Magnetic impurity coupled to a quantum spin chain: A quantum Monte Carlo study

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We study by Monte Carlo simulations a magnetic impurity coupled antiferromagnetically to a one-dimensional quantum spin model. The impurity susceptibility and the spin-correlation function are calculated. By defining and evaluating an energy scale from the inverse of the impurity susceptibility at zero temperature, we find a scaling relation for the impurity susceptibility in agreement with the prediction of the conformal field theory. We analyze the problem by mapping the spin model onto the resonant-level model, and interpret the energy scale as the resonant-level width. The spin-correlation function between the impurity spin and the spins in the chain is found to extend over long range at low temperatures. We show that the system can be considered as a model of an insulator with heavy-fermion behavior. [S0163-1829(96)05745-1]

I. INTRODUCTION

The study of a magnetic impurity embedded in a system of strongly interacting conduction electrons has recently attracted much interest. In the conventional Kondo problem where conduction electrons are noninteracting,[1] an impurity spin forms a singlet at low temperatures through the antiferromagnetic Kondo coupling. The interaction between conduction electrons is expected to affect considerably the formation of this singlet state.

Recently this problem has been studied in a simplified version by considering the ground state of a magnetic impurity coupled to a chain of strongly interacting conduction electrons at half-filling.[2] In the strong interaction limit, the low-lying excitations of the system are well described by a spin-1/2 antiferromagnetic Heisenberg model:

$$H = H_c + H_{fc}, \tag{1.1}$$

where

$$H_c = J\sum_{i=1}^{L} [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z], \tag{1.2}$$

$$H_{fc} = J'[S_f^x S_1^x + S_f^y S_1^y + \lambda' S_f^z S_1^z], \tag{1.3}$$

with $J>0$, $J'>0$, $\lambda=1$, $\lambda'=1$. Here $\mathbf{S}_i$ $(i=1,\ldots,L)$ and $\mathbf{S}_f$ denote the spin-1/2 operators attached to site i of the chain and to the impurity, respectively. Furthermore L is the number of sites on the chain and we require the periodic boundary condition, $\mathbf{S}_{L+1}=\mathbf{S}_1$. The system is schematically shown in Fig. 1. The Hamiltonian was previously diagonalized for finite-size clusters. The binding energy of the impurity spin to the spins in the chain was calculated as well as the pair-correlation function between the impurity spin and the ones in the chain. Thereby insight was gained as regards the formation of a spin singlet in the ground state of the system.[2] Recently the ground state was also studied for filling factors different from half-filling.[3,4]

The aim of this paper is to report work which extends the previous calculations to finite temperatures. Eggert and Affleck[5] have already studied the magnetic impurity problem with the use of the conformal field theory. The system studied in this paper belongs to the open chain fixed point in their classification, and the scaling behavior was predicted in the impurity susceptibility as well as the impurity specific heat. In this paper, we study the problem with the help of quantum Monte Carlo computations, which has the advantage that by this direct method quantitative statements can be made. Thereby we concentrate on determining the susceptibility of the impurity and the correlation function between the spin of the impurity and the ones in the chain. In order to obtain a comprehensive understanding of the problem, we study not only the case of $\lambda=\lambda'=1$ but also the ones with $\lambda=\lambda'=0$ and $\lambda=0$, $\lambda'=1$. The case of $\lambda=\lambda'=0$ can be solved analytically by mapping the Hamiltonian onto one of a resonant-level model with spinless fermions.[6–9] It yields special insight into the problem and also serves as a bench mark for testing the accuracy of the numerical Monte Carlo results. It is well known that the susceptibility of the impurity $\chi_{\rm imp}$ remains finite in the zero-temperature limit and that the impurity contribution to the specific heat $C_{\rm imp}$ is proportional to

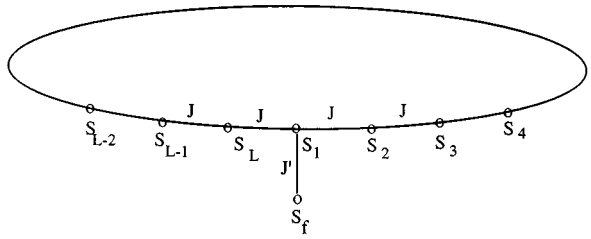

FIG. 1. Schematic drawing of the system. Open circles represent spins. J and J' denote the exchange interactions between spins in the chain and between an impurity spin and a spin in the chain, respectively.

temperature T. The model with $\lambda=0$ ($\lambda'\neq 0$) has been shown to be formally equivalent to the s-d Hamiltonian within the long-time approximation.[8,9] The exact solution was obtained by the Bethe ansatz technique in the continuum limit.[10] We will show that the Monte Carlo data reproduces well these exact results.

Finite values of λ introduce interactions among the spinless fermions and the model is no longer analytically solvable. Numerical calculations become mandatory in that case. We will show for $\lambda=\lambda'=1$ that the impurity susceptibility approaches a finite value with decreasing temperatures, owing to the formation of a spin singlet between the impurity spin and the spins in the chain. It is also shown that at low temperatures spin correlations between the impurity spin and the ones in the chain are rather long ranged. However, thermal fluctuations are rather effective in destroying them. A characteristic energy scale is given by $\chi_{\rm imp}^{-1}(T=0)/\pi$. It can be obtained from the Monte Carlo data. We find that the data for $T\chi_{\rm imp}(T)$ lies on a universal curve, i.e., it does not depend on the coupling J'. This is similar to the case of $\lambda=\lambda'=0$, where analytic results are available. Indeed, this similarity makes us speculate that interactions between spinless fermions give rise to a renormalization of the energy scale only. This scaling relation is consistent with the prediction of the conformal field theory.[5]

The scaling behavior of $T\chi_{\rm imp}$ is similar to that in the Kondo problem,[11] where a singlet is formed between a magnetic impurity and conduction electrons. We show, however, that here the energy scale is greatly enhanced as compared with the Kondo temperature, an effect of the strong interactions between the electrons in the chain. This is in accordance with a previous discussion based on the binding energy at zero temperature.[2] The analogy to the Kondo problem goes even farther. Like there we find for $\lambda=\lambda'=0$ a low-temperature specific-heat contribution of the impurity which is of the form $C_{\rm imp}=\gamma T$ with a γ coefficient given by the same energy scale as $\chi_{\rm imp}^{-1}(T=0)/\pi$. Moreover, the so-called Wilson ratio[11] $(T\chi_{\rm imp}/C_{\rm imp})(\pi^2/3)$ is found here to be close to unity, whereas in the Kondo problem it equals 2 for an impurity with a $N=2$ orbital degeneracy. A specific heat and susceptibility of the above form together with a Wilson ratio of order 1 are usually taken as indications of a local Fermi liquid.[12] A one-dimensional interacting electron system is known to be a Luttinger liquid, the low-temperature thermodynamics of which is the same as that of a Fermi liquid. We shall adopt the generally accepted convention to speak of a *local Fermi liquid*, despite the fact that we could use as well the expression *local Luttinger liquid* in view of the one-dimensional character of the problem treated here.

Additionally, another point deserves attention. A quantum spin system with or without an impurity coupled to it is an insulator. Therefore it seems useful to distinguish between a local *neutral* Fermi liquid and a local *charged* Fermi liquid. The first case applies here, because the conductivity is zero like for a system of uncharged particles. The second case applies to a Kondo ion in a system of nearly-free electrons which is metallic. Speculating that the above findings for $\lambda=\lambda'=0$ remain qualitatively unmodified when $\lambda=\lambda'=1$ (i.e., up to a change in energy scale), the lattice version of the impurity system we are studying here may be viewed as a model of a so-called Kondo insulator. According to the above, the notation heavy neutral-fermion system would be preferable. Indeed, a number of semimetals and insulators have low-temperature thermodynamic properties which resemble those of metallic heavy-fermion systems. One of them is Yb_4As_3, and a recent theory for its description[13] has features which are similar to the ones discussed here.

The paper is organized as follows. In Sec. II, we map the present spin model onto a resonant-level model and present the analytical results for $\lambda=\lambda'=0$. In Sec. III, we outline the quantum Monte Carlo computational scheme which we apply in order to compute the above-mentioned properties of our system. We also discuss the results obtained. Section IV contains concluding remarks.

II. RESONANT-LEVEL MODEL

In order to map the spin model to the resonant-level model, we apply the Jordan-Wigner transformation and express the spin operators in terms of fermion annihilation and creation operators at each site:

$$S_f^z=f^\dagger f-\frac{1}{2},\quad S_f^+=(S_f^-)^\dagger=f^\dagger, \tag{2.1}$$

$$S_i^z=c_i^\dagger c_i-\frac{1}{2},$$

$$S_i^+=(S_i^-)^\dagger=c_i^\dagger\exp\left\{i\pi\left(f^\dagger f+\sum_{j=1}^{i-1}c_j^\dagger c_j\right)\right\}. \tag{2.2}$$

Imposing the periodic boundary condition $\mathbf{S}_{L+1}=\mathbf{S}_1$ to spins in the chain, we find the boundary condition for the fermion operator, $c_{L+1}^\dagger=c_1^\dagger\exp(-i\pi\Sigma_{j=1}^L c_j^\dagger c_j)$. It depends on the total number N_F of fermions *in the chain*, and is periodic for even N_F and antiperiodic for odd N_F. Inserting Eqs. (2.1) and (2.2) into Eqs. (1.2) and (1.3), we obtain a Hamiltonian for spinless fermions $H=H_c+H_{fc}$ with

$$H_c=\sum_k\epsilon_k c_k^\dagger c_k+\lambda J\sum_{j=1}^{L}\left(c_j^\dagger c_j-\frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1}-\frac{1}{2}\right), \tag{2.3}$$

$$H_{fc}=\frac{J'}{2}\frac{1}{\sqrt{L}}\sum_k(c_k^\dagger f+f^\dagger c_k)+\frac{\lambda' J'}{4}$$

$$\times(f^\dagger f-ff^\dagger)\frac{1}{L}\sum_k(c_k^\dagger c_{k'}-c_{k'}c_k^\dagger). \tag{2.4}$$

Here $c_k=L^{-1/2}\Sigma_{j=1}^L c_j\exp(-ikj)$ and $\epsilon_k=J\cos k$ with $-\pi<k<\pi$.

For $\lambda=\lambda'=0$ we can diagonalize the Hamiltonian analytically,[6–9] since it is quadratic with respect to c_k and f. Following Wiegmann and Finkelstein,[8] we introduce the temperature Green's functions:

$$G(\tau)=-\langle T_\tau(f(\tau)f^\dagger(0))\rangle, \tag{2.5}$$

where $\langle\cdots\rangle$ denotes a thermal average, and $f(\tau)=e^{H\tau}fe^{-H\tau}$. The Fourier transform of $G(\tau)$ is found to be

$$G(\omega_n)=[i\omega_n-(J'/2)^2F(\omega_n)]^{-1}, \tag{2.6}$$

where $\omega_n=(2n+1)\pi T$, and

$$F(\omega_n)=\frac{1}{L}\sum_k \frac{1}{i\omega_n-\epsilon_k}. \tag{2.7}$$

The change of the thermodynamic potential due to the impurity spin is simply given by

$$\Delta\Omega=-T\sum_n \{\ln[i\omega_n-(J'/2)^2F(i\omega_n)]-\ln(i\omega_n)\}. \tag{2.8}$$

Note that the chemical potential μ is zero. The retarded function $F_R(x)$ is obtained from $F(\omega_n)$ by replacing $i\omega_n$ by $x+i\delta$:

$$\frac{J'^2}{4}F_R(x)\equiv A(x)-iB(x)=-i\frac{J'^2/4}{\sqrt{J^2-x^2}} \quad \text{for } |x|<J,$$

$$=\frac{J'^2\mathrm{sgn}(x)/4}{\sqrt{x^2-J^2}} \quad \text{for } |x|>J. \tag{2.9}$$

This defines the two functions $A(x)$ and $B(x)$. With the help of this formula, we can write

$$\Delta\Omega=-\frac{1}{\pi}\int_0^J \theta(x)\tanh\frac{x}{2T}\,dx-\int_J^{x_c}\tanh\frac{x}{2T}\,dx, \tag{2.10}$$

where the phase shift $\theta(x)$ is defined by

$$\tan\theta(x)=\frac{1}{x}\frac{J'^2/4}{\sqrt{J^2-x^2}}. \tag{2.11}$$

The bound-state energies $\pm x_c$ are determined from the relation $x_c-(J'/2)^2/\sqrt{x_c^2-J^2}=0$. The specific-heat contribution of the impurity spin is given by $C_{\mathrm{imp}}=-T\partial^2\Delta\Omega/\partial T^2$.

We define the impurity susceptibility χ_{imp} by the response of the system to an external magnetic field which acts on the impurity spin only:

$$\chi_{\mathrm{imp}}(J',T)=\int_0^\beta d\tau\langle S_f^z(\tau)S_f^z(0)\rangle. \tag{2.12}$$

In terms of the Green's function, we can write $\chi_{\mathrm{imp}}(J',T)=-T\Sigma_{\omega_1}G(\omega_1)G(\omega_n+\omega_1)$ with $\omega_n\to 0$. This expression can be rewritten as

$$\chi_{\mathrm{imp}}(J',T)=\int\int dx\,dy\rho(x)\rho(y)\times\frac{1}{x-y}\left[\frac{1}{e^{y/T}+1}-\frac{1}{e^{x/T}+1}\right], \tag{2.13}$$

where $\rho(\chi)$ is given by

$$\rho(x)=\frac{1}{\pi}\frac{B(x)}{x^2+B(x)^2}+\frac{1}{|1-dA(x)/dx|}\,\delta(x-x_c)+\frac{1}{|1-dA(x)/dx|}\,\delta(x+x_c). \tag{2.14}$$

At low temperatures, C_{imp} and χ_{imp} become[7]

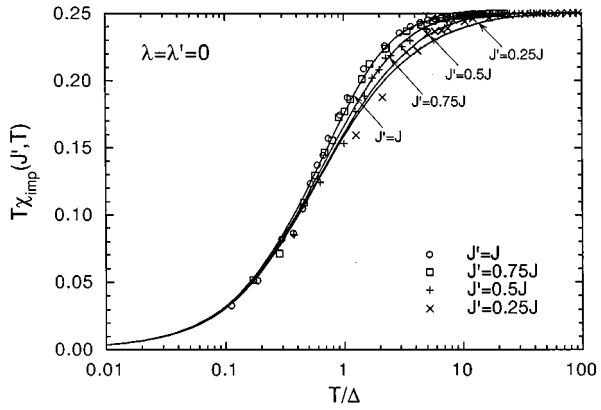

FIG. 2. $T\chi_{\mathrm{imp}}$ vs T/Δ for $\lambda=\lambda'=0$. The energy scale Δ is given by $J'^2/(4J)$. Solid lines represent the exact results of the resonant-level model. Also shown are Monte Carlo data.

$$C_{\mathrm{imp}}(J',T)\approx\frac{\pi^2}{3}\frac{T}{\pi\Delta}, \quad \chi_{\mathrm{imp}}(J',T)\approx\frac{1}{\pi\Delta}, \tag{2.15}$$

where $\Delta[=J'^2/(4J)]$ represents the resonant-level width. These expressions lead to a Wilson ratio[8] of one, i.e., $(T\chi_{\mathrm{imp}}/C_{\mathrm{imp}})(\pi 2/3)=1$. The resonant-level width Δ defines the energy scale at low temperatures. Figure 2 shows $T\chi_{\mathrm{imp}}$ as a function of T/Δ. As is suggested from Eq. (2.15), all curves for different values of J' merge at low temperatures into a single one. Figure 3 shows C_{imp} as a function of T/Δ. There a similar scaling behavior is seen to hold at low temperatures.

For finite values of λ' (λ is still zero), the model can be exactly solved by the Bethe ansatz technique in the continuum limit that the fermions in the chain have a linear dispersion. For finite values of λ, the system is no longer exactly solvable. By performing Monte Carlo simulations for $\lambda'=0$, $\lambda'=1$, and for $\lambda=\lambda'=1$, we will show in the next section that the behavior of the susceptibility is similar to that for $\lambda=\lambda'=0$.

III. MONTE CARLO SIMULATIONS

A. Computational method

We use a Monte Carlo method based on the Suzuki-Trotter decomposition.[14] It is of the checkerboard type.[15,16]

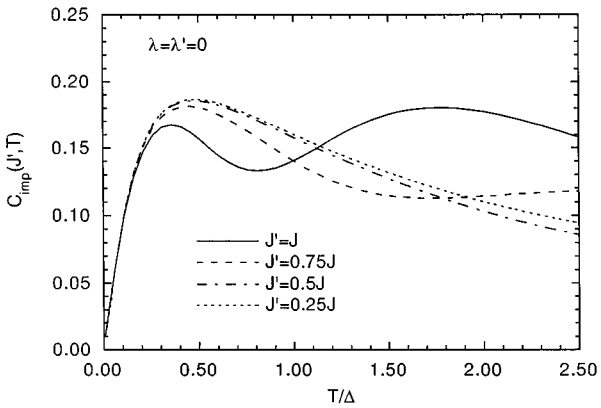

FIG. 3. Impurity specific heat as a function of T/Δ for $\lambda=\lambda'=0$.

To avoid the well-known sign problem,[17] we assume L to be even and transform the Hamiltonian by the unitary matrix $U=\exp[-i\pi\Sigma_{i=\text{odd}}S_i^z]$. As a consequence the Hamiltonian is decomposed into a sum of local Hamiltonians:

$$H=\sum_i h_{i,i+1}, \tag{3.1}$$

with

$$\begin{aligned} h_{i,i+1}&=J(\lambda S_i^z S_{i+1}^z-S_i^x S_{i+1}^x-S_i^y S_{i+1}^y), \quad \text{for } i\neq 1,\\ &=J(\lambda S_1^z S_2^z-S_1^x S_2^x-S_1^y S_2^y)+J'(\lambda' S_f^z S_1^z-S_f^x S_1^x\\ &\quad -S_f^y S_1^y), \quad \text{for } i=1. \end{aligned} \tag{3.2}$$

Dividing the Hamiltonian into two parts, $H=H_1+H_2$, with $H_1=\Sigma_{i=\text{odd}}h_{i,i+1}$, $H_2=\Sigma_{i=\text{even}}h_{i,i+1}$, we approximate the partition function Z as

$$Z\approx[\exp(-\beta H_1/N)\exp(-\beta H_2/N)]^N. \tag{3.3}$$

Here N is the Trotter number, and $\beta=1/T$. The quantum problem is found to be approximately equivalent to a two-dimensional Ising system. Its configuration is governed locally by the operator $h_{i,i+1}$. The Boltzmann factor $\exp[-\beta h_{i,i+1}/N]$ can be exactly evaluated in terms of a four-body interaction for $i\neq 1$ and of a six-body interaction for $i=1$.

In order to evaluate the impurity susceptibility χ_{imp}, we introduce the base states $|\alpha_m\rangle$ which diagonalize S_f^z, i.e., $S_f^z|\alpha_m\rangle=\sigma_f^z(\alpha_m)|\alpha_m\rangle$ for $m=1,\ldots,2N$. In terms of them we have[18]

$$X_{\text{imp}}=\frac{\beta}{(2N)^2}\left\langle\left[\sum_{m=1}^{2N}\sigma_f^z(\alpha_m)\right]^2\right\rangle_{\text{MC}}, \tag{3.4}$$

where $\langle\cdots\rangle_{\text{MC}}$ denotes a thermal average over the two-dimensional Ising board. Note that the spin-correlation function $\langle S_f^z S_i^z\rangle$ is straightforwardly evaluated, since $S_f^z S_i^z$ is a diagonal operator. As regard the impurity contribution to the specific heat, we may evaluate it by taking a numerical derivative of the impurity energy with respect to temperature. However, the numerical derivative gives rise to large numerical errors. For that reason we were unable to obtain reliable values for low temperatures.

We carried out a Monte Carlo simulation for finite-size systems with $L=32$, 40, 48, 64, 128, and four values of the Trotter number N. For $T\leqslant 0.1J$, the values of N are between 60 to 120. For $T>0.1J$, they are required to satisfy $0.01<(J\beta/N)^2<0.05$. For high temperatures, the smallest value of N is 4. In all the cases we performed the calculations in steps of 5.5×10^5 in order to get sufficiently high acceptance of states and the first 5×10^4 steps are discarded as the system is warming up. The values evaluated by the Monte Carlo simulation are extrapolated to the thermodynamic limit by a least-squares method. Specifically we used the formula

$$A_{L,N}=A_\infty+\frac{a_1}{L}+\frac{a_2}{L^2}+\frac{b_1}{N^2}+\frac{b_2}{N^4}. \tag{3.5}$$

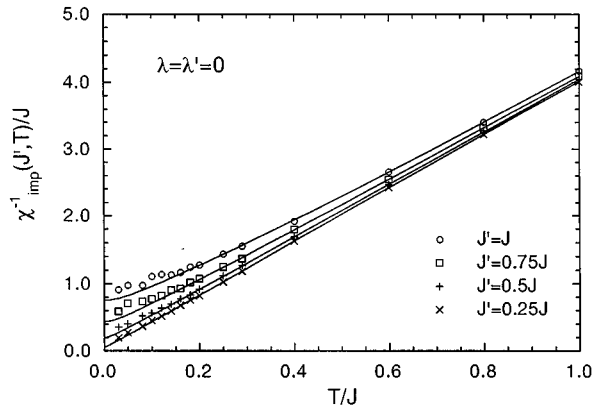

FIG. 4. Inverse of the impurity susceptibility as a function of T, for $\lambda=\lambda'=0$. Solid lines represent exact results for the resonant-level model.

B. Results for $\lambda=\lambda'=0$

We study first the case of $\lambda=\lambda'=0$ in order to check the accuracy of the Monte Carlo data. Figure 4 shows the inverse of the impurity susceptibility extrapolated to the thermodynamic limit according to Eq. (3.5). The results are in good agreement with the exact ones of the resonant-level model. The temperature dependence of $\chi_{\text{imp}}(J',T)$ is shown in Fig. 2, from which it is seen that the scaling relation is well reproduced. In order to evaluate Δ from the Monte Carlo data, we use the relation $\Delta=\chi_{\text{imp}}^{-1}(J',T=0)/\pi$. The inverse of the impurity susceptibility is extrapolated to zero temperature by applying a least-squares fitting of the finite-temperature data ($T=0.05J\sim 2J$). Thereby a power series expansion up to T^3 is used. The values obtained this way are compared in Fig. 5 with the exact ones. The Monte Carlo data is found to be slightly larger.

C. Results for $\lambda=0$, $\lambda'=1$

Next we consider the case of $\lambda=0$, $\lambda'=1$. Note the resemblance of the present case to the one-impurity problem coupled to a ''Kondo necklace'' studied by Doniach.[19] Figure 6 shows the numerical results for the inverse of the im-

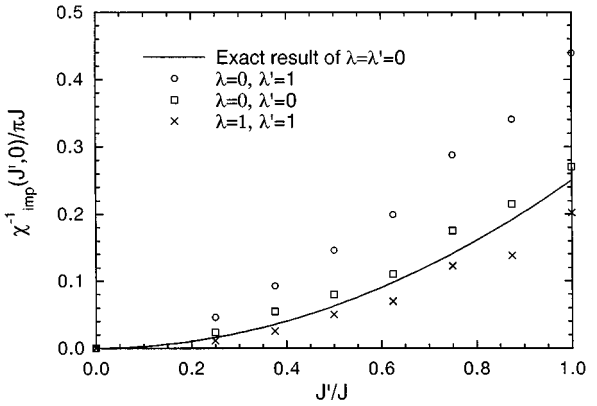

FIG. 5. Energy scale Δ defined by $\chi_{\text{imp}}^{-1}(J',\ T=0)/\pi$ as a function of J'/J. The solid line represents the exact results for $\Delta=J'^2/(4J)$ when $\lambda=\lambda'=0$.

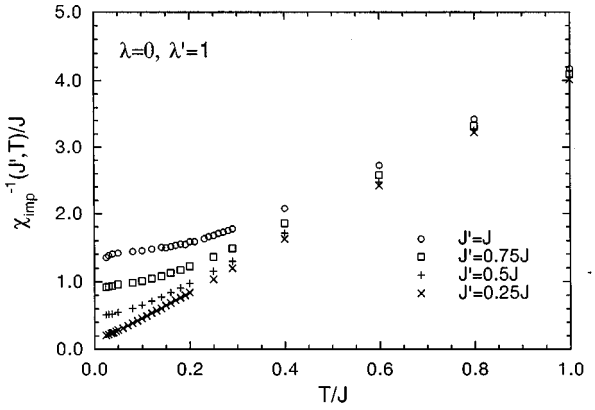

FIG. 6. Inverse of the impurity susceptibility as a function of T, for $\lambda=0$, $\lambda'=1$.

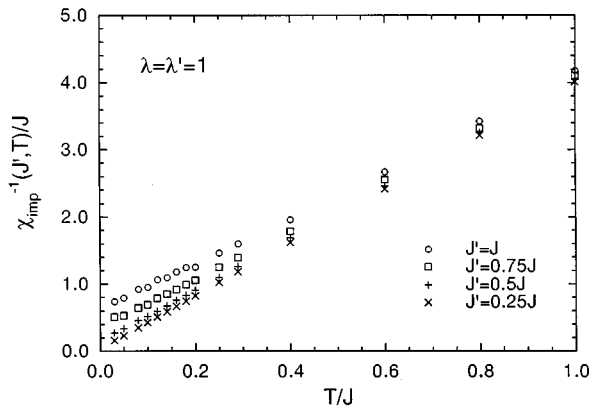

FIG. 8. Inverse of the impurity susceptibility as a function of T, for $\lambda=\lambda'=1$.

purity susceptibility as a function of T, extrapolated to the thermodynamic limit according to Eq. (3.5). Its behavior resembles that for $\lambda=\lambda'=0$. We tentatively assume that the energy scale Δ is given by $\chi_{\rm imp}^{-1}(J',T=0)/\pi$, i.e., by the same relation as for $\lambda=\lambda'=0$. Figure 7 shows $T\chi_{\rm imp}(J',T)$ as a function of T/Δ. For small values of T/Δ, the data for different values of J' falls nearly onto a single curve. This indicates that evaluating the energy scale as indicated above is justified within the accuracy of the data. In Fig. 5, the results for Δ are shown as a function of J'; note that they are larger than those for $\lambda=\lambda'=0$. They are consistent with the exact solution in the continuous limit,[10] which predicts $\chi_{\rm imp}^{-1}(J',T=0)\propto D[(\rho J')^2]^{\pi/(\pi+\rho J')}$ with D and ρ denoting the bandwidth and the density of states for the fermions in the chain. For small values of J', $\chi_{\rm imp}^{-1}(J',T=0)$ behaves like $\propto J'^2$.

D. Results for $\lambda=\lambda'=1$

We finally consider the case of $\lambda=\lambda'=1$. Figure 8 shows the inverse of the impurity susceptibility as a function of T after extrapolating to the thermodynamic limit according to Eq. (3.5). The energy scale Δ is evaluated again from $\Delta=\chi_{\rm imp}^{-1}(J',T=0)/\pi$. Figure 9 shows $T\chi_{\rm imp}(J',T)$ as a function of T/Δ. For small values of T/Δ, the data for different values of J' falls nearly on a single curve. This indicates again that the energy scale is properly chosen. Note that the data for $J'/J=0.25$ does not reach the low T/Δ regime. In Fig. 5, the energy scale Δ is shown as a function of J'; the energy scale is the smallest in the three cases. Therefore it is not clear whether or not for small values of J' it behaves like $\Delta\sim e^{-a/J'}$.

Figure 10 shows the absolute value of the spin-correlation function $|\langle \mathbf{S}_f\cdot\mathbf{S}_i\rangle|$ between the impurity spin and the spin at site i in the chain, at $T/J=0.025$. Spin correlations for $i=1$ have previously been calculated for zero temperature by diagonalizing exactly the Hamiltonian for finite clusters (see Fig. 3 of Ref. 2). The present values are close to the previous ones. With increasing values of J', they increase toward 0.75, which is the value for a perfect singlet. As for the site dependence, the correlations are rather long ranged particularly for small values of J'/J. Figure 11 shows the absolute value of the spin-correlation function $|\langle \mathbf{S}_f\cdot\mathbf{S}_1\rangle|(i=1)$ as a function of T/Δ. This quantity decreases rapidly with increasing values of T/Δ. A scaling relation is not satisfied in this case.

IV. CONCLUDING REMARKS

We have studied finite-temperature properties of a magnetic impurity coupled to a one-dimensional quantum spin

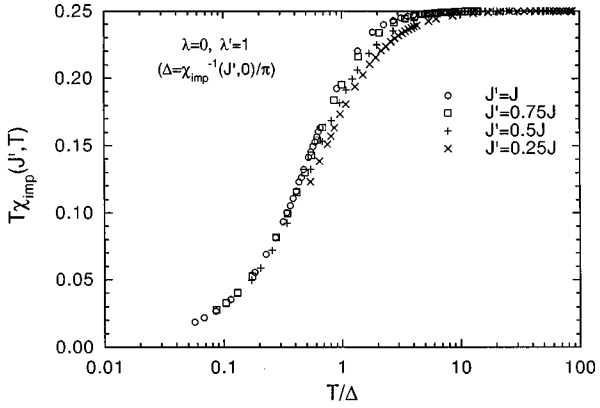

FIG. 7. $T\chi_{\rm imp}$ vs T/Δ for $\lambda=0$, $\lambda'=1$. The energy scale Δ is evaluated from $\chi_{\rm imp}^{-1}(J',\ T=0)/\pi$.

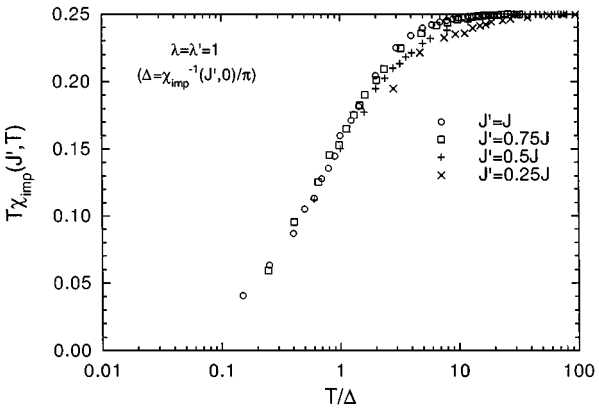

FIG. 9. $T\chi_{\rm imp}$ vs T/Δ for $\lambda=\lambda'=1$. The energy scale Δ is evaluated from $\chi_{\rm imp}^{-1}(J',\ T=0)/\pi$.

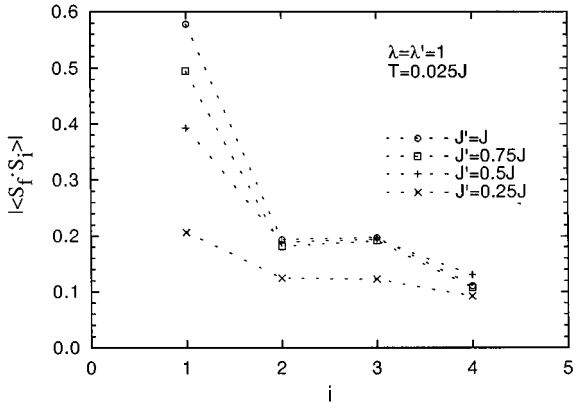

FIG. 10. Absolute value of the spin-correlation function $|\langle \mathbf{S}_f \cdot \mathbf{S}_i \rangle|$ between the impurity spin and the spin at site i in the chain. $T/J = 0.025$, and $\lambda = \lambda' = 1$.

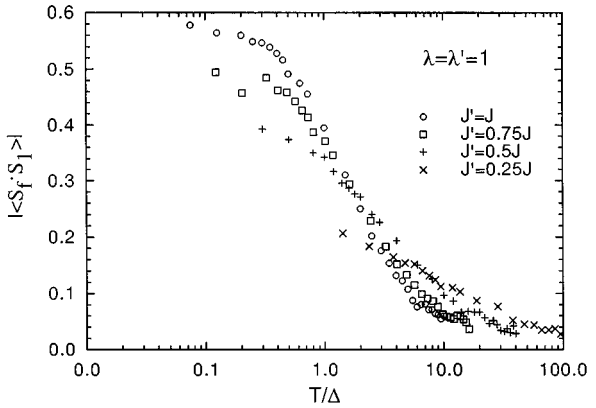

FIG. 11. Absolute value of the spin-correlation function $|\langle \mathbf{S}_f \cdot \mathbf{S}_1 \rangle|$ as a function of T/Δ. $\lambda = \lambda' = 1$. The energy scale Δ is evaluated from $\chi_{\rm imp}^{-1}(J', T=0)/\pi$.

model. After mapping the spin model onto a resonant-level model of spinless fermions, we have discussed the exactly solvable case $\lambda = \lambda' = 0$. It is shown that the resonant-level width sets the energy scale, and that the impurity susceptibility and the impurity contribution to the specific heat show a scaling behavior. The accuracy of the present Monte Carlo data is checked by comparison with the exact results.

Then we proceeded to study the cases of $\lambda = 0$, $\lambda' = 1$, and $\lambda = \lambda' = 1$. By using the Monte Carlo method, we have calculated the impurity susceptibility and the spin-correlation function between the impurity spin and the ones in the chain. We find that the spin-correlation function is rather long ranged at low temperatures, but that the long-ranged part is easily destroyed when thermal fluctuations become of order Δ. The scaling behavior of the impurity susceptibility is found to be quite similar to that for $\lambda = \lambda' = 0$. From this similarity we speculate that the interactions between the spinless fermions caused by finite values of λ, λ' do not change the physics and merely renormalize the energy scale. In order to draw a definite conclusion though, we need to improve the accuracy of the Monte Carlo simulation, so that we can obtain data for smaller values of T and J'. Also we need to calculate the impurity contribution to the specific heat.

If our speculation should turn out to be right, then the Hamiltonian Eq. (1.1) is a model of an insulator with low-temperature properties which correspond to those of a local neutral Fermi liquid. The properties found here for $\lambda = \lambda' = 0$ and expected to hold also for $\lambda = \lambda' = 1$ are an impurity susceptibility of the form $\chi_{\rm imp}(T=0) = (\pi\Delta)^{-1}$, a specific-heat contribution $C_{\rm imp}(T) = \gamma T$, where γ scales with Δ^{-1}, and a Wilson ratio $(T\chi_{\rm imp}/C_{\rm imp})(\pi^2/3) = 1$. They are very similar to those of a Kondo impurity coupled to nearly-free conduction electrons.[12] Because we are dealing here with an insulator, the behavior of the impurity is that of a local neutral Fermi liquid, in contrast to the conventional Kondo problem. Generalizing this concept from an impurity to a lattice results in a heavy neutral Fermion system. As pointed out in the introduction, the semimetal Yb_4As_3 comes close to that physical situation.[20–22]

In the conventional Kondo problem with weak coupling,[1] the energy scale, i.e., the Kondo temperature T_K, is given by $T_K \approx 4te^{-1/\rho J'}$, where $4t$ is the bandwidth and $\rho = (2\pi t)^{-1}$ is the density of states of the conduction electrons at the Fermi energy. For $t \simeq 1$ eV and $J' \simeq 0.25$ eV this gives $T_K = 4e^{-10\pi}$ eV, which actually is zero. If the Heisenberg spin model is regarded as the strong-coupling limit of the Hubbard model, the exchange interaction between different sites may be estimated as $J(=4t^2/U) \simeq 1$ eV when the values $U \simeq 4$ eV and $t \simeq 1$ eV are used. For $J' \simeq 0.25$ eV and $J'/J = 0.25$, the energy scale Δ becomes ~ 0.1 eV, according to the present calculation. This indicates that the interactions between the conduction electrons enhance greatly the energy scale.

For $\lambda = \lambda' = 0$, the energy scale Δ obeys a power law with respect to J'. Our present Monte Carlo data suggests a similar dependence for $\lambda = 0$, $\lambda' = 1$, in agreement with the exact solution in the continuous limit.[10] However, for $\lambda = \lambda' = 1$, the data is not sufficient in order to exclude or confirm a singular dependence of the energy scale as a function of J', $\Delta \sim e^{-a/J'}$. The conformal field theory[5] predicts the exponential form. For a one-dimensional system away from half-filling,[23] a power-law dependence of the energy scale was predicted even when the coupling to the impurity is weak.

When the impurity spin is symmetrically coupled to two spins in the chain, analogies to the two-channel Kondo model have been discussed.[5,24] Due to frustration, one must deal here with the negative sign problem,[25] and therefore a Monte Carlo study is difficult.

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