Magnetic susceptibility of the impure spin-$\frac{1}{2}$ XY chain

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We use a pseudofermion representation to study the formation and magnetic-field dependence of split-off energy levels in a spin-$\frac{1}{2}XY$ chain with a small concentration of magnetic impurities. Of particular interest are split-off states whose energy at a certain magnetic field crosses the zero level corresponding to the chemical potential of pseudofermions. If this condition is satisfied, then at sufficiently low temperature the magnetic-field dependence of the chain susceptibility is significantly altered by even a small number of impurities.

I. INTRODUCTION

The purpose of this work is to investigate the magnetization curve of an isotropic spin-$\frac{1}{2}$ XY chain with a small concentration of identical magnetic impurities. We show that formation of split-off energy levels outside of the pseudofermion energy band may lead to a drastic, and at least in principle, observable modification of the magnetic-field dependence of the macroscopic susceptibility.

The spin-$\frac{1}{2}$ XY chain is often invoked as the simplest case of an essentially quantum one-dimensional antiferromagnet.[1] Its principal advantage in theoretical studies is an exact pseudofermion representation established by way of a Wigner-Jordan transformation.[2] For an ideal chain, this allows an exact computation of thermodynamic properties and magnetic susceptibility,[1,3-5] and greatly assists in the investigations of correlation functions and nonequilibrium effects.[6-8]

Subsequent investigations have shown that an exact solution is also possible for a spin-$\frac{1}{2}$ XY chain with a random distribution of identical nonmagnetic impurities which break the infinite chain into a set of finite chains with free ends.[9-13] In particular, it was found that finite-size effects change the low-temperature behavior of the specific heat from linear to exponential[10,11] and are responsible for a nonmonotonic magnetic-field dependence of magnetic susceptibility.[9,12] Mathematically, the presence of nonmagnetic impurities is equivalent to a discrete distribution of coupling constant which either vanishes completely or takes the value corresponding to the ideal chain. An opposite case of the spin-$\frac{1}{2}$ XY chain with a random but smooth distribution of coupling constants has been solved in Ref. 14.

In this work we return to the case of the spin-$\frac{1}{2}$ XY chain with identical impurities. Unlike the treatments given in Refs. 9–13, we consider magnetic impurities. In order to trace the consequences of the impurity-induced localized states, we limit our analysis to the case of small impurity concentrations. The resulting magnetization curves are significantly different from those obtained in Refs. 9 and 12.

The paper proceeds as follows. In Sec. II we derive conditions for the formation of split-off states in an XY chain with a single impurity of a reasonably general type. Section III contains an analytical approximation for the contribution of split-off states to magnetic susceptibility. The results of numerical computations of susceptibility are presented in Sec. IV.

II. SPLIT-OFF STATES

The Hamiltonian of the isotropic spin-$\frac{1}{2}$ XY chain with a single impurity can be written as

$$H=H_0+V \ , \tag{1}$$

where

$$H_0=J\sum_j (S_j^xS_{j+1}^x+S_j^yS_{j+1}^y)+h\sum_j S_j^z \tag{2}$$

denotes the Hamiltonian of the ideal chain, and the perturbation

$$V=\Delta J\sum_{j=\pm 1}(S_j^xS_0^x+S_j^yS_0^y)+J\Delta h S_0^z \ . \tag{3}$$

In these expressions, J is the coupling constant, S_j^x and S_j^y denote the components of spin at site j, $h=-g\mu_B B$ is the normalized magnetic field, g is the Lande factor, μ_B is Bohr's magneton, and B is the magnetic field. The impurity is located at site $j=0$, its exchange interaction with two nearest neighbors is characterized by a new coupling constant $J'=J+\Delta J$, and $\Delta h=-\Delta g\mu_B BJ$ or $\Delta h=(h/J)(\Delta g/g)$, where Δg denotes the change of g factor at the impurity site. In what follows we assume $J>0$ since the sign of J can be changed by a unitary transformation.[4]

The pseudofermion representation is introduced by a Wigner-Jordan transformation[1,2]

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

and

$$C_j^+=(-2)^{j-1}S_j^+\prod_{m=1}^{j-1}S_m^z \tag{5}$$

where $S_j^{\pm}=S_j^x \pm i S_j^y$. Operators C_j and C_j^+ satisfy the standard Fermi anticommutation rules

$$\{C_j^+, C_{j'}\}=\delta_{jj'} \tag{6}$$

$$\{C_j, C_{j'}\}=0 , \tag{7}$$

and can be used to present H_0 and V as follows:

$$H_0=h\sum_j C_j^+C_j+(J/2)\sum_j (C_j^+C_{j+1}+\text{H.c.}) , \tag{8}$$

$$V=J\Delta h C_0^+C_0+(\Delta J/2)\sum_{j=\pm 1}(C_j^+C_0+\text{H.c.}) . \tag{9}$$

In the absence of an impurity the eigenvalues of H_0 for an infinite chain form a single energy band

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

In this work, we are interested in the localized or "split-off" states with the energies outside the band (i.e., with $|E-h|>J$) and their contribution to the normalized magnetic susceptibility:

$$k=-\frac{d}{dh}\left[\frac{J}{N}\sum_j \langle S_j^z\rangle\right] . \tag{11}$$

Here N is the total number of spins in the chain (when convenient we put $N\to\infty$), and $\langle \cdots \rangle$ denotes the canonical average corresponding to an absolute temperature T. In a Wigner-Jordan representation

$$S_j^z=C_j^+C_j-\tfrac{1}{2} , \tag{12}$$

and

$$k=-\frac{d}{dh}\left[\frac{J}{N}\sum_j \langle C_j^+C_j\rangle\right] . \tag{13}$$

The impurity problem described by Eqs. (1)–(9) has been posed in Refs. 15–19. The analysis based on perturbation theory (small ΔJ, $\Delta h=0$) has led to the prediction of long-range Friedel-type oscillations of the pseudofermion density $\langle C_j^+C_j\rangle$ and corresponding oscillations of the local magnetization for $T=0$.[16] The exact solution of this problem was given in Ref. 17 using a Green-function method. The temperature damping of the oscillations of local magnetization, which limits the range of indirect interaction between impurities, was studied numerically in Ref. 18. The formation of split-off states for a particular case of zero magnetic field (and hence $\Delta h=0$) was investigated in Ref. 15 while Ref. 19 deals with local critical exponents for the $T=0$ magnetic phase transition in the impure chain.

The split-off energy levels can be found as the poles of the retarded Green function

$$G_{ij}(E)=-i\int_{-\infty}^{\infty}\theta(t)\exp(iEt/\hbar)\langle\{C_i(t),C_j^+(0)\}\rangle dt , \tag{14}$$

where $\theta(t)$ denotes the unit step ("inclusion") function. The corresponding equation of motion in the site representation is

$$[\underline{H}-(E+i0)\underline{I}]\underline{G}=\underline{I} , \tag{15}$$

where $\underline{I}$ denotes the unit matrix and

$$H_{ij}=h\delta_{ij}+J/2(\delta_{i,j+1}+\delta_{i,j-1})+J\Delta h\delta_{i0}\delta_{j0} + \tfrac{1}{2}\Delta J[(\delta_{j,1}+\delta_{j,-1})\delta_{i0}+(\delta_{i,1}+\delta_{i,-1})\delta_{j0}] . \tag{16}$$

The solution of Eq. (15) has been found in the form[17]

$$G_{ij}=g_{ij}+\Delta G_{ij} , \tag{17}$$

where g_{ij} denotes the Green function of the ideal chain[15] and ΔG_{ij} is the change introduced by an impurity. Denoting $f=(E-h)/J$ we have

$$g_{jj}=2Q^{|j|+1}/J(1-Q^2) , \tag{18}$$

$$\Delta G_{jj}=\frac{(\sigma-1)(1+\delta_{0j})[(1-\delta_{0j})Q^{2|j|+1}+Q^{2|j|+3}]+4\Delta h Q^{2|j|+2}}{J(1-Q^2)(1-\sigma Q^2-2\Delta h Q)} , \tag{19}$$

where

$$Q=f-i\sqrt{1-f^2} , \quad |f|\le 1 , \tag{20}$$

$$Q=f-\text{sgn}(f)\sqrt{f^2-1} , \quad |f|>1 . \tag{21}$$

Parameter σ is defined as

$$\sigma=2(J'/J)^2-1 , \quad J'=J+\Delta J . \tag{22}$$

According to (21) for states outside the pseudofermion band $0<|Q|<1$, and $f=\frac{1}{2}(Q+1/Q)$. Consequently, the energy of the split-off state is given by

$$E_s=h+(J/2)(Q+1/Q) , \tag{23}$$

where Q is the solution (if any) of the equation

$$1-2\Delta h Q-\sigma Q^2=0 \tag{24}$$

satisfying the additional condition $|Q|<1$.

The existence of such solutions depends on the values of σ and Δh. There are three possible cases. If

$$|\Delta h|\le(1-\sigma)/2=1-(J'/J)^2 \tag{25}$$

then there are no split-off states. For

$$\left.\begin{aligned}|\Delta h|&>(1-\sigma)/2=1-(J'/J)^2\\ |\Delta h|&\ge(\sigma-1)/2=(J'/J)^2-1\end{aligned}\right\} \tag{26}$$

there is one split-off state with the energy

$$E_s=h+J\frac{\Delta h(\sigma-1)}{2\sigma}+J\frac{\text{sgn}(\Delta h)}{2\sigma}(\sigma+1)\sqrt{(\Delta h)^2+\sigma} , \quad \sigma\ne 0 \tag{27}$$

and

$$E_s = h + J(\Delta h + 1/4\Delta h)\ , \quad \sigma = 0\ . \tag{28}$$

Note that taking the limit $\sigma \to 0$ in (27) results in (28) so that $E_s(\sigma)$ remains continuous for $\sigma = 0$.

Finally, for

$$|\Delta h| < (\sigma - 1)/2 = (J'/J)^2 - 1 \tag{29}$$

there are two localized states with energies given by

$$E_{s\pm} = h + (J/2\sigma)[\Delta h(\sigma - 1) \pm (\sigma + 1)\sqrt{(\Delta h)^2 + \sigma}\,]\ . \tag{30}$$

The graphic representation of conditions (25), (26), and (29) is shown in Fig. 1. If $|J'| \le J$ then there is at most one split-off state provided that the absolute value of the site energy perturbation Δh is sufficiently large. For $|J'| > J$ there are two split-off states at $h = 0$, one of which may be suppressed by an increase in the magnetic field, provided that $\Delta g \ne 0$. Note also that the formation of localized states and the effect discussed in the next section do not depend on the sign of the coupling constant $J' = J + \Delta J$ in the immediate vicinity of the impurity. Indeed, the sign of J' can be changed by a unitary transformation $H \to UHU^+$, $U = 2S_0^z$.

The formation of split-off states for $h = 0$ was considered in Ref. 15. In this particular case, $\Delta h = 0$ and according to Eqs. (25)–(30) there is no split-off state unless $|J'| > J$. If the latter condition is satisfied, then there are precisely two split-off states with energies

$$E_{s\pm} = h \pm (\sigma + 1)J/2\sqrt{\sigma}\ . \tag{31}$$

III. MAGNETIC SUSCEPTIBILITY

We now investigate the possible experimental manifestation of split-off states. With reference to Eq. (16)

$$H = \sum_{i,j} H_{ij} C_i^+ C_j\ . \tag{32}$$

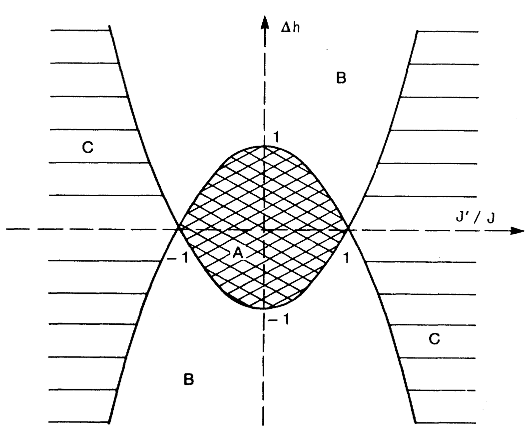


FIG. 1. Conditions for the formation of split-off states in a spin-$\frac{1}{2}$ XY chain with a single impurity. A, no split-off states; B, one split-off state; C, two split-off states. Boundary lines are included in region B for $|J'/J| > 1$ and in region A for $|J'/J| \le 1$.

This Hamiltonian can be diagonalized by a canonical transformation

$$a_p = \sum_n \Psi_n^{(p)} C_n\ , \tag{33}$$

where $\Psi_n^{(p)}$ denotes the nth component of the pth eigenvector of $\underline{H}$ corresponding to the eigenvalue E_p. The vectors $\Psi^{(p)}$ are assumed to be orthonormalized.

In terms of the new operators (which satisfy the same anticommutation rules as C_j)

$$H = \sum_p E_p a_p^+ a_p\ . \tag{34}$$

Consequently,

$$\langle a_p^+ a_p \rangle = [1 + \exp(\beta E_p)]^{-1}\ , \tag{35}$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant, and T denotes the absolute temperature. Since, according to (33), $\Sigma_p a_p^+ a_p = \Sigma_j C_j^+ C_j$, we can express the normalized magnetization

$$\frac{1}{N}\sum_j \langle S_j^z \rangle = \frac{1}{N}\sum_j (\langle C_j^+ C_j \rangle - \tfrac{1}{2}) \tag{36}$$

as

$$\frac{1}{N}\sum_j \langle S_j^z \rangle = \frac{1}{N}\sum_p \{[1 + \exp(\beta E_p)]^{-1} - \tfrac{1}{2}\}\ . \tag{37}$$

Consequently, the normalized magnetic susceptibility defined by expression (11) is given by

$$k = \frac{\beta J}{2N}\sum_p \frac{dE_p/dh}{1 + \cosh(\beta E_p)}\ . \tag{38}$$

Separating the contributions of the in-band (k_b) and split-off states (k_s) we write $k = k_b + k_s$, where

$$k_b = \frac{\beta J}{2}\int_{h-J}^{h+J} D(E)\frac{dE/dh}{1 + \cosh(\beta E)}dE \tag{39}$$

and $D(E)$ denotes the in-band density of states, which is, of course, affected by the presence of impurities.

For the contribution of the split-off states with energies E_s we have

$$k_s = \frac{\beta J}{2N}\sum_s N_s \frac{dE_s/dh}{1 + \cosh(\beta E_s)}\ , \tag{40}$$

where N_s denotes the degeneracy factor and the summation is extended over all (if any) split-off energy levels. For a single impurity, $N_s = 1$ as discussed above. If, however, we consider a chain with $N_i \ll N$ identical impurities and neglect the splitting of the localized states associated with the indirect [Ruderman-Kittel-Kasuya-Yosida (RKKY)-type] impurity-impurity interaction, then $N_s = N_i$ and

$$k_s = \frac{\beta J n_i}{2}\sum_s \frac{dE_s/dh}{1 + \cos(\beta E_s)}\ , \tag{41}$$

where $n_i = N_i/N$ denotes the fraction of chain sites occupied by impurities.

The accuracy of approximation (41) is discussed in the next section. Here we note only that it requires $n_i \ll 1$. Hence, the contribution of split-off states is negligible except for a particular case when E_s reaches zero for a certain value of the magnetic field $h=h_0$ (and consequently for $h=-h_0$). When this occurs, Eq. (41) predicts two characteristic peaks at points $h=\pm h_0$ on the magnetic-field dependence of susceptibility (see Fig. 2). What happens is that according to Eq. (35), at sufficiently low temperatures, the occupation number $\langle a_s^+ a_s \rangle$ changes rapidly with $E_s=E_s(h)$ near the point h_0 corresponding to $E_s(h)=0$. This is a common feature of systems of particles described by Fermi-Dirac statistics. The only special feature of the present problem is that the chemical potential of pseudofermions (whose total number is not fixed) is equal to zero.[1] The abrupt charge of the occupation number near $h=h_0$ results in a steplike behavior of the average magnetization [see Eq. (37)] corresponding to the peak of magnetic susceptibility shown in Fig. 2.

The magnetic-field dependence of split-off energy levels for two different types of impurities is shown in Fig. 3. In accordance with Fig. 1, the number of split-off states which exist in the chain depends on the magnitude of the magnetic field. Furthermore, even if an impurity (described by parameters J' and g') is such that split-off states do exist in a certain range of magnetic fields, the equation $E_s(h)=0$ may not have a solution in this range [cf. Fig. 3(b)]. Indeed, expressions (27) and (30) can be used to show that split-off states do not cross the zero energy level unless

$$(J'/J)^2 > g'/g > 0 \ . \tag{42}$$

If condition (42) is satisfied, then the magnetic field corresponding to the center of the peak

$$h_0 = J\frac{(J'/J)^2}{\{[2(J'/J)^2 - g'/g](g'/g)\}^{1/2}} \tag{43}$$

is determined by the coupling constant J' and the g factor $g'=g+\Delta g$ of the impurity.

In Eq. (41) the dE_s/dh vs h dependence is relatively weak as compared with that of $\cosh[\beta E_s(h)]$. Approximating this derivative by its value at $h=h_0$ and using the expressions for E_s given above, we find, after some algebra,

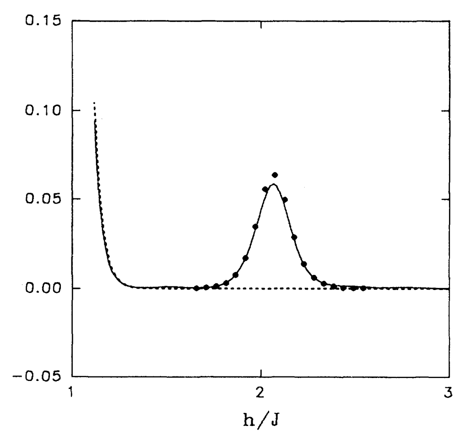


FIG. 2. Normalized magnetic susceptibility of the impure (solid line) and ideal (dashed line) spin-$\frac{1}{2}$ XY chains. Symbols represent Eq. (44); $J'=2J$, $g'=g/2$, $T=0.04J/k_B$, $n_i=0.015$.

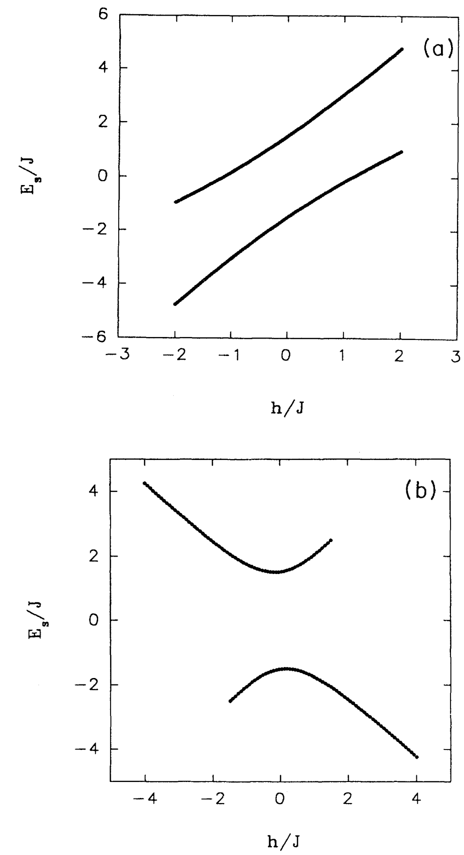


FIG. 3. Energy levels of split-off states as functions of the normalized magnetic field for (a) $J'=2J$, $g'=2g$; (b) $J'=2J$, $g'=-g$.

$$k_s = \frac{J\beta n_i(1+\Delta g/g)(\sigma-\Delta g/g)}{[\sigma(2+\Delta g/g)-\Delta g/g][1+\cosh(\beta E_s)]} \tag{44}$$

and

$$E_s = h[1+(\Delta g/g)(\sigma-1)/2\sigma] + \eta J[(\sigma+1)/2\sigma][\sigma+(\Delta h)^2]^{1/2} \ . \tag{45}$$

The sign of

$$\eta = -\mathrm{sgn}\{h[2\sigma+(\Delta g/g)(\sigma-1)]\} \tag{46}$$

is chosen in such a way that if there is more than one split-off state then E_s corresponds to the one with the energy closest to zero.

The magnitude of the peak predicted by Eq. (44) is proportional to $J\beta n_i$. Hence, even for small impurity concentrations, $n_i \ll 1$, the impurity-induced peak is observable if, in addition to condition (42), the temperature is sufficiently low ($J\beta \sim 1/n_i$) and h_0 falls within the range where the magnetic susceptibility of the ideal chain is negligible. The latter is given by the author of Ref. 3 as

$$k_0 = \frac{\beta J}{4\pi}\int_0^{\pi} \mathrm{sech}^2\{(\beta J/2)[(h/J)+\cos y]\}dy \ . \tag{47}$$

For $\beta(|h|-J) \gg 1$, $\beta J \gg 1$, evaluation of the integral using the Laplace method results in

$$k_0 \simeq \sqrt{\beta J/2\pi}\exp[-\beta(|h|-J)] \ . \tag{48}$$

Thus, if $\beta(h_0-J) \gg 1$, then h_0 corresponds to the range where k_0 is exponentially small (see Fig. 2). Physically, this means that for $|h|=h_0$ the split-off energy level (which is equal to zero) is separated from the pseudofermion band by a few $k_B T$.

IV. VIRIAL EXPANSION

Expression (44) for the contribution of the split-off states to magnetic susceptibility is first order with respect to the impurity concentration n_i. It is derived by neglecting the indirect (RKKY-type) interaction of magnetic impurities.

In principle, the validity of (44) may be assured by reducing n_i or increasing the temperature (which limits the range of the indirect impurity-impurity interaction.[18]) However, if $J\beta n_i$ is too small then the peaks on the $k(h)$ dependence described by Eq. (44) become insignificant. To extend the computations into a somewhat wider range of concentrations, we use the virial expansion of Ref. 20. For a one-dimensional problem with integer coordinates of impurities this gives

$$k=k_0+n_i f_1+n_i^2\sum_{r=1}^{\infty}[f_2(r)-2f_1]+\cdots \ . \tag{49}$$

In this expression k is the normalized magnetic susceptibility given by Eq. (11), k_0 is the normalized susceptibility of the ideal chain,

$$f_1=F_1-F_0 \tag{50}$$

and

$$f_2=F_2(r)-F_0 \ , \tag{51}$$

where $F_0=k_0 N$,

$$F_1=-J\frac{d}{dh}\sum_{j=1}^{N}\langle S_j^z\rangle\Bigg|_{\text{one impurity}} \ , \tag{52}$$

$$F_2(r)=-J\frac{d}{dh}\sum_{j=1}^{N}\langle S_j^z\rangle\Bigg|_{\text{two impurities separated by a distance } r} \ . \tag{53}$$

In what follows we neglect terms of order $O(n_i^3)$, i.e., the clusters of more than two impurities. For temperatures and concentrations considered below, the resulting error is less than 1% for the peak values of k.

Expansion (49) is written assuming that coordinates of impurities are not correlated. The length N of the chain is chosen sufficiently large to make size effects insignificant. In particular, while computing susceptibilities F_1 and $F_2(r)$, impurities are positioned well outside the range of boundary-induced oscillations of local magnetization.[18] Note also that for $N\to\infty$, F_0, F_1, $F_2=O(N)$ while f_1, $f_2=O(1)$. The magnetic susceptibility of the chain with two impurities was computed numerically using the expression

$$F_2(r)=-J\frac{d}{dh}\sum_p[1+\exp(\beta E_p)]^{-1} \ , \tag{54}$$

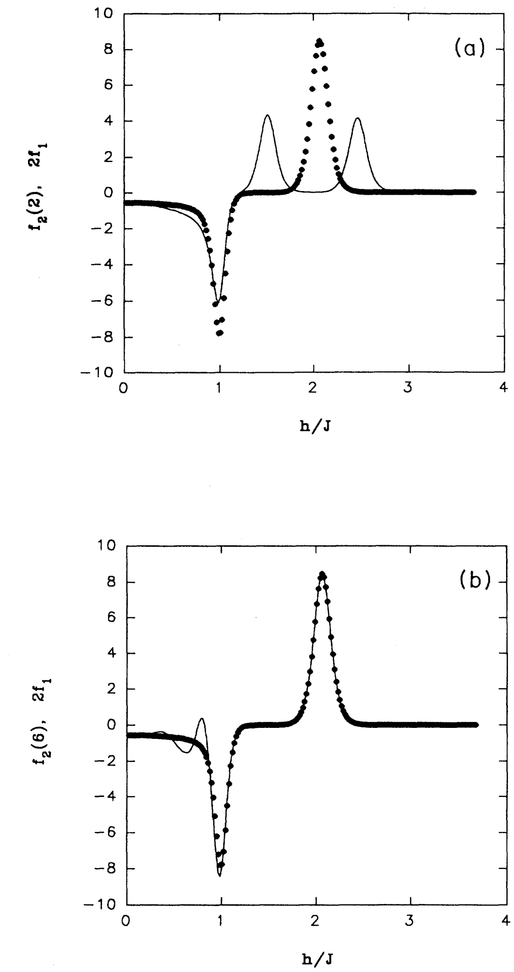


FIG. 4. Magnetic-field dependence of $f_2(r)$ (solid line) and $2f_1$ (circles) for (a) $r=2$ and (b) $r=6$; $J'=2J$, $g'=g/2$, $T=0.04J/k_B$.

where now E_p are the eigenvalues of the Hamiltonian matrix describing the two-impurity problem.

Typical results for f_2 and f_1 are shown in Fig. 4. For $r=2$ the additional splitting of the split-off energy levels associated with individual impurities significantly modifies the high-field ($|h|>J$) susceptibility. In contrast, for $r\geq 5$, in the high-field region $f_2(r)\approx 2f_1$, which assures a rapid convergence of $\Sigma_r[f_2(r)-2f_1]$. For $|h|<J$, $f_2(r)$ may be different from $2f_1$ for higher r [see Fig. 4(b)].

Physically, this difference in $f_2(r)$ field dependence for high and low magnetic fields is related to the temperature-dependent range of impurity-induced Friedel-type oscillations of local magnetization.[18] Indeed, the indirect interaction between impurities is negligible unless the oscillations of $\langle S_j^z\rangle$ produced by the first impurity can reach the second. For $T=0$ at large distances r from the impurity site $j=0$ the oscillations of local magnetization are described by the following expression:[17]

$$\Delta S_r = \frac{[(1-\sigma)\cos(k_F)-2\Delta h]\{\sin[(2r+1)k_F]-\sigma\sin[(2r-1)k_F]\}-2\Delta h\sin(2rk_F)}{2\pi r[1+4\Delta h^2+\sigma^2+4\Delta h(\sigma-1)\cos(k_F)-2\sigma\cos(2k_F)]}, \tag{55}$$

where, $\Delta S_r = \langle S_r^z \rangle - \langle S_r^z \rangle_{\text{ideal}}$ and

$$k_F = \cos^{-1}(-h/J) . \tag{56}$$

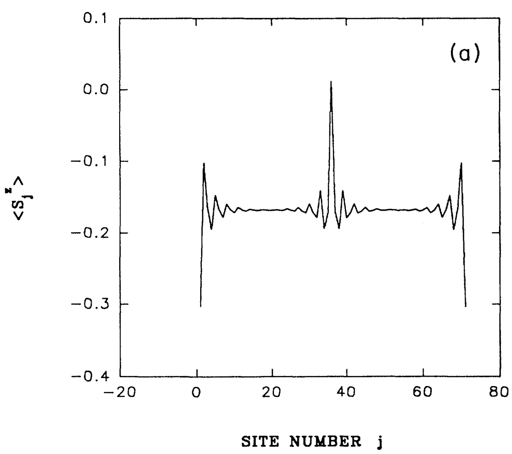
Thus, for $T=0$, $\Delta S_r \propto 1/r$. However, at finite temperatures, the range of the oscillations is significantly reduced[18] (in direct analogy with Friedel oscillations in metals which for $T>0$ decay exponentially with distance from the impurity[21]).

This description is illustrated in Fig. 5 where $\langle S_j^z \rangle$ is computed using a numerical procedure outlined in Ref. 18. The size of the chain in Fig. 5 is kept intentionally small in order to show both boundary and impurity-induced oscillations of local magnetization. For $h=0.5J$ the oscillations of the local magnetization $\langle S_j^z \rangle$ are clearly seen at a distance $r=10$ from the boundary or impurity. This agrees with the fact that for this field $f_2(6)$ is significantly different from $2f_1$. In contrast, as shown in Fig. 5(b), a strong field ($h=2J$) suppresses the oscillations of local magnetization everywhere except in the vicinity of the impurity. Consequently, for this field, indirect impurity-impurity interaction is negligible for $r \geq 5$, so that $f_2(r) \approx 2f_1$ for $h=2J$ and $r \geq 5$.

The magnetic susceptibility of an impure spin-$\frac{1}{2}$ XY chain computed using the first three terms of the virial expansion (49) is shown in Figs. 6–8 for three different types of impurities. For $J'=J/2$ and $g'=3g/2$, the equation $E_s(h)=0$ has no solution for $|h|>J$, and k remains exponentially small in the high-field region (Fig. 6). In this case, the introduction of impurities results in a modification of the $k(h)$ dependence for $|h|<J$.

For $J'=2J$ and $g'=g$ (Fig. 7) or $J'=2J$ and $g'=g/2$ (Fig. 8), high-field peaks associated with split-off energy levels are clearly seen. Equation (43) for the magnetic field corresponding to the center of the peak remains valid, but the shape of the peak is altered by the indirect interaction between impurities [Fig. 8(b)]. In addition to the first-order peaks at $h=\pm h_0$, in Fig. 8 one can also observe secondary peaks corresponding to the pairs of impurities with $r=1$ and 2. The magnitudes of these peaks are of the order of $J\beta n_i^2$. In general, clusters of more than two impurities described by higher-order terms in the virial expansion (49) produce the peaks of the order of $J\beta n_i^q$, $q>2$ on the $k(h)$ dependence. These high-order peaks can be ignored for $J\beta=25$, $n_i=0.05$ corresponding to Figs. 6–8. However, as shown in Fig. 8(b), the quadratic term in the virial expansion cannot be neglected for these values of β and n_i.

Let us now compare these results with an essentially exact solution obtained for spin-$\frac{1}{2}$ XY chains with nonmagnetic impurities.[9–12] A single nonmagnetic impurity breaks the infinite chain into two semiinfinite parts. This effect can be treated formally by putting $\Delta J=-J$ (i.e., by



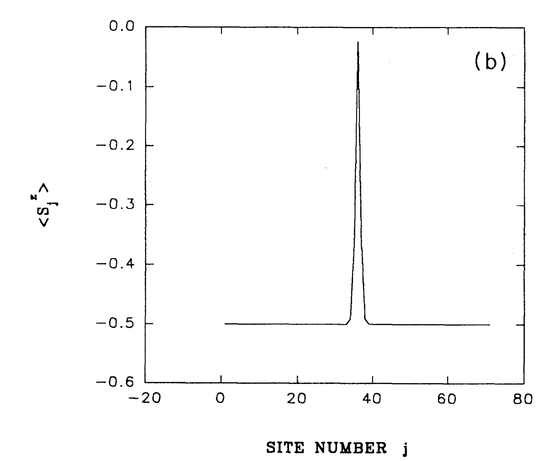


FIG. 5. Local magnetization in the finite-size ($N=70$) spin-$\frac{1}{2}$ XY chain with a single impurity, for (a) $h=0.5J$ and (b) $h=2J$; $J'=2J$, $g'=g/2$, $T=0.04J/k_B$.

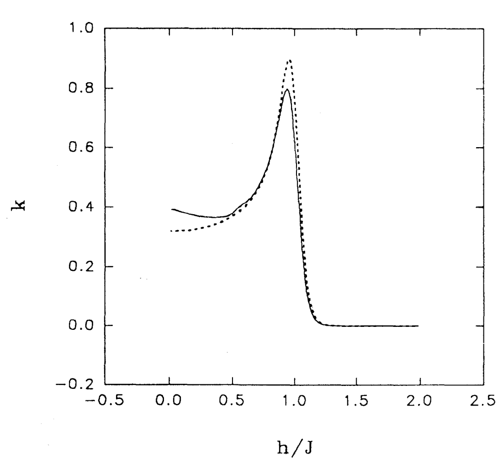


FIG. 6. Normalized magnetic susceptibility of impure (solid line) and ideal (dashed line) spin-$\frac{1}{2}$ XY chains; $J'=J/2$, $g'=3g/2$, $T=0.04J/k_B$, $n_i=0.05$.

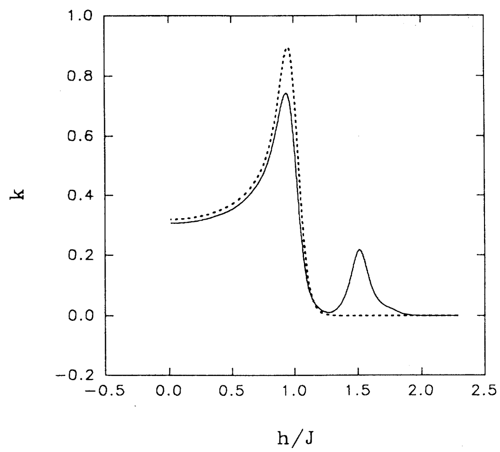


FIG. 7. Same as Fig. 6 for $J'=-2J$, $g'=g$.

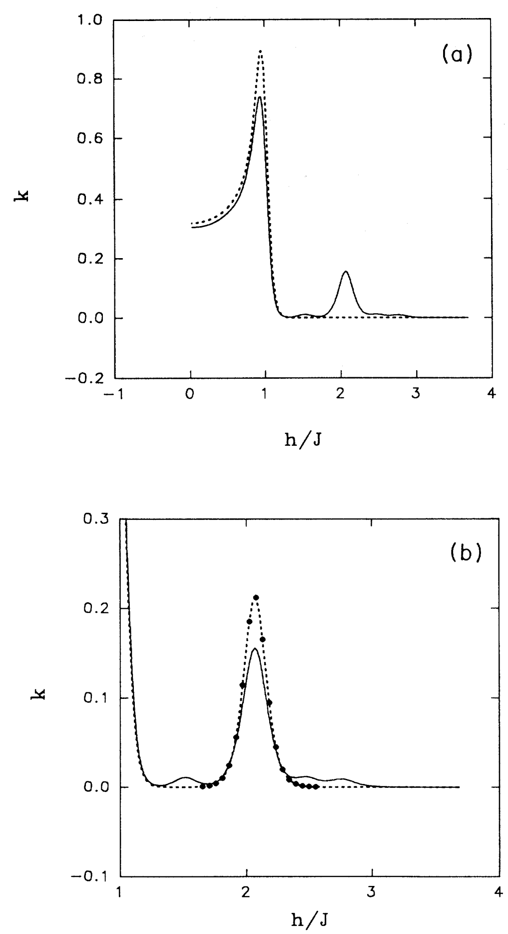


FIG. 8. (a) Same as Fig. 6 for $J'=2J$, $g'=g/2$. (b) The high-field region of the $k(h)$ dependence computed using first-order (dashed line) and second-order (solid line) virial expansions. Circles represent an analytical approximation (44) for the contribution of split-off energy levels; $J'=2J$, $g'=g/2$, $T=0.04J/k_B$, $n_i=0.05$.

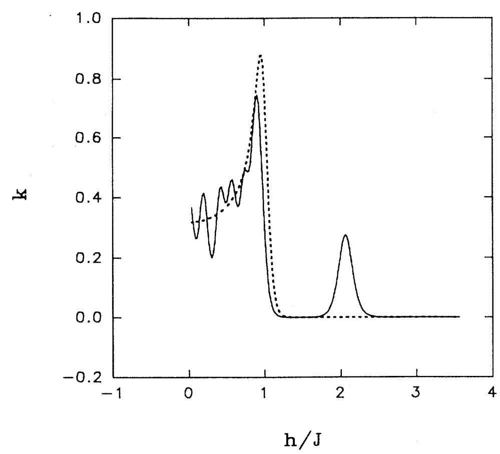


FIG. 9. Normalized magnetic susceptibility of a finite-size ($N=15$) spin-$\frac{1}{2}XY$ chain with free ends and a single impurity (solid line); $J'=2J$, $g'=g/2$, $T=0.04J/k_B$. The dashed line corresponds to the infinite ideal chain.

assigning a new coupling constant $J'=0$). For $J'=0$, according to condition (25) or Fig. 1, there are no split-off states and the magnetic susceptibility remains exponentially small for $h > h_c = J$ [h_c is a singular point for the $k(h)$ dependence of the ideal chain at $T=0$; in Refs. 10–12 the definition of h differs from the one used in this work by a factor of $2/J$ so that $h_c = 2$].

However, when we deal with a finite concentration of nonmagnetic impurities, the chains of the finite size become important and the transition to integration in Eq. (39) for $k_b(h)$ is no longer justified. At sufficiently low temperatures, the $\langle S_j^z \rangle$ vs h dependence is stepwise, corresponding to the peaks of the $k_b(h)$ dependence. The physics is the same as discussed above: a stepwise change in the occupation of discrete energy levels of the finite chains.[9,12] These peaks, which occur for $|h| < h_c$, are easily distinguishable from those which are caused by magnetic impurity-induced split-off states crossing the zero energy level. Indeed, the latter correspond to $|h| = h_0 > h_c$. This is further illustrated in Fig. 9 where we show impurity-indiced peak simultaneously with the finite-size effects.

V. CONCLUSIONS

We have calculated the magnetic susceptibility for an isotropic spin-$\frac{1}{2}$ XY chain with a small number of magnetic impurities. If condition (42) above is satisfied, then at low temperatures formation of split-off states outside of the pseudofermion energy band gives rise to an anomalous $k(h)$ dependence in the strong-field region $|h| > J$. This effect is caused by an abrupt change of occupation numbers of pseudofermions for the split-off states and is clearly distinguishable from the finite-size effects produced by nonmagnetic impurities.[9–12] The latter occur for $|h| < J$. The $k(h)$ dependence of the impure chain is invariant with respect to the sign of the coupling constant J' in the immediate vicinity of the impurity.

As suggested earlier,[10,12,19] impurity related effects may be experimentally observable in compounds like Cs_2CoCl_4,[22–24] $PrCl_3$,[25–27] and $Pr(C_2H_5SO_4)_3 \cdot 9H_2O$ (Refs. 28 and 29) representing isotropic spin-$\frac{1}{2}$ XY chains, provided that impurities with desirable properties are identified. The temperature range of interest is between the temperature of the three-dimensional ordering (which may be affected by the presence of impurities[30]) and J/k_B.

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[1]E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[2]P. Jordan and E. Wigner, Z. Phys. **47**, 631 (1928).
[3]S. Katsura, Phys. Rev. **127**, 1508 (1962).
[4]C. N. Yang and C. P. Yang, Phys. Rev. **147**, 303 (1966).
[5]Th. Niemeijer, Physica (Utrecht) **36**, 377 (1967).
[6]B. McCoy, E. Barouch, and D. Abraham, Phys. Rev. A **4**, 2331 (1971).
[7]J. D. Johnson, B. McCoy, and M. Dresden, Phys. Rev. A **4**, 2314 (1971).
[8]E. Barouch, B. McCoy, and M. Dresden, Phys. Rev. A **2**, 1075 (1970).
[9]F. Matsubara and S. Katsura, Prog. Theor. Phys. **49**, 367 (1973).
[10]M. F. Thorpe and S. Miyazima, Phys. Rev. B **24**, 6686 (1981).
[11]M. F. Thorpe, A. R. McGurn, and S. Miyazima, in *Excitations in Disordered Systems,* edited by M. F. Thorpe (Plenum, New York, 1982), p. 601.
[12]M. Maccio, A. Rettori, and M. G. Pini, Phys. Rev. B **31**, 4187 (1985).
[13]M. Maccio, M. G. Pini, and A. Rettori, J. Magn. Magn. Mater. **54-57**, 863 (1986).
[14]R. Smith, J. Phys. C **3**, 1419 (1970).
[15]T. Oguchi and I. Ono, J. Phys. Soc. Jpn. **26**, 1378 (1969).
[16]G. Baskaran, Phys. Rev. Lett. **40**, 1521 (1978).
[17]G. Gildenblat, J. Magn. Magn. Mater. **43**, 96 (1984).
[18]G. Gildenblat, Phys. Rev. B **30**, 6539 (1984).
[19]G. Gildenblat, Phys. Rev. B **32**, 3006 (1985).
[20]I. M. Lifshitz, Adv. Phys. **13**, 483 (1964).
[21]M. T. Beal-Monod, J. Phys. Chem. Solids **28**, 1261 (1967).
[22]H. A. Algra, L. J. de Jongh, M. W. L. Blote, W. J. Huiskamp, and R. L. Carlin, Physica B **82**, 239 (1976).
[23]L. J. de Jongh, J. Appl. Phys. **49**, 1305 (1978).
[24]K. Hirakawa, H. Yoshizawa, G. Shirane, and H. Shiba, J. Magn. Magn. Mater. **31-34**, 1137 (1983).
[25]P. M. Duxbury, J. Oitmaa, M. N. Barber, A. Van der Bilt, K. O. Joung, and R. L. Carlin, Phys. Rev. B **24**, 5149 (1981).
[26]J. P. Harrison, J. P. Hessler, and D. R. Taylor, Phys. Rev. B **14**, 2979 (1976).
[27]M. Bevis, A. J. Sievers, J. P. Harrison, D. R. Taylor, and D. J. Thouless, Phys. Rev. Lett. **41**, 987 (1978).
[28]M. D'Iorio, R. L. Armstrong, and D. R. Taylor, Phys. Rev. B **27**, 1664 (1983).
[29]E. Goovaertz, H. De Taedt, and D. Schoemaker, Phys. Rev. Lett. **52**, 1649 (1984).
[30]D. R. Taylor and E. Zaremba, Phys. Rev. B **23**, 3384 (1981).