Impurity effect on the singularity of the local magnetization in the spin-$\frac{1}{2}$ XY chain

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A Green's-function method is used to obtain the exact expression for the local susceptibility of the impure spin-$\frac{1}{2}$ XY chain at zero temperature. The presence of the impurity (or boundary) affects the singularity of the magnetic field dependence of the local susceptibility. The corresponding critical exponent changes from $-\frac{1}{2}$ to $+\frac{1}{2}$ at an arbitrary distance from the impurity site. In contrast with the transverse Ising model, the critical exponent is independent of the perturbation strength. This phenomenon is related to the spatial oscillations of the local density of states in the nonideal XY chain. It is also shown that experimental investigation of the field dependence of the finite-temperature macroscopic susceptibility of the one-dimensional XY-like system (such as Cs_2CoCl_4) may reveal the formation of the localized states associated with impurities.

I. INTRODUCTION

The first part of this work deals with the hypothetical "zero-temperature magnetic phase transition" in a spin-$\frac{1}{2}$ XY chain containing a single impurity. It is shown that Green's-function theory in the pseudofermion representation leads to the exact expression for the critical exponent which describes the singularity of the local susceptibility at the arbitrary distance from the impurity. A comparison of this result with similar calculations for the classical and transverse Ising model (TIM) demonstrates the sensitivity of the local critical behavior to the details of the spin-spin interaction in the model Hamiltonian. The experimentally observable effects are discussed in Sec. III. It is shown that formation of the localized states in the diluted XY chain can be (at least in principal) detected by measuring its macroscopic magnetization in the strong-field region at sufficiently low temperature.

II. LOCAL CRITICAL EXPONENT

It is well known that the ground-state magnetization curves of the anisotropic Heisenberg chains have a singular point which corresponds to a certain critical field h_c.[1] Corresponding susceptibilities also exhibit a singular behavior with the critical exponents depending on the details of the exchange interaction.[2,4] Since the local magnetization of the quasi-one-dimensional magnets is strongly affected by the presence of the boundary[5,6] or impurity,[6–9] it is of interest to investigate the details of the critical behavior at the local level (a single impurity does not affect the macroscopic magnetization curve).

Uselac, Jullien, and Pfeuty[10] investigated the impurity-site magnetization within the TIM,[2,3] using the real-space renormalization-group technique as well as the exact results of Bariev[11] and McCoy and Perk[12] for the two-dimensional Ising model applied to the TIM via Suzuki mapping theorem.[13] They have found that the presence of the impurity changes the local critical exponent which becomes dependent on the relative strength of the perturbation.[10]

Sensitivity of the singularities of the local magnetization to the type of the model Hamiltonian of the ideal chain[1] suggests that the same should be true for the local magnetization of the nonideal chain. Indeed, the exact results of the present work show that for the linear isotropic spin-$\frac{1}{2}$ XY model[14] the presence of the boundary or impurity removes the discontinuity of the local susceptibility at an arbitrary distance from the impurity site for $h=h_c$.

Consider Hamiltonian $H=H_0+V$, where H_0 describes the ideal infinite (c-cyclic[14]) XY chain and V introduces the impurity located at site I.

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

$$V=\Delta J\sum_{j=I\pm1}(S_I^xS_j^x+S_I^yS_j^y)\ , \tag{2}$$

where J denotes the exchange coupling constant in the bulk of the chain, ΔJ describes its change in the immediate vicinity of the impurity, and h is the normalized magnetic field.

To facilitate the exact calculation of the local susceptibility $\kappa_j(h)=-d\langle S_j^z\rangle/dh$ we make use of the pseudofermion representation of the impure XY chain.[5–9] After Jordan-Wigner transformation one finds

$$H_0=h\sum_j C_j^\dagger C_j+\frac{J}{2}\sum_j (C_j^\dagger C_{j+1}+\text{H.c.})\ , \tag{3}$$

$$V=\frac{\Delta J}{2}\sum_{j=I\pm1}(C_I^\dagger C_j+\text{H.c.})\ , \tag{4}$$

where the operators

$$C_j^\dagger=(-2)^{j-1}(S_j^x+iS_j^y)\prod_{n=1}^{j-1}S_n^z\ , \tag{5}$$

$$C_j=(-2)^{j-1}(S_j^x-iS_j^y)\prod_{n=1}^{j-1}S_n^z \tag{6}$$

satisfy Pauli anticommutation rules and can be considered as creation-annihilation operators for the pseudofermions.[14]

Since in the pseudofermion representation $S_j^z = C_j^\dagger C_j - \frac{1}{2}$, the ground-state local susceptibility can be written as $\kappa_j = -d\langle C_j^\dagger C_j \rangle / dh$, or

$$\kappa_j(h) = -\frac{d}{dh}\left[\int_{-\infty}^{\mu} \rho_j(h,E)dE\right], \quad (7)$$

where the chemical potential of the pseudofermions $\mu = 0$,[14,15] and $\rho_j(h,E)$ denotes the local density of states (LDS) as a function of the external magnetic field h and energy E.

Introducing double-time Green's function

$$G_{ij}(E) = -i\int_{-\infty}^{\infty} \Theta(t)\exp(iEt/\hbar) \times \langle [C_i(t), C_j^\dagger(0)]_+ \rangle dt , \quad (8)$$

where $\Theta(t)$ denotes the unit step ("inclusion") function, one can present the LDS in the standard form

$$\rho_j(h,E) = -\frac{1}{\pi}\mathrm{Im}G_{ij}(E) . \quad (9)$$

Since the Hamiltonian given by expressions (3) and (4) describes essentially a one-particle problem, the equation of motion for $G_{ij}(E)$ can be brought into the form

$$[\underline{H} - (E + i0)\mathbb{1}]\underline{G} = \mathbb{1} , \quad (10)$$

where $\mathbb{1}$ denotes the unit matrix and the Hamiltonian matrix $\underline{H}$ is a particular case of the matrix $\underline{H}^{\mathrm{HF}}$ introduced in Ref. 6 ($\underline{H} = \underline{H}^{\mathrm{HF}}|_{J_z=0}$). The solution of the last equation can be presented in the form

$$G_{ij} = g_{ij} + \Delta G_{ij} , \quad (11)$$

where g_{ij} is the Green's function of the uniform chain and ΔG_{ij} denotes the perturbation caused by the presence of the impurity. Expressions for g_{jj} (Ref. 16) and ΔG_{jj} (Refs. 8 and 9) can be written in the following form.

$$g_{jj} = \frac{2Q}{J(1-Q^2)} , \quad (12)$$

$$\Delta G_{ij} = \frac{(\sigma-1)(1+\delta_{Ij})[(1-\delta_{Ij})Q^{2|j-I|+1} + Q^{2|j-I|+3}]}{J(1-Q^2)(1-\sigma Q^2)} , \quad (13)$$

where

$$\sigma = 2(1+\Delta J/J)^2 - 1 , \quad (14)$$

$$Q = \begin{cases} f - \mathrm{sgn}(f)(f^2-1)^{1/2}, & |f| > 1 , \\ f - i(1-f^2)^{1/2}, & |f| < 1 , \end{cases} \quad (15)$$

and $f = (E-h)/J$.

After defining $\rho_j^{(0)} = -\pi^{-1}\mathrm{Im}g_{jj}$ and $\Delta\rho_j = -\pi^{-1}\mathrm{Im}\Delta G_{jj}$ so that $\rho_j = \rho_j^{(0)} + \Delta\rho_j$, one finds from expressions (12)—(15)

$$\rho_j^{(0)} = (\pi J \sin K)^{-1}, \quad K = \cos^{-1}[(E-h)/J] , \quad (16)$$

$$\Delta\rho_j = \Theta(J - |E-h|)\frac{(\sigma-1)\cos K\{\cos[(2r_j+1)K] - \sigma\cos[(2r_j-1)K]\}}{\pi J \sin K[1+\sigma^2 - 2\sigma\cos(2K)]} + \Theta(\sigma-1)\frac{\sigma^2-1}{4\sigma^{r_j+1}}[\delta(E-E_+) + \delta(E-E_-)] , \quad (17)$$

where $r_j = |j - I| \neq 0$ and

$$E_\pm = h \pm \frac{J(\sigma+1)}{2\sigma^{1/2}} \quad (18)$$

denote the energy levels of the localized states that exists only for $\sigma > 1$.[8,16] For $j = I$ expression (17) is not valid and should be replaced by

$$\Delta\rho_I = \Theta(J - |E-h|)\frac{(\sigma-1)[\cos(2K) - \sigma]}{\pi J \sin K[1+\sigma^2 - 2\sigma\cos(2K)]} + \Theta(\sigma-1)\frac{\sigma-1}{2\sigma}[\delta(E-E_+) + \delta(E-E_-)] . \quad (19)$$

The last terms in Eqs. (17) and (19) give the LDS associated with the localized states.

An examination of expressions (16)—(19) shows that the LDS of the impure spin-$\frac{1}{2}$ XY chain posesses the property

$$\rho_j(h,E) = \rho_j(0, E-h) . \quad (20)$$

Then by putting $\mu = 0$ and using the variable $E' = E - h$, expression (7) for the local susceptibility can be rewritten as

$$\kappa_j(h) = -\frac{d}{dh}\left[\int_{-\infty}^{-h} \rho_j(0,E')dE'\right] ,$$

or

$$\kappa_j(h) = \rho_j(0, -h) . \quad (21)$$

In the absence of impurity the Hamiltonian (3) corresponds to a single energy band with the energy dispersion law

$$\epsilon_k = h + J\cos K, \quad -\pi < K \le \pi . \quad (22)$$

Then Fermi wave number of the quasiparticles is defined by the condition $\epsilon_{k_F} = \mu = 0$, or[7]

$$k_F = \cos^{-1}(-h/J) . \quad (23)$$

Using this notation and substituting Eqs. (16)—(19) into Eq. (21) one finds that for $|h| < J$

$$\kappa_o(h) = \frac{2(1-h^2/J^2)^{1/2}(\sigma+1)}{\pi J[(1+\sigma)^2 - 4\sigma h^2/J^2]} , \quad (24)$$

$$\kappa_j(h)=(1-h^2/J^2)^{1/2}\frac{(1-\sigma)^2\left\{1+2h^2\left[\frac{\sin(r_jk_F)}{J\sin k_F}\right]^2\right\}+4\sigma-h(1-\sigma)^2\frac{\sin(2r_jk_F)}{J\sin k_F}}{\pi J[(1+\sigma)^2-4\sigma h^2/J^2]}, \tag{25}$$

where in the last equation $r_j=|j-I|\neq 0$, and k_F is given by expression (23).

For $|h|>J$

$$\kappa_j(h)=\Theta(\sigma-1)\frac{(\sigma-1)[1+(1-\delta_{jI})\sigma]}{2(2-\delta_{jI})\sigma^{r_j+1}} \times[\delta(h-h_c')+\delta(h+h_c')], \tag{26}$$

where

$$h_c'=J(\sigma+1)/2\sigma^{1/2}. \tag{27}$$

Expressions (24)—(27) show that unlike the local susceptibility of the ideal chain[1] given by expression (4),

$$\kappa_j^{(0)}(h)=(J^2-h^2)^{-1/2}\Theta(J-|h|), \tag{28}$$

the ground-state local susceptibility of the perturbed chain $\kappa_j(h)$ remains continuous as a function of h for $|h|=J$ ($\sin k_F=0$) at an arbitrary distance from the impurity. (For a uniform chain the macroscopic susceptibility κ_M per unit spin coincides with the local susceptibility.) The second critical point $|h|=h_c'>J$ on the $\kappa_j(h)$ dependence exists only for $\sigma>1$. Physically, condition $\sigma>1$ corresponds to formation of two localized states with the energy levels $E_\pm=h\pm h_c'$ lying outside the pseudofermion energy band.[8] Then the second critical point on the $\kappa_j(h)$ dependence appears when the Fermi level of the quasiparticles coincides with the energy level of the localized state.

Qualitatively, the strong change of the critical exponent (from $-\frac{1}{2}$ to $\frac{1}{2}$) at an arbitrary distance from the impurity can be understood in terms of the Friedel-type oscillations of the local magnetization in the nonideal antiferromagnetic chains.[5-9] The localized perturbation (4) results in the oscillation of the pseudofermion density as a function of a distance from the impurity. This oscillation decays with the amplitude $\propto r^{-d}$, where d is the dimensionality of the system. Corresponding perturbation of the LDS decays as r^{1-d} and for $d=1$ does not vanish for $r\to\infty$, which is a specific feature of the one-dimensional problem. One notices also that since $\kappa_j(h)=0$ for $|h|=J$, the differentiation with respect to h and transition to the thermodynamic limit are not interchangeable operations for $|h|=J$. Indeed, the macroscopic susceptibility

$$\kappa_M=-\frac{d}{dh}\lim_{N\to\infty}\left[\frac{1}{N}\sum_{j=1}^{N}\langle S_j^z\rangle\right],$$

which is unaffected by the presence of a single impurity, for $|h|=J$ cannot be written as $\lim_{N\to\infty}[(1/N)\sum_{j=1}^N\kappa_j]=0$.

III. MACROSCOPIC SUSCEPTIBILITY OF THE IMPURE *XY* CHAIN IN THE PRESENCE OF LOCALIZED STATES

In the remaining part of this work we examine the role of the localized states which are formed if $\sigma>1$. At zero temperature they are responsible for the δ-type singularity on the microscopic level. In order to deal with experimentally observable effects, consider temperature $T=1/k_B\beta>0$ (k_B is the Boltzmann constant) and small but finite concentration of the impurity n_0 per unit site of the chain. As a first approximation for $n_0\ll 1$ one can neglect the interference effects on the oscillations of the local magnetization in the impure antiferromagnetic chain. Then the perturbation of the macroscopic magnetization (per unit site) becomes

$$\Delta S\approx n_0\sum_{j=-\infty}^{\infty}\Delta S_j, \tag{29}$$

where ΔS_j is a perturbation of the local magnetization at site j caused by a single impurity. Since the quasiparticles are described by Fermi statistics with zero chemical potential, one can write

$$\Delta S_j=\Delta\langle C_j^\dagger C_j\rangle=\int_{-\infty}^{\infty}\frac{\Delta\rho_j}{1+\exp(\beta E)}dE. \tag{30}$$

Consider next the part of the magnetization curve near the point $h=h_c'>h_c=J$. As has been shown previously[8] at zero temperature the in-band pseudofermions do not contribute to ΔS_j for $|h|>h_c$. For $T>0$ their contribution decreases exponentially with $|h|-h_c$. Then assuming that the perturbation is sufficiently strong (or the temperature is low enough) so that $T\ll h_c'-h_c$, one can neglect the contribution of the in-band pseudofermions for $|h|\approx h_c'$. Then

$$\Delta S\approx n_0\sum_{j=-\infty}^{\infty}\left[\int_h^{\infty}+\int_{-\infty}^{-h}\right]\frac{\Delta\rho_j(E)}{1+\exp(\beta E)}dE, \tag{31}$$

where only the contribution from the localized states is accounted for. Substituting Eqs. (17) and (19) for $\Delta\rho_j$ one finds

$$\Delta S\approx\Theta(\sigma-1)n_0\{[1+\exp(\beta E_-)]^{-1}+[1+\exp(\beta E_+)]^{-1}\}. \tag{32}$$

The corresponding equation for the macroscopic susceptibility κ_M near $|h|=\pm h_c'$ can be written as

$$\kappa_M\approx\frac{\Theta(\sigma-1)\beta n_0/2}{1+\cosh[\beta(h_c'-|h|)]}. \tag{33}$$

The last equation predicts an experimentally observable peak on the $\kappa_M(h)$ dependence of the impure magnetic chain. For a diluted chain its amplitude is proportional to the impurity concentration and is inversely proportional to the temperature, which may be useful for the experimental investigation of the effect.

In its present form, this analysis is limited to the case of the spin-$\frac{1}{2}$ XY chain (experimentally represented by Cs_2CoCl_4).[17–20] However, qualitatively it is clear that in the more general case of the impure Heisenberg antiferromagnet[6] the formation of the localized states corresponds to the peaks of susceptibility for $h > h_c$.

These peaks are well resolved only at sufficiently low temperatures ($T \ll J$) so that the best conditions for their observation are expected just above the temperature of the three-dimensional ordering T_c' (or just above the temperature of the spin-Peierls phase transition).[21] Since for the spin chains $T_c' \ll J$, there is a sufficient temperature range $T_c' < T \ll J$ where the effect is expected to exist.

Corresponding magnetic field can be estimated by putting $h = g\mu_B B$, where g denotes the Lande factor, μ_B is the Bohr magneton and B is the external magnetic field (in usual units). Then $B_c = 1.488(J/k_B)g^{-1}$ T and $B_c' = B_c(\sigma+1)/2\sigma^{1/2}$. Here B_c and B_c' are the values of B corresponding to h_c and h_c'. For Cs_2CoCl_4 susceptibility measurements[20] give $J/k_B = 1.54$ K in a reasonable agreement with the heat-capacity data showing $J/k_B = 1.47$ K.[22] Accordingly $B_c \approx 2.2g^{-1}$ T, while the new critical field B_c' has the same order of magnitude but is a function of σ (i.e., of $\Delta J/J$) and thus depends on the particular type of the impurity introduced into the magnetic chain.

We note in conclusion that macroscopic magnetization of the spin-$\frac{1}{2}$ XY chain with randomly distributed nonmagnetic impurities was calculated numerically in Ref. 23. In the notations of the present work the nonmagnetic impurity corresponds to a particular value of $\Delta J = -J$. In this case $\sigma < 1$ and the localized states with the energy levels outside the pseudofermion energy band do not exist. The "conspicuous" steplike features of the macroscopic magnetization curve described in Ref. 23 appear only for $|h| < h_c = J$ and sufficiently large impurity concentration. This manifestation of the one-dimensional nature of the problem does not affect the results of the present work dealing with the case of a single impurity or with a slightly diluted chain ($n_0 \ll 1$) and $|h| > h_c$. In fact numerical calculations[24] based on the procedure described in Ref. 6 show that for $|h| > h_c$ and regularly distributed impurities there are only two steps on the macroscopic magnetization curve located precisely at $|h| = h_c$ as predicted by the approximate theory developed in the present work.

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