Specific heat of the impure spin-$\frac{1}{2}$ XY chain

G. Gildenblat
Electronic Materials and Processing Research Laboratory, The Pennsylvania State University, University Park, Pennsylvania 16802
(Received 12 May 1993)

We use a pseudofermion representation to investigate strong-field anomalies of the magnetic-field (h) dependence of the specific heat (c) of a spin-$\frac{1}{2}$ XY chain doped with magnetic impurities. If at certain magnetic field the impurity-induced split-off energy levels come sufficiently close to the chemical potential of pseudofermions (zero), then at low temperatures the specific heat of the chain is significantly altered by even a small number of impurities. The impurity-induced peaks of the $c(h)$ dependence correspond to magnetic fields in a range where the specific heat of the ideal spin-$\frac{1}{2}$ XY chains is exponentially small. They have the same physical origin, but different structure, as compared to the high-field anomalies of longitudinal magnetic susceptibility investigated previously.

I. INTRODUCTION

In a recent work,[1] we described strong-field anomalies of the longitudinal magnetic susceptibility of the impure spin-$\frac{1}{2}$ XY chain. The purpose of this work is to investigate a similar effect on the magnetic-field dependence of the specific heat. The specific heat of the spin-$\frac{1}{2}$ XY chain was obtained in Ref. 2 for the ideal chain and in Refs. 3 and 4 for the chain containing nonmagnetic impurities. The latter transform the infinite chain into an ensemble of finite-sized free-end segments with a known distribution of the segment length.[3,5] The corresponding problem has an exact solution for an arbitrary impurity concentration.[3,4] Thermodynamic properties of the impure spin-$\frac{1}{2}$ XY chain can be also computed exactly in the case of the random exchange interaction with a smooth distribution of the coupling parameter.[6] The opposite case of the spin-$\frac{1}{2}$ XY chain with identical magnetic impurities has been studied in relation to the impurity-induced oscillations of local magnetization,[7–9] formation of split-off energy levels outside of the pseudofermion band,[1,10] and high-field anomalies of the magnetic susceptibility.[1,11] In this work, we show that under certain conditions the magnetic-field (h) dependence of the specific heat (c) of a spin-$\frac{1}{2}$ XY chain can be significantly altered by even a small number of magnetic impurities. The anomalous $c(h)$ dependence of the impure spin-$\frac{1}{2}$ XY chain is closely related to that of magnetic susceptibility and may present another opportunity for an experimental investigation of the effect.

II. SPECIFIC HEAT

The Hamiltonian of the impure spin-$\frac{1}{2}$ XY chain with free ends and the nearest-neighbor interaction can be written in the form

$$H=\sum_{j=1}^{N} J_j(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y)+\sum_{j=1}^{N} h_jS_j^z \ . \tag{1}$$

Here N denotes the number of sites in the chain, J_j is the coupling constant for the sites j and $j+1$, S_j^α denotes the components of the spin at site j ($\alpha=x,y,z$), $h_j=-g_j\mu_B B$ where g_j is the Lande factor corresponding to site j, μ_B is the Bohr magneton, and B is the magnetic field applied along the z axis. If at least one of the sites j or $j+1$ is occupied by an impurity spin, we put $J_j=J'$, otherwise $J_j=J$. Finally, $g_j=g$ if the site j is occupied by the host spin and $g_j=g'$ if impurity is located at this site. In what follows, we use the notations $\Delta J=J'-J, h=g\mu_B B$ (normalized magnetic field), $\Delta g=g'-g$, and $\Delta h=(h/J)(\Delta g/g)$. Since the sign of J_j can be changed by a unitary transformation $H\rightarrow UHU^\dagger$, $U=2S_j^z$, we assume $J>0$. In the pseudofermion representation[12,13]

$$H=\sum_j H_{ij}C_i^\dagger C_j \ , \tag{2}$$

where

$$H_{ij}=(J_j/2)(\delta_{j,i+1}+\delta_{j,i-1})+(h_j/2)\delta_{ij} \ , \tag{3}$$

and the operators

$$C_j=(-2)^{j-1}\left[\prod_{m=1}^{j-1} S_m^z\right]S_m^- \tag{4}$$

satisfy the Fermi anticommutation rules $[C_i^\dagger,C_j]=\delta_{ij},[C_i,C_j]=0$.

The Hamiltonian (2) is diagonalized by a second canonical transformation

$$a_p=\sum_j \Psi_j^{(p)}C_j \ , \tag{5}$$

where $\Psi_j^{(p)}$ denotes the jth component of the pth eigenvector of H_{ij} corresponding to the eigenvalue E_p. As long as $\Psi^{(p)}$ are orthonormalized, the operators a_p satisfy the usual Fermi anticommutation rules. In terms of the new operators,

$$H=\sum_p E_p a_p^\dagger a_p \ . \tag{6}$$

Since the total number of pseudofermions is not fixed, the free energy is given by the expression

$$F=-\beta^{-1}\sum_{p=1}^{N}\ln(1+e^{-\beta E_p}) \ , \tag{7}$$

where $\beta=1/k_B T$, k_B is the Boltzmann constant, and T is the absolute temperature. Consequently, the average energy E and specific heat $c=-N^{-1}k_B^{-1}T(\partial^2 F/\partial T^2)_h$ (in a constant magnetic field) are given by the expressions

$$E=N^{-1}\sum_{p=1}^{N}E_p(1+e^{-\beta E_p})^{-1} \tag{8}$$

and

$$c=N^{-1}\sum_p[(\beta E_p/2)\,\mathrm{sech}(\beta E_p/2)] \ . \tag{9}$$

In particular, for an ideal infinite spin-$\frac{1}{2}$ XY chain, the energy levels of pseudofermions form a single energy band

$$E=h+J\cos k, \quad 0\le k<2\pi \ , \tag{10}$$

and[2]

$$c=\int_0^{2\pi}\left[\frac{\beta}{2}(h+J\cos k)\,\mathrm{sech}\left[\frac{\beta}{2}(h+J\cos k)\right]\right]^2 dk \ . \tag{11}$$

Approximation of this integral using the Laplace method shows that in the high-field, low-temperature region

$$\beta(|h|-J)\gg 1, \quad \beta J\gg 1 \ , \tag{12}$$

the specific heat of the pure chain

$$c\approx\frac{[\beta(|h|-J)]^2}{\sqrt{2\pi\beta J}}\exp[-\beta(|h|-J)] \ , \tag{13}$$

is exponentially small.

For the impure spin-$\frac{1}{2}$ XY chain it is convenient to separate contributions of the in-band (c_b) and split-off (c_s) states of the pseudofermions:

$$c=c_b+c_s \ . \tag{14}$$

For the in-band states $|E_p-h|<J$ and according to (9), $c_b\propto\exp(-\beta|h|)$ remains negligible in the high-field region (12). To investigate the contribution c_s of the split-off states outside the pseudofermion band we first neglect the indirect Ruderman-Kittel-Kasuya-Yosida impurity-impurity interaction. Under this assumption, each split-off energy level has degeneracy N_i (the number of impurities) and

$$c_s=n_i\sum_{s:|E_s-h|>J}\varphi(\beta E_s/2) \ , \tag{15}$$

where

$$\varphi(x)=(x\,\mathrm{sech}x)^2 \ , \tag{16}$$

$n_i=N_i/N$ is the fraction of the chain sites occupied by impurities, and E_s are split-off energy levels in an infinite chain with a single impurity. The following conditions for the formation of impurity-induced energy levels in a spin-$\frac{1}{2}$ XY chain with a single impurity were obtained in Ref. 1 by investigating the poles of the pseudofermion propagator.

If

$$|\Delta h|\le(1-\sigma)/2=1-(J'/J)^2 \ , \tag{17}$$

where $\sigma=2(J'/J)^2-1$, then there are no split-off states. For

$$\left.\begin{aligned}|\Delta h|&>(1-\sigma)/2=1-(J'/J)^2 \quad (18)\\ |\Delta h|&\ge(\sigma-1)/2=(J'/J)^2-1 \quad (19)\end{aligned}\right\} ,$$

there is one split-off state with the energy

$$E_s=h+J\frac{\Delta h(\sigma-1)}{2\sigma}+J\frac{\mathrm{sgn}(\Delta h)}{2\sigma}(\sigma+1)\sqrt{(\Delta h)^2+\sigma} \tag{20}$$

and

$$E_s=h+J(\Delta h+1/4\Delta h), \quad \sigma=0 \ . \tag{21}$$

Note that taking the limit $\sigma\to 0$ in (20) results in (21) so that $E_s(\sigma)$ remains continuous for $\sigma=0$.

Finally, for

$$|\Delta h|<(\sigma-1)/2=(J'/J)^2-1 \ , \tag{22}$$

there are two localized states with energies given by

$$E_{s\pm}=h+(J/2\sigma)[\Delta h(\sigma-1)\pm(\sigma+1)\sqrt{(\Delta h)^2+\sigma}\,] \ . \tag{23}$$

According to expression (15), the contribution of split-off states to the specific heat of the chain remains negligible unless $\beta E_s/2\approx\pm x_0$, where $x_0\approx 1.1997$ (the positive solution of equation $x\tanh x=1$) corresponds to the maximum of $\varphi(x)$. Corresponding magnetic fields are found as solutions (if any) of equation

$$E_s(h)/J=\pm 2x_0/\beta J \ . \tag{24}$$

Since in the temperature range of interest $\beta J\gg 1$, conditions for Eq. (24) to have solutions are essentially the same as for the equation

$$E_s(h)=0 \ . \tag{25}$$

The last equation has the solution[1]

$$h_0=J\frac{(J'/J)^2}{\{2(J'/J)^2-g'/g\,](g'/g)\}^{1/2}} \ , \tag{26}$$

provided

$$(J'/J)^2>g'/g>0 \ . \tag{27}$$

If condition (27) is satisfied, and $\beta J\gg 1$, then the solutions $h_\pm$ of Eq. (24) are given by

$$h_\pm=h_0\pm\frac{2x_0}{\beta}\left[\frac{dE_s}{dh}\right]^{-1}_{h=h_0} . \tag{28}$$

If there is more than one split-off energy level, then the derivative in (28) is taken for the one satisfying Eq. (25). This gives

$$h_{\pm}=h_0 \pm \frac{x_0}{\beta}\frac{\sigma(2+\Delta g/g)-\Delta g/g}{(1+\Delta g/g)(\sigma-\Delta g/g)} . \tag{29}$$

Physically, Eq. (25) is a requirement that at a certain magnetic field one of the split-off energy levels crosses the zero energy representing the chemical potential of pseudofermions.[1] If this occurs, then the rapid change in the corresponding occupation numbers results in the peaks of the specific heat for $h=h_{\pm}$ (and hence for $h=-h_{\pm}$). Since these peaks are located in the high-field region (12), where the specific heat of the ideal chain is exponentially small, even a small number of impurities can drastically alter the $c(h)$ dependence (Fig. 1). We note also that if condition (25) is satisfied, then h_0 corresponds to the center of impurity-induced peak of the magnetic susceptibility.[1]

III. VIRIAL EXPANSION

The above analysis is limited to the case when the indirect interaction between magnetic impurities can be neglected. In this section we show that for small concentrations of impurities ($n_i \leq 0.05$ in the computations below) the impurity-impurity interaction changes the shape but not the position of strong-field anomalies on the magnetic-field dependence of the specific heat of the impure spin chain. To account for the random distribution of impurities we use Lifshitz virial expansion[14]

$$c=c_0+n_i(F_1-F_0)+n_i^2\sum_{r=1}^{\infty}[F_0-2F_1+F_2(r)]+O(n_i^3) , \tag{30}$$

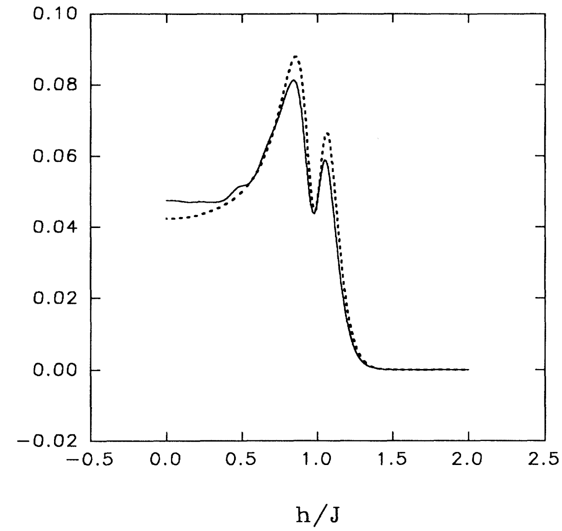

FIG. 2. Same as in Fig. 1 for $J'=J/2$, $g'=3g/2$, $T=0.04J/k_B$, $n_i=0.05$.

where c_0 is the normalized specific heat of the ideal chain, $F_0=Nc_0$, F_1 is the specific heat of the chain with a single impurity, and $F_2(r)$ denotes the specific heat of the chain with two impurities separated by a distance of r lattice periods. Unlike c and c_0, F_1 and $F_2(r)$ are not normalized to the chain length. A similar virial expansion has been used earlier in the study of high-field magnetic susceptibility of the impure spin-$\frac{1}{2}$ XY chain.[1] Since our prime objective is to relate high-field peaks on the $c(h)$ dependence to split-off states produced by the individual impurities, we consider relatively small impurity concen-

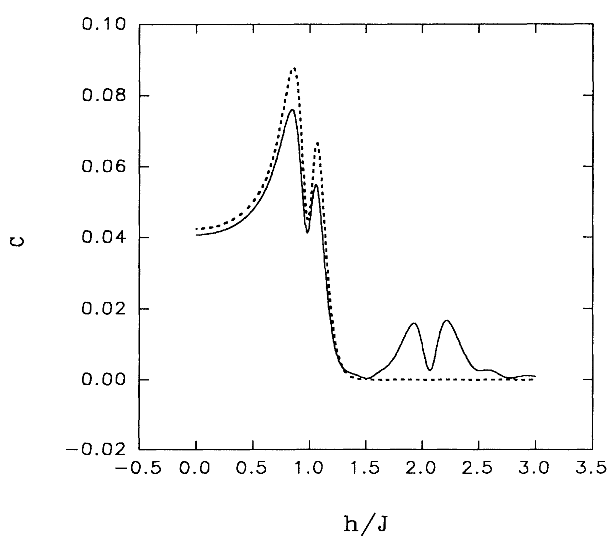

FIG. 1. Magnetic-field dependence of the normalized specific heat of the impure (solid line) and ideal (dashed line) spin-$\frac{1}{2}$ XY chains; $J'=2J$, $g'=g/2$, $T=0.04J/k_B$, $n_i=0.05$.

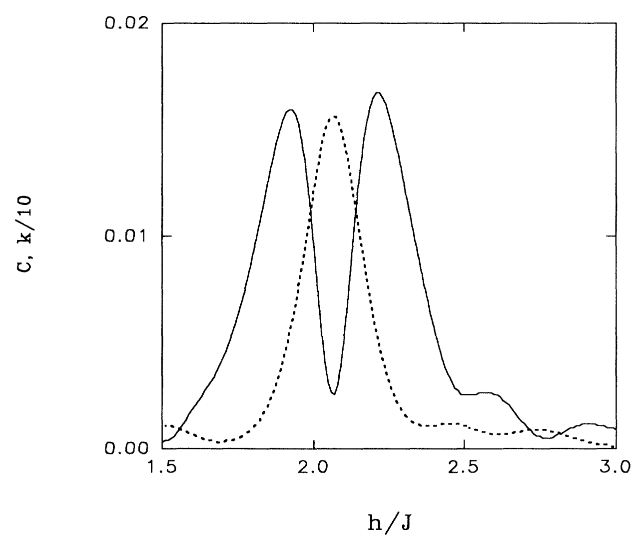

FIG. 3. Strong-field anomalies of the normalized specific heat (solid line) and magnetic susceptibility (dashed line) of the impure spin-$\frac{1}{2}$ XY chain; $J'=2J$, $g'=g/2$, $T=0.04J/k_B$, $n_i=0.05$.

trations. Consequently, the terms $O(n_i^3)$ corresponding to clusters of three or more impurities are negligible in the computations performed in this work. The maximum error for the impurity-induced peaks on the $c(h)$ dependence introduced by neglecting $O(n_i^3)$ terms does not exceed 1%.

The results of computations are shown in Figs. 1–3. For $J'=J/2$ and $g'=3g/2$, condition (26) is not satisfied and there is no impurity-induced peaks on the $c(h)$ dependence (Fig. 2); the high-field specific heat of the chain remains exponentially small. The impurity peaks appear for $J'=2J$ and $g'=g/2$ (Fig. 1), and the position of the peaks are accurately given by expression (29). The secondary peaks in Fig. 1 are produced by the indirect impurity-impurity interaction, which is responsible for an additional splitting of the split-off energy levels corresponding to individual impurities. The physical origin and the range of this interaction are discussed elsewhere.[1,9]

It is interesting to compare high-field magnetic anomalies of the specific heat and magnetic susceptibility k of the impure spin-$\frac{1}{2}$ XY chain. Although the physical origin of these anomalies is the same (the rapid change in the occupation of split-off energy levels with magnetic field), the details are somewhat different. As shown in Fig. 3, in agreement with Eq. (29), a single peak on the $k(h)$ dependence is positioned in the middle of the two impurity-induced peaks of the specific heat.

The specific heat of the spin-$\frac{1}{2}$ XY chain with nonmagnetic impurities has been studied in Refs. 3 and 4. In this case the exact solution can be obtained for an arbitrary impurity concentration. In particular, the formation of the gap in the spectrum of pseudofermions is responsible for the exponential $c(T)$ dependence for $h=0$, $\beta J \ll 1$ [as compared to $c(T) \propto T$ for an ideal chain].[3] For a non-magnetic impurity $J'=0$, condition (27) is not satisfied and specific heat remains exponentially small in the high-field region (12). However, nonmagnetic impurities split the otherwise infinite chain into noninteracting segments with discrete energy levels of pseudofermions.[3–5] The abrupt change in the occupation numbers of these discrete energy levels produce the double peaks of the $c(h)$ dependence.[4] The main difference with the case of magnetic impurities considered in this work is that at low temperature ($\beta J \gg 1$) finite-size effects are important for $|h| \le J$, while magnetic impurities are responsible for the high-field ($|h| > J$) anomalies of the $c(h)$ dependence.

In conclusion, we have shown that if condition (25) is satisfied, impurity-induced energy levels outside of the pseudofermion band produce strong-field anomalies of the magnetic-field dependence of the specific heat of the spin-$\frac{1}{2}$ XY chain. The conditions for possible experimental observation of the impurity-related anomalies of specific heat and magnetic susceptibility are essentially the same and have been discussed elsewhere.[1,3,4,11]

[1] G. Gildenblat, Phys. Rev. B **47**, 2611 (1993).
[2] S. Katsura, Phys. Rev. **127**, 1508 (1962).
[3] M. F. Thorpe and S. Miyasima, Phys. Rev. B **24**, 6686 (1981).
[4] M. Maccio, A. Rettori, and M. G. Pini, Phys. Rev. B **31**, 4187 (1985).
[5] F. Matsubara and S. Katsura, Prog. Theor. Phys. **49**, 367 (1973).
[6] R. Smith, J. Phys. C **3**, 1419 (1970).
[7] G. Baskaran, Phys. Rev. Lett. **40**, 1521 (1978).
[8] G. Gildenblat, J. Magn. Magn. Mater. **43**, 96 (1984).
[9] G. Gildenblat, Phys. Rev. B **30**, 6539 (1984).
[10] T. Oguchi and I. Ono, J. Phys. Soc. Jpn. **26**, 1378 (1969).
[11] G. Gildenblat, Phys. Rev. B **32**, 3006 (1985).
[12] P. Jordan and E. Wigner, Z. Phys. **47**, 631 (1928).
[13] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[14] I. M. Lifshitz, Adv. Phys. **13**, 483 (1964).