change of sign of ε_n occurs at the origin. The correction to the $T=0$ solution of ε_n due to a small but finite temperature is then proportional to T^2. It is then possi-

ble to write $\varepsilon_n = \varepsilon_n^{(0)} + T^2 \varepsilon_n^{(2)}$ and perform a Sommerfeld expansion of the Fermi distribution function, where $\varepsilon_n^{(0)}$ is the zero-temperature solution and $\varepsilon_n^{(2)}$ is the contribution proportional to T^2. Since the ε_k for $k < n$ do not have a zero at finite Λ a Sommerfeld expansion for them is not possible. The correction due to small temperatures is again proportional to T^2, i.e., $\varepsilon_k = \varepsilon_k^{(0)} + \varepsilon_k^{(2)}$. In this way integral equations for the $\varepsilon_k^{(2)}$ are obtained, which are nonlinear and require the knowledge of the zero-temperature solution. The asymptotic conditions for the new integral equations can be obtained from Eqs. (10).

In summary, we solve the thermodynamic Bethe-ansatz equations by employing two different numerical procedures: a standard one giving good results for $H/T < 10$ and the 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.

IV. RESULTS

We restrict ourselves to the solution of the n-channel Kondo problem for the situation $n > 2S = 1$. The case $n = 2S = 1$ (subspace μ is two dimensional corresponding to two channels of spinless fermions) just corresponds to the ordinary Kondo problem for which the thermodynamic Bethe-ansatz equations have been solved numerically in Ref. 25. The properties for $n = 1$ are Fermi-liquid-like at low temperatures and, in general, similar to those of a resonant level for all fields.

For $n > 2S = 1$ the effective conduction-electron spin S_e is larger than $S = \frac{1}{2}$, i.e., larger than needed to compensate the impurity spin at low T. In this case the model scales into a strong-coupling fixed point with a finite value of the interaction constant.[11] This contrasts the situation for $n = 2S = 1$, which has an infinite coupling fixed point giving rise to Fermi-liquid-like behavior. A fixed point with finite coupling leads to critical behavior[27] and to power-law dependences in thermodynamic properties as H and T tend to zero (the critical point is $H = T = 0$).

The zero-temperature limit has been solved analytically[12,13,22] and, for small fields, one obtains ($S = \frac{1}{2}$)

$$M_{\text{imp}} \propto (H/T_K)^{2/n}, \quad \chi_{\text{imp}} \propto (H/T_K)^{(2/n)-1}, \tag{11}$$

for $n > 2$. For $n = 2$ and $S = \frac{1}{2}$, the critical exponent of the susceptibility vanishes and a logarithmic divergence is obtained instead:

$$M_{\text{imp}} \propto (H/T_K)\ln(H/T_K), \quad \chi_{\text{imp}} \propto \ln(H/T_K) . \tag{12}$$

Similarly, for zero field and low temperatures, one obtains[23]

$$\begin{aligned} C_{\text{imp}} &\propto (T/T_K)^{\tau} , \\ C_{\text{imp}}/T &\propto (T/T_K)^{\tau-1} , \\ \chi_{\text{imp}} &\propto (T/T_K)^{\tau-1} , \end{aligned} \tag{13}$$

where $\tau = 4/(n+2)$. Once again for $n = 2$ and $S = \frac{1}{2}$, the exponents of C_{imp}/T and χ_{imp} vanish, giving rise to a logarithmic dependence.[23]

Hence, for $n > 1$ and $S = \frac{1}{2}$, the susceptibility diverges as H and T tend to zero. As a consequence the TLS is unstable to a level splitting Δ, i.e., to an asymmetry of the energy levels of the two positions of the tunneling atom (asymmetric double well). In other words, assume we initially have a symmetric TLS and allow a small coupling to a phonon deformation field. The divergent susceptibility of the TLS and the coupling to the phonons will induce a local distortion of the environment which then leads to a level splitting. At high temperatures this splitting will be zero, but there is a critical temperature T_c below which $\Delta \neq 0$ is the stable situation. The transition at T_c is continuous, i.e., Δ tends to zero as $T \to T_c$. The transition is similar to the one expected for the quadrupolar Kondo effect.[28–30]

We are representing the TLS interacting with the electron gas by the n-channel Kondo model. We have assumed in Sec. II that only one subspace μ is relevant. The validity of our argument is then restricted by the role of other subspaces. At low T one subspace is believed to be the dominant one. When the temperature is raised or for higher-energy excitations, other representations will influence the physical properties. We will, however, present our numerical results for the entire temperature range, with the understanding that the applicability to the TLS is restricted to low T.

Equations (11) and (12) show that the limits $H \to 0$ and $T \to 0$ cannot be interchanged, since the temperature and the field have different scaling dimensions $d_T = 4/(n+2)$ and $d_H = 2/n$. Both scaling dimensions are equal to one only for the case $n = 2$ and, consequently, the same logarithmic dependence in H and T is found.

The numerical zero-field results for the specific heat over temperature and the susceptibility as a function of T/T_K are shown in Figs. 1(a) and 1(b), respectively, for $n = 1, \ldots, 6$. Since $S = \frac{1}{2}$, only for $n = 1$, both χ and C/T are finite as $T \to 0$. In this case the ground state is a singlet, implying Fermi-liquid behavior. As discussed above, for $n = 2$ a logarithmic dependence and for $n > 2$, a power-law dependence, are obtained at low T. Note that, within our numerical accuracy, all the susceptibility curves cross each other at about $T = 0.1 T_K$.

Inserting Eq. (10) for $k = 1$ into the expression for the impurity free energy ($S = \frac{1}{2}$), Eq. (9), one obtains that the zero-field zero-temperature entropy is given by[23]

$$S(T \to 0, H = 0) = \ln\{2\cos[\pi/(n+2)]\} . \tag{14}$$

Hence, for $n \neq 1$, the $T = 0$ entropy is nonzero, which implies that the ground state is not a singlet. This is consistent with the divergence in the susceptibility discussed above.

In a finite field the situation is qualitatively different. If $H \neq 0$, the susceptibility is always finite (for all n and S) and, consequently, the ground state is expected to be a singlet. Hence, the zero-temperature entropy is zero as pointed out previously by Tsvelick,[23] $S(T = 0, H \neq 0) = 0$. This is the case irrespective of the strength of the field. The entropy then has an essential singularity at the critical point $H = T = 0$. As a consequence of the singlet ground state for $H \neq 0$, the TLS has Fermi-liquid proper-

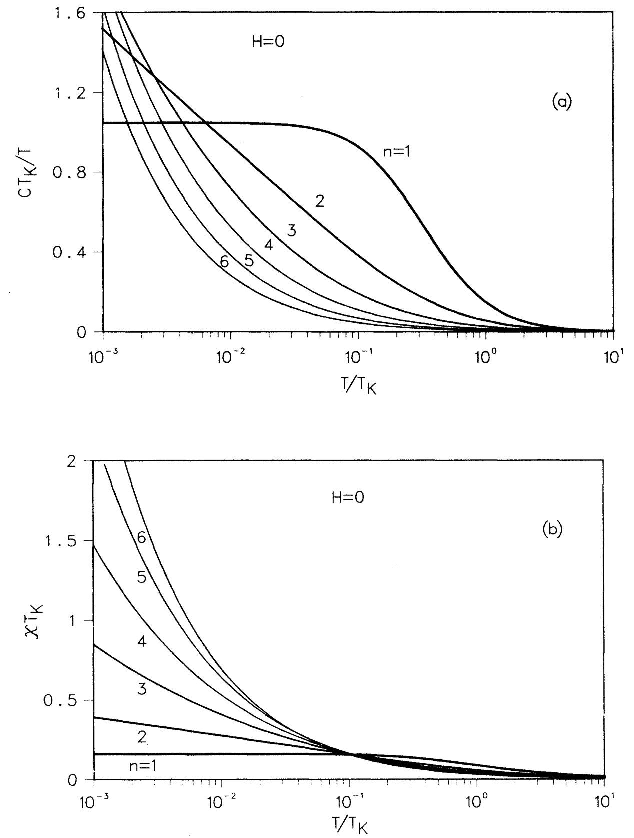

FIG. 1. Numerical zero-field results for (a) the specific heat over temperature and (b) the susceptibility as a function of T/T_K for $n=1,2,\ldots,6$. Note that both C/T and χ diverge as $T\to0$ for $n>1$.

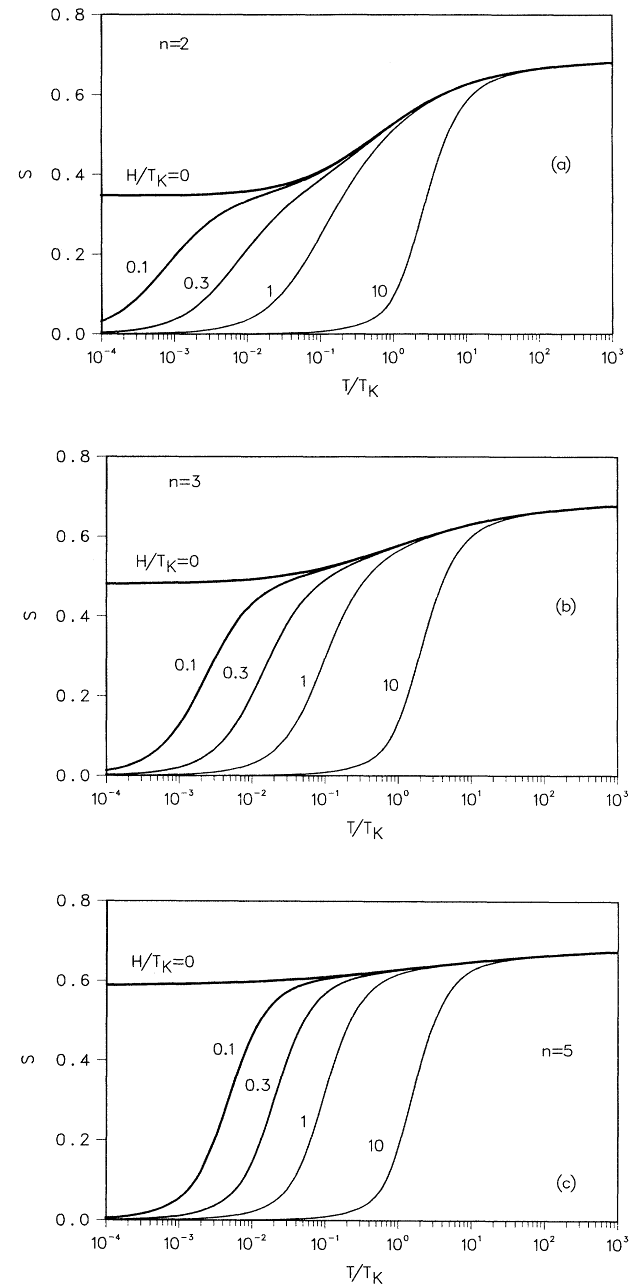

FIG. 2. Entropy as a function of T/T_K for (a) $n=2$, (b) $n=3$, and (c) $n=5$ and five values of the field $H/T_K=0$, 0.1, 0.3, 1, and 10. The entropy is singular at $H=T=0$; if $H=0$ the entropy at $T=0$ is finite and given by Eq. (14), while it vanishes if $H\neq0$. For $H\neq0$ the low-T entropy is proportional to T.

ties over a limited range of temperature. For small fields the characteristic energy scale is the field strength rather than the Kondo temperature.

The low-T (Fermi-liquid) behavior has to be calculated using the second numerical procedure described in Sec. III. In a previous paper[30] we obtained the entropy and specific heat in constant field for $n=2$ and $S=\frac{1}{2}$ using an interpolation scheme between the numerical results for the free energy as a function of temperature and field and the analytical solution for the ground state. Unfortunately, the numerical derivatives of the free energy obtained through the interpolation turned out to be inaccurate at very low T. The procedure yielded a finite entropy in the presence of a small field at low T.[31] All other features[30] found, i.e., the double-peak structure in the specific heat, the very large γ values, and the shoulders in the susceptibility, are qualitatively correct and quantitatively not far off. In order to rectify our previous results we also show in this paper our accurate numerical results for $n=2$ and $S=\frac{1}{2}$.

The entropy curves in constant fields as a function of T/T_K for $n=2$, 3 and 5 are shown in Figs. 2(a)–2(c), respectively. In zero field the entropy of the TLS interpolates smoothly between the value given by Eq. (14) for low temperatures and the asymptotic free-spin entropy, ln(2), at high T. In a nonvanishing field, the entropy tends to zero proportionally to T at low temperatures as discussed above. At high T, i.e., for $T\ll H$, again the asymptotic free-spin value of ln(2) is reached. The drop in the entropy at low T, a consequence of the magnetic field (asymmetry of the double well in the case of the

TLS), for $n=2$ begins on a temperature scale of the order of H^2/T_K, i.e., at very low T if the field is small. The reduction of the entropy at high temperatures is a consequence of the Kondo screening. Hence, there are two independent energy scales involved, namely H^2/T_K and T_K, which are well separated if the field is small, as seen in Fig. 2(a). The situation is similar for larger n. As n increases the Kondo screening is less pronounced. The field-dependent energy scale can be shown to be $T_K(H/T_K)^{1+2/n}$ using the exponents in Eqs. (11) and (13). For very large n this energy scale is just the magnetic field. This is consistent with the gradual decrease of the Kondo compensation with n, so that, for $n\rightarrow\infty$, the impurity behaves like a free spin with Zeeman splitting.

The entropy for $H=0.1T_K$ is shown in Fig. 3 for $n=1,\ldots,6$. This figure summarizes the low-field behavior discussed above. The curve for $n=1$ corresponds to the traditional Kondo problem with the impurity degrees of freedom being gradually frozen out by spin compensation from the conduction electrons. The $n=2$ curve displays the shoulder due to the second energy scale. This behavior is still present for higher values of n, but the feature due to the field is much more pronounced than the Kondo effect. The larger n, the faster the singlet state is reached at low T, as well as the high-temperature asymptotics, showing once more that a Schottky anomaly is asymptotically approached.

The specific heat as a function of T/T_K in constant fields is shown for $n=2$, 3, and 5 in Figs. 4(a)–4(c). These curves just correspond to the slope of those in Figs. 2(a)–2(c). The zero-field specific heat has one peak at $T\sim T_K$, which arises from the Kondo screening that reduces the entropy from ln(2) to the zero-temperature value given by Eq. (14). In a small magnetic field, e.g., $H=0.1T_K$, this Kondo peak basically remains unchanged but at low T, a second peak develops, a consequence of the second energy scale. The two peaks are well separated at low fields and merge into one at intermediate fields, e.g., $H\sim T_K$. At very high fields the free-spin Schottky resonance is asymptotically reached on a logarithmic scale (characteristic of asymptotic freedom). For larger values of n, the height of the resonance for low fields is large, since a large amount of entropy has to be removed. As $n\rightarrow\infty$ the height of the peak (only one can be seen) is that of a spin-$\frac{1}{2}$ Schottky anomaly.

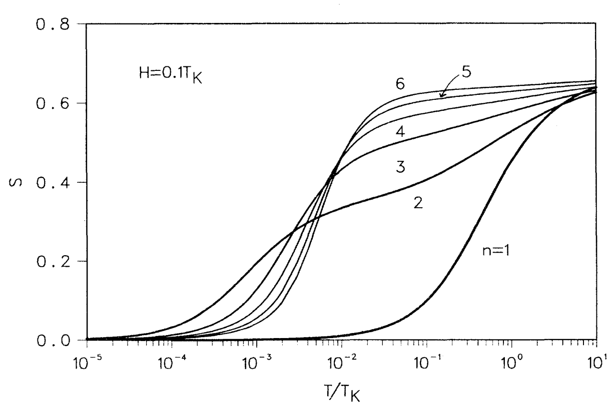

FIG. 3. Entropy for $H=0.1T_K$ as a function of T/T_K for $n=1,2,\ldots,6$. Note the dramatically different behavior for $n>1$ as compared to the traditional Kondo problem. The entropy change from $S=0$ to ln(2) becomes more abrupt with growing n.

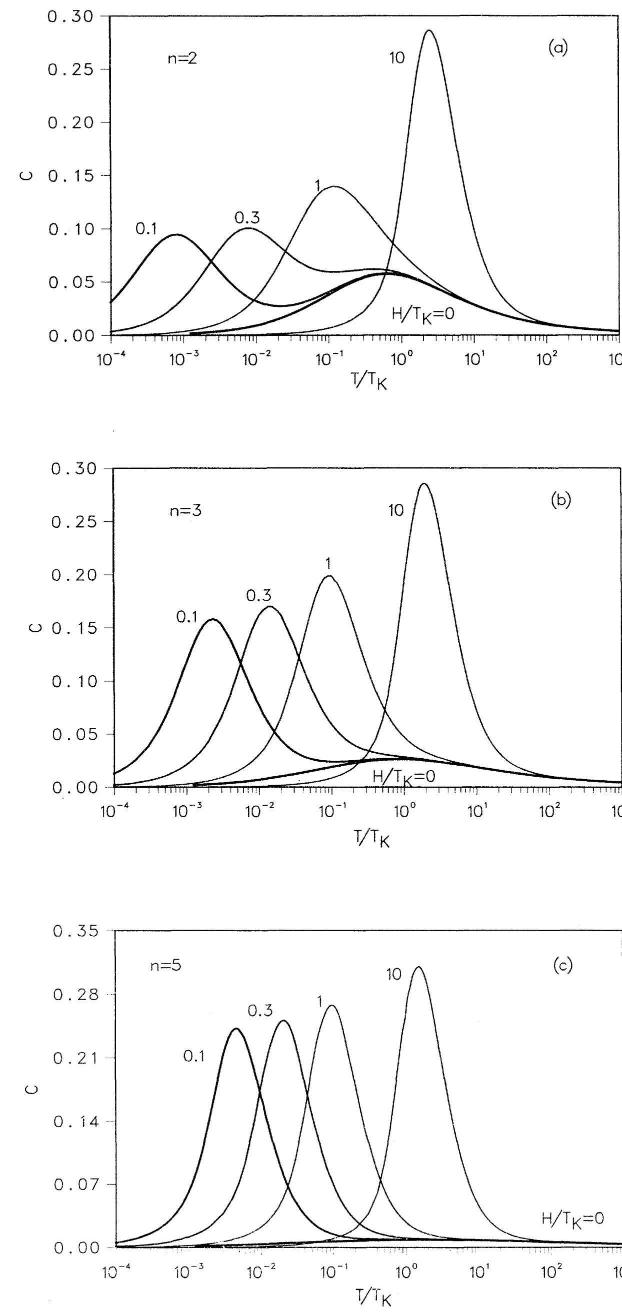

FIG. 4. Specific heat as a function of T/T_K for (a) $n=2$, (b) $n=3$, and (c) $n=5$ and five values of the field $H/T_K=0$, 0.1, 0.3, 1, and 10. The $H=0$ curve shows the Kondo resonance. A two-peak structure is observed in small fields. At high fields the two peaks merge into a Schottky anomaly.

In Figs. 5 we display the specific-heat curves for constant H ($0.1T_K$ and T_K) as a function of temperature for $n=1-6$ to explicitly show the dependence on the number of channels. The qualitatively different behavior for $n=1$ is apparent. In Fig. 5(a) the double-peak structure is evidenced for $n\geq 2$, with the weight of the low-temperature peak growing with n, while the importance of the Kondo compensation decreases. The shift of the magnetic field peak with n is also clearly seen. In Fig. 5(b) the case of $H=T_K$ is shown. The two peaks are merged, the height of the peak grows with n and asymptotically approaches a spin-$\frac{1}{2}$ Schottky resonance. The peaks are now positioned at about the same temperature.

In view of the Fermi-liquid properties for $H\neq 0$, the low-temperature specific heat is proportional to the temperature and can be characterized by a coefficient γ. C/T in constant field as a function of T/T_K for $n=2$, 3, and 5 are shown in Figs. 6(a)–6(c), respectively. The $H=0$ curves do not, of course, saturate as $T\to 0$. γ is, however, finite if H is nonzero. For $n>1$, C/T increases dramatically at low T if the field is small, giving rise to giant γ values. A maximum in C/T develops for larger fields (C/T no longer decreases monotonically with T), which is the consequence of the developing Schottky anomaly. At very high temperatures ($T\gg H$), the curves approach the high-temperature Kondo asymptotics. The comparison of C/T for several n in the same fixed field of $H=0.1T_K$ is shown in Fig. 7. Note that the γ value for $n=2$ is roughly 300 times larger than the corresponding one for $n=1$. For $n>2$, the γ values decrease as a func-

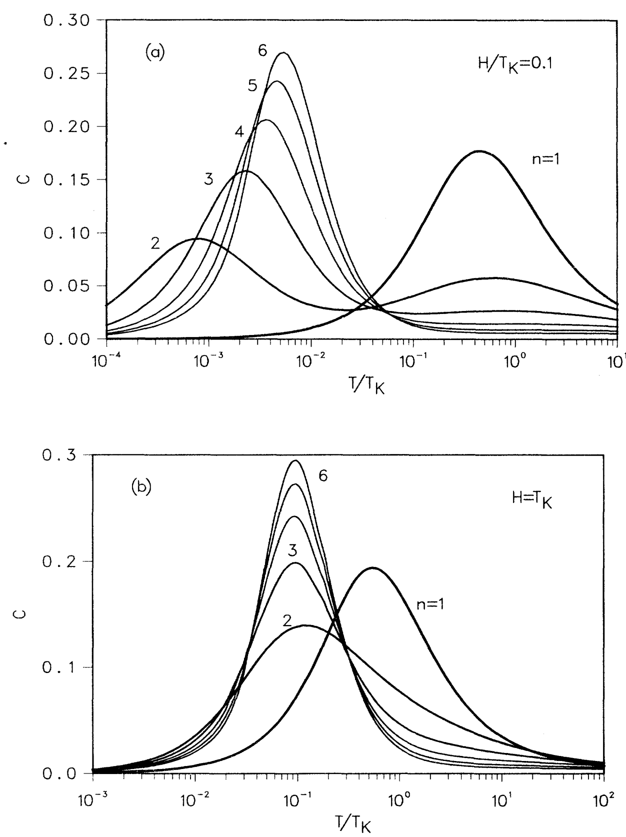

FIG. 5. Specific heat as a function of T/T_K in constant field (a) $H/T_K=0.1$ and (b) $H/T_K=1$ for $n=1,2,\ldots,6$. Note the distinct behavior of the traditional Kondo problem. With increasing n the Kondo resonance becomes less important, while the size of the field-dependent peak grows. In (b) the two peaks have already merged into one peak.

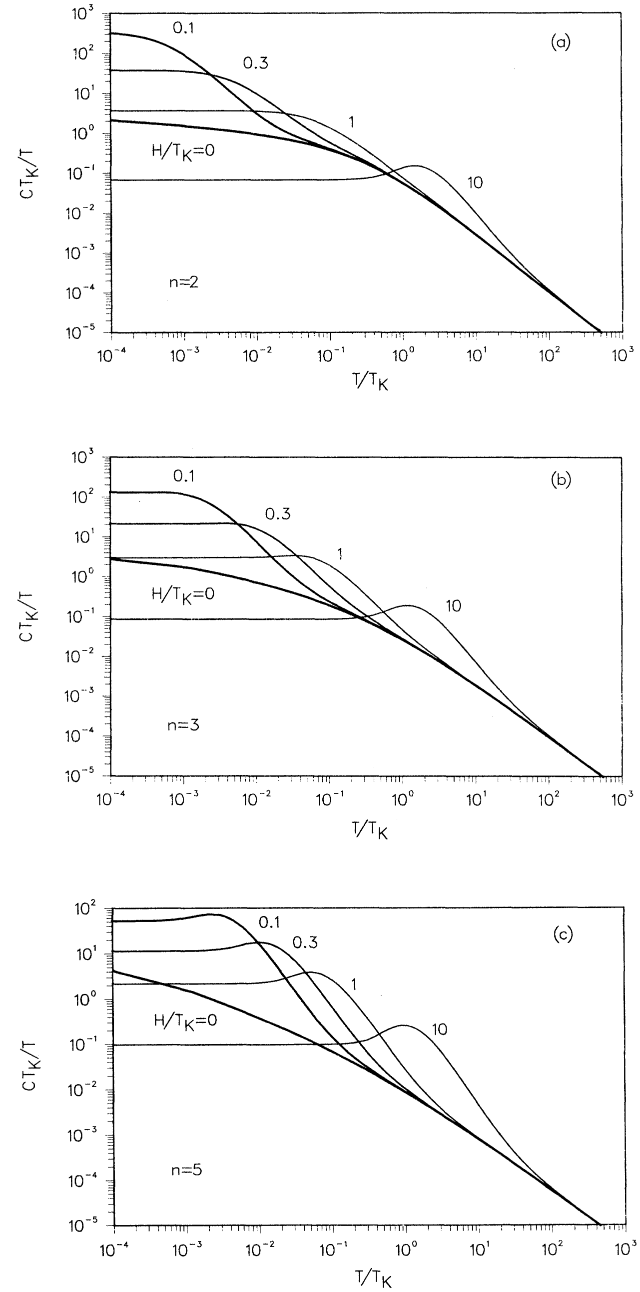

FIG. 6. C/T as a function of T/T_K for (a) $n=2$, (b) $n=3$, and (c) $n=5$ in constant field $H/T_K=0$, 0.1, 0.3, 1, and 10. Giant γ values are obtained in small fields. The shoulders are due to the incipient Schottky anomaly in higher fields.

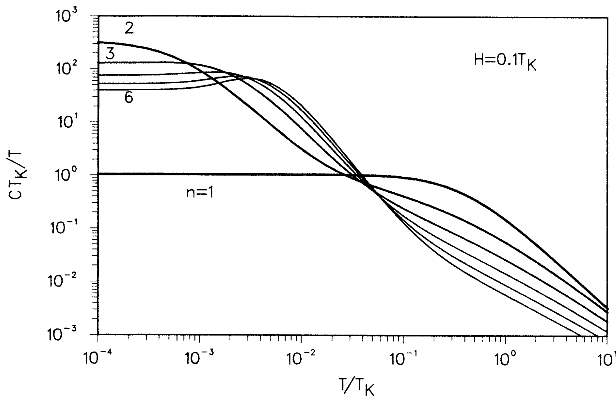

FIG. 7. C/T as a function of T/T_K in a constant field of $H=0.1T_K$ for $n=1,2,\ldots,6$. Again a distinct behavior for $n=1$ is observed. The γ values decrease with n as a consequence of the developing Schottky anomaly.

tion of n.

In Fig. 8 the γ value (as obtained by extrapolating C/T to zero temperature) is plotted versus the $T=0$ susceptibility for $n=2$, 3, and 5. γ/χ, which is the inverse of the Wilson ratio, grows rapidly as $H\to 0$. For instance, for $n=2$, $H=0.1T_K$ is about 1260, i.e., 200 times larger than for the traditional Kondo impurity. This is, in the first place, the consequence of the giant γ values, required to quench the large zero-temperature zero-field entropy. The low-field γ/χ ratios decrease with the number of orbitals. Since one gradually approaches a Schottky anomaly with increasing n, the fraction of entropy removed via a linear specific heat (Fermi liquid) necessarily has to decrease. For large H, γ/χ is supposed to asymptotically reach the value $2\pi^2/3n$.

We had obtained similar results for $n=2$ in Refs. 30 and 31. The γ values obtained there are substantially smaller than those obtained here, as a consequence of the extrapolated nonvanishing $T=0$ entropy for $H\neq 0$. The

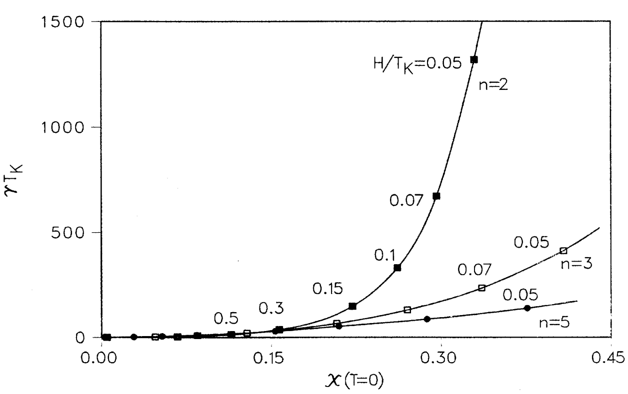

FIG. 8. γ values as a function of the zero-temperature susceptibility for $n=2$, 3, and 5 with the field as the parameter. Note the rapid increase of γ as $H\to 0$.

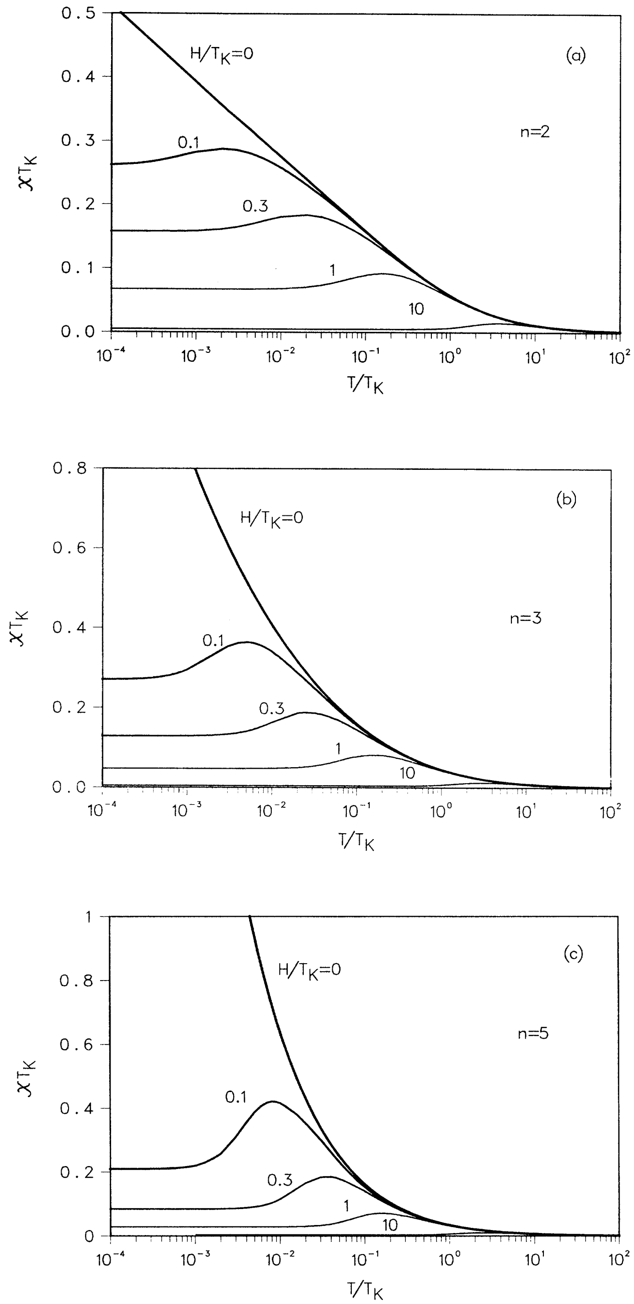

FIG. 9. Susceptibility as a function of T/T_K for (a) $n=2$, (b) $n=3$, and (c) $n=5$ in constant fields of $H/T_K=0$, 0.1, 0.3, 1, and 10. The divergent response in zero field is clearly seen. The shoulders correlate with the field-dependent peak in the specific heat.

giant γ values are actually the cause of the imprecision in the procedure employed in Refs. 30 and 31. A more detailed analysis of the increase of γ for $n=2$ as $H\to 0$ shows that, approximately, $\gamma\propto H^{-2}$, which is consistent with the field-dependent energy scale of H^2/T_K argued above.

The susceptibility as a function of temperature for constant fields is shown in Figs. 9(a)–9(c) for $n=2$, 3, and 5, respectively. χ decreases montonically with field, but has a maximum as a function of temperature. This maximum in $\chi(T)$ correlates with the low-T peak of the specific heat.

V. CONCLUDING REMARKS

We considered an atom in a double-well potential (parametrized by a TLS) interacting with screened conduction electrons. The hopping of the atom between the two positions is assumed to be assisted by scattering of the electrons. The spin of the electron remains invariant in this process, but the electron can change its orbital character. This is similar to the n-channel Kondo problem if the role of spin and orbit is interchanged.

Close to the strong-coupling fixed point, the renormalization-group equations for the noncommutative model lead to a structure resembling the infinitesimal generators of an irreducible unitary representation of the rotation group. Assuming that only one subspace μ (of dimension $g_\mu = 2S_\mu + 1$) is relevant, we have shown that, in the case of no spin degeneracy, the TLS Hamiltonian in the strong-coupling regime ($T \le T_K$), reduces to the n-channel Kondo problem with $S=\frac{1}{2}$ and $n=g-1$, where g is the dimensionality of the relevant subspace. This result extends the proofs given in Refs. 7 and 8 to arbitrary degeneracy.

The n-channel Kondo problem has been exactly diagonalized by means of the Bethe ansatz.[12,13] By solving the thermodynamic Bethe-ansatz equations[12,23] numerically in the presence of a field, we gained insight into the low-T properties of the TLS model using the above-mentioned equivalence. The magnetic field in the n-channel Kondo problem plays the same role as the energy difference between the two positions of the tunneling atom. We have presented our results for all temperatures even though the equivalence only holds for low temperatures, since the results for the n-channel Kondo model are interesting by themselves.

The magnetic susceptibility in the Kondo problem corresponds to the response of the TLS to a change in the asymmetry of the double-well Δ. $\chi(H,T)$ diverges at $(H=0, T=0)$ along both lines, $(H\to 0, T=0)$ and $(H=0, T\to 0)$. This implies that the symmetric TLS (symmetric double well) is unstable at low T. Even a very small coupling to a local lattice distortion field (e.g., pseudospin-phonon coupling) is going to produce a significant asymmetry in the potential minima. The total free energy of the system consists of three terms: the one of the TLS interacting with the electrons, the pseudospin-phonon coupling (Zeeman energy), and the elastic energy of the phonon mode. The first one is given by Eq. (9), the coupling to the phonons is proportional to Δ and the elastic energy to Δ^2. The minimization of the total free energy with respect to Δ yields an equilibrium condition of the form $\langle S_z \rangle = aH$, where a is proportional to the elastic constant. At $T=0$ there is always a nontrivial solution H_c, which is gradually reduced with increasing temperature and vanishes above T_c given by $\chi(H=0, T_c) = a$. This is similar to the situation found for the quadrupolar Kondo effect,[29–31] where the instability is with respect to a quadrupolar distortion. A divergent correlation length is associated with the critical behavior of the susceptibility. Hence, even if the concentration of TLS is very small, they are going to interfere with each other at low T. This interference competes with the local lattice distortion induced by a single TLS.

Since the ground-state equilibrium situation for an isolated TLS corresponds to $H \neq 0$, the ground-state entropy vanishes and a Fermi-liquid-like picture applies, i.e., the susceptibility is finite and the specific heat is proportional to T. The specific-heat γ values can become very large, giving rise to very large γ/χ ratios. For small fields the specific heat shows a double-peak structure which is specially evident for $n=2$. The low-T peak is reminiscent of the Zeeman splitting, while the high-T peak is caused by the Kondo screening. For large n the magnitude of the low-T peak is considerably larger than the Kondo resonance. At larger fields ($H \sim T_K$) the two peaks merge. The same field-dependent structure shows up as a shoulder in the susceptibility as a function of temperature.

ACKNOWLEDGMENTS

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