

THERMODYNAMICS OF A DILUTE XX CHAIN IN A FIELD

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Gapless phases in ground states of low-dimensional quantum spin systems are rather ubiquitous. Their peculiarity is a remarkable sensitivity to external perturbations due to permanent criticality of such phases manifested by a slow (power-low) decay of pair correlations and the divergence of the corresponding susceptibility. A strong influence of various defects on the properties of the system in such a phase can then be expected. Here, we consider the influence of vacancies on the thermodynamics of the simplest quantum model with a gapless phase, the isotropic spin-$1/2$ XX chain. The existence of the exact solution of this model gives a unique opportunity to describe in detail the dramatic effect of dilution on the gapless phase — the appearance of an infinite series of quantum phase transitions resulting from level crossing under the variation of a longitudinal magnetic field. We calculate the jumps in the field dependences of the ground-state longitudinal magnetization, susceptibility, entropy, and specific heat appearing at these transitions and show that they result in a highly nonlinear temperature dependence of these parameters at low T. Also, the effect of enhancement of the magnetization and longitudinal correlations in the dilute chain is established. The changes of the pair spin correlators under dilution are also analyzed. The universality of the mechanism of the quantum transition generation suggests that similar effects of dilution can also be expected in gapless phases of other low-dimensional quantum spin systems.

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1. INTRODUCTION

The discovery of the equivalence of XY spin chains with spin $1/2$ to free fermions [1] was a breakthrough in the studies of quantum phase transitions. Such a transition takes place in the XY chain at $T = 0$ under a variation of the transverse field H when its modulus becomes equal to the modulus of the average nearest-neighbor exchange $J = (J_x + J_y)/2$, $J_x J_y > 0$ [1–5]. Usually, it features the ordinary scaling behavior with the order parameter being the magnetization component with the largest exchange, i. e., M_x if $|J_x| > |J_y|$. Then M_x vanishes at $|H| > |J|$ and only M_z along the field exists.

Apparently, this scenario does not hold in the special case of an isotropic (XX) chain with $J_x = J_y = J$, where rotational symmetry and low dimension makes $M_x = M_y = 0$ at all H [1–5]. Nevertheless, the XX chain also experiences a ground-state quantum transition at $|H| = |J|$ from a saturated phase with $M_z = 1/2\,\mathrm{sign}(H)$ into the so-called quasi-long-range-ordered (QLRO) phase at $|H| < |J|$ characterized by the vanishing of the gap between the ground and excited states in the energy spectrum of free fermions [5–7] and a power-law decay of spin correlators [8–10]. Thus, the XX chain is always in a critical state at all $|H| < |J|$, while the anisotropic XY chain is gapless only at the transition point.

This specificity of the isotropic chain can be easily understood by noting that in the fermionic language, QLRO is a “metal” phase, while the saturated one at $|H| > |J|$ is an “insulator”. Indeed, the one-fermion spectrum of this chain is [1–4]

$$\varepsilon(q) = J(\cos \pi q - h), \quad h = H/J, \tag{1}$$

where q is a continuous wave number in the interval $0 \le q \le 1$ for an infinite chain. Here, the number of fermions is not conserved, and therefore both the chemical potential μ and the Fermi energy ε_F are zero, $\mu = \varepsilon_F = 0$. At $|h| < 1$, the Fermi energy lies within the “conduction band” and the spectrum is gapless. Under a variation of h, the state of this “metal” changes continuously with changes in the Fermi wave number

$$q_F(h) = \frac{1}{\pi} \arccos h, \tag{2}$$

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whence $q_F(0) = 1/2$, and we therefore have a half-filled band, while $q_F(1) = 0$ and the band is fully filled or empty depending on the sign of J.

A further insight into the nature of this permanent criticality in the QLRO phase stems from the studies of ground states of finite XX chains [6,7]. In finite chains, the critical state splits into a series of quantum transitions due to discrete (rational) values of q in the same dispersion law (1). The transitions occur when $q_F(h)$ becomes equal to one of the allowed rational q. At these points, the ground state is changed by adding or deleting a fermion with the wave number nearest to $q_F(h)$. Right at the transition point, the ground state is doubly degenerate because both states with and without a fermion with $\varepsilon_F = 0$ have the same energy. Thus, the level crossing in the energy spectrum constitutes the mechanism of quantum phase transitions in the XX chain [6, 7] and the QLRO phase in the infinite-chain limit is a consequence of level crossing at every q.

In real crystals with noninteracting XX chains, the detection of the QLRO phase at a low temperature T can be rather complicated because the only pronounced feature of macroscopic chains is the power-law decay of correlators [8–10]. Yet the manifestations of this phase can be more visual in dilute crystals where nonmagnetic ions substitute magnetic ones in the chains. Then discrete level-crossing transitions in finite magnetic segments can be seen in usual macroscopic experiments at low T as anomalies in field dependences of the magnetization, specific heat, and so on. Hence, there should be some quantitative predictions regarding these anomalies to recognize the presence of XX chains in real crystals. Here, we present the study of macroscopic thermodynamics of dilute XX chains showing spectacular features of the QLRO phase at low T.

2. THERMODYNAMICS OF THE QLRO PHASE

We first recall the fermionization procedure for a finite XX chain with spin 1/2 [1, 6, 7]. We start with the Hamiltonian for N spins with free boundaries,

$$\frac{\mathcal{H}_N}{J} = \frac{1}{4}\sum_{n=1}^{N-1}\left(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y\right) - \frac{h}{2}\sum_{n=1}^{N}\sigma_n^z,$$

where σ_n^α, $\alpha = x, y, z$, are the Pauli matrices defining operators of local magnetic moments $s_n^\alpha = \sigma_n^\alpha/2$.

Introducing the fermionic creation and annihilation operators through the Jordan–Wigner transformation

$$a_n^+ = \sigma_n^+\prod_{i=1}^{n-1}\left(-\sigma_i^z\right), \quad a_n = \sigma_n^-\prod_{i=1}^{n-1}\left(-\sigma_i^z\right), \qquad \sigma_n^\pm = \frac{1}{2}\left(\sigma_n^x \pm i\sigma_n^y\right) \quad (3)$$

and using the relation

$$\sigma_n^z = 2\sigma_n^+\sigma_n^- - 1 = 2a_n^+a_n^- - 1, \quad (4)$$

we obtain

$$\frac{\mathcal{H}_N}{J} = \frac{1}{2}\sum_{n=1}^{N-1}\left(a_n^+a_{n+1} + a_{n+1}^+a_n\right) - h\sum_{n=1}^{N}a_n^+a_n + \frac{Nh}{2}.$$

This Hamiltonian is diagonalized via the transformation to new fermionic operators b_k:

$$a_n = \sqrt{\frac{2}{N+1}}\sum_{k=1}^{N} b_k \sin\frac{\pi k n}{N+1}. \quad (5)$$

In terms of b_k and b_k^+, we have the Hamiltonian of free fermions,

$$\frac{\mathcal{H}_N}{J} = \sum_{k=1}^{N}\left(\cos\frac{\pi k}{N+1} - h\right) b_k^+ b_k + \frac{Nh}{2}.$$

With this simple expression, we can easily obtain the thermodynamic potential of a dilute XX chain as the sum of independent contributions from finite fragments appearing under dilution. Therefore, the average potential per site in the case of random dilution is

$$F = -T\sum_{l=1}^{\infty}\frac{N_l}{N}\ln\operatorname{Tr}\exp\left(-\frac{\mathcal{H}_l}{T}\right),$$

where N_l is the average number of magnetic clusters with l sites. If magnetic ions appear independently on all sites with a probability p, then, for large N [11],

$$N_l \approx N(1-p)^2 p^l$$

and hence in the limit as $N \to \infty$,

$$F = -T\sum_{l=1}^{\infty}(1-p)^2 p^l \ln\operatorname{Tr}\exp(-\beta\mathcal{H}_l) = -T(1-p)^2\sum_{l=1}^{\infty}p^l\sum_{k=1}^{l}\ln(1 + e^{2u_{k,l}}) + \frac{phJ}{2}, \quad (6)$$

where

$$u_{k,l} = \frac{J}{2T}\left[h - \cos\left(\frac{\pi k}{l+1}\right)\right]. \quad (7)$$

The thermodynamic potential in Eq. (6) allows finding macroscopic observables of a dilute XX chain averaged over disorder. The average magnetization along the field is

$$M = \frac{1}{2}\left\langle\langle\sigma^z\rangle_T\right\rangle_p = -\frac{1}{J}\frac{\partial F}{\partial h} =$$

$$= (1-p)^2\sum_{l=1}^{\infty}p^l\sum_{k=1}^{l}\left(1+e^{-2u_{k,l}}\right)^{-1} - \frac{p}{2} =$$

$$= \frac{(1-p)^2}{2}\sum_{l=1}^{\infty}p^l\sum_{k=1}^{l}\tanh u_{k,l}, \quad (8)$$

where $\left\langle\langle\ldots\rangle_T\right\rangle_p$ is a shorthand notation for the Gibbs average followed by the average over possible realizations of disorder.

Similarly, we obtain the expressions for the longitudinal magnetic susceptibility

$$\chi_{zz} \equiv \chi = \frac{\partial M}{J\,\partial h}, \qquad \chi = \frac{(1-p)^2}{4T}\sum_{l=1}^{\infty}p^l\sum_{k=1}^{l}\cosh^{-2}(u_{k,l}), \quad (9)$$

entropy S, and specific heat C:

$$S = -\frac{\partial F}{\partial T} = (1-p)^2\sum_{l=1}^{\infty}p^l \times \sum_{k=1}^{l}\left[\ln(2\cosh u_{k,l}) - u_{k,l}\tanh u_{k,l}\right], \quad (10)$$

$$C = T\frac{\partial S}{\partial T} = \frac{(1-p)^2}{2}\sum_{l=1}^{\infty}p^l\sum_{k=1}^{l}u_{k,l}^2\cosh^{-2}(u_{k,l}). \quad (11)$$

As $p \to 1$, Eqs. (6), (8)–(11) become the corresponding expressions for a pure infinite chain. To see this, we note that in this limit, the major contribution to the sum over k transforms into an integral as

$$(1-p)^2\sum_{l=100}^{\infty}p^l\sum_{k=1}^{l}X\left(\pi\frac{k}{l+1}\right) \to (1-p)^2 \times \sum_{l=100}^{\infty}p^l(l+1)\int_0^{\pi}\frac{d\theta}{\pi}X(\theta) \to \int_0^{\pi}\frac{d\theta}{\pi}X(\theta).$$

For example, at $p = 1$, we obtain the known expression for the magnetization of an infinite XX chain [2–4]

$$M = \int_0^{\pi}\frac{d\theta}{2\pi}\tanh\frac{J}{2T}(h-\cos\theta). \quad (12)$$

The above expressions for thermodynamic quantities can be obtained only approximately at $T > 0$ because only finite sums can be calculated. Because the lth term of series (8)–(11) is of the order of lp^l, the finite sums with $l < L$ give approximate values with a relative error ε that we can roughly estimate as

$$\varepsilon \approx \sum_{l=L+1}^{\infty}lp^l \Big/ \sum_{l=1}^{\infty}lp^l = p^L\left[L(1-p)+1\right]. \quad (13)$$

Hence, to achieve, e.g., $\varepsilon = 0.05$ for $p = 0.25$, 0.5, 0.75, we should respectively take $L = 3$, 7, 16 terms in Eqs. (8)–(11). The results of such calculations with $\varepsilon < 0.02$ ($L = 20$) are shown in Fig. 1. Here, the field dependences of M, χ, S, and C at $T = 0.1J$ feature somewhat smeared anomalies reminiscent of ground-state quantum transitions in finite magnetic clusters.

Actually, at $T = 0$, the dilute XX chain has an infinite set of these anomalies at all fields for which $q_F(h)$ is rational. We consider the field dependence of M at $T = 0$. From (6), we then obtain

$$2M = (1-p)^2\sum_{l=1}^{\infty}p^l\sum_{k=1}^{l}\operatorname{sign}\left[k - q_F(h)(l+1)\right], \qquad \operatorname{sign}(0) = 0.$$

Summation over k then gives

$$2M = (1-p)^2\sum_{l=1}^{\infty}p^l\left\{l - 2m_l^F + \delta_{m_l^F,\,q_F(h)(l+1)}\right\}, \quad (14)$$

where $m_l^F \equiv [q_F(l+1)]$ is the integer part of $q_F(l+1)$ and the Kronecker delta is 1 when $q_F(h)(l+1)$ is integer and 0 otherwise.

Apparently, M in (14) has jumps at every rational $q_F(h)$. This means that there are infinitely many jumps in every field interval. However, most of them are tiny and unobservable in real experiments. The approximate M with largest jumps at $h < 1$ is shown in Fig. 2 for $p = 0.25$, 0.5, 0.75 as compared with $p = 1$. We note that according to (12), at $T = 0$, $p = 1$, and $h < 1$, we have the known result [2–4]

$$M = \frac{1}{2} - q_F(h) \quad (15)$$

while the data for $p < 1$ are obtained from (14) by reducing the sum to $l < 20$ terms. As Fig. 2 shows, a noticeable feature of the dilute chain magnetization is that it can be larger than that of a pure chain at the same field. Qualitatively, this effect is a consequence of the freedom of finite magnetic fragments to orient their magnetizations along the field, which can overcome the diminishing of the overall M due to dilution.

We can obtain simple expressions for some largest M jumps near some rational $q_F(h)$. For irrational

$$q_F(h) = \frac{1}{k} + \delta, \quad \delta \to 0,$$

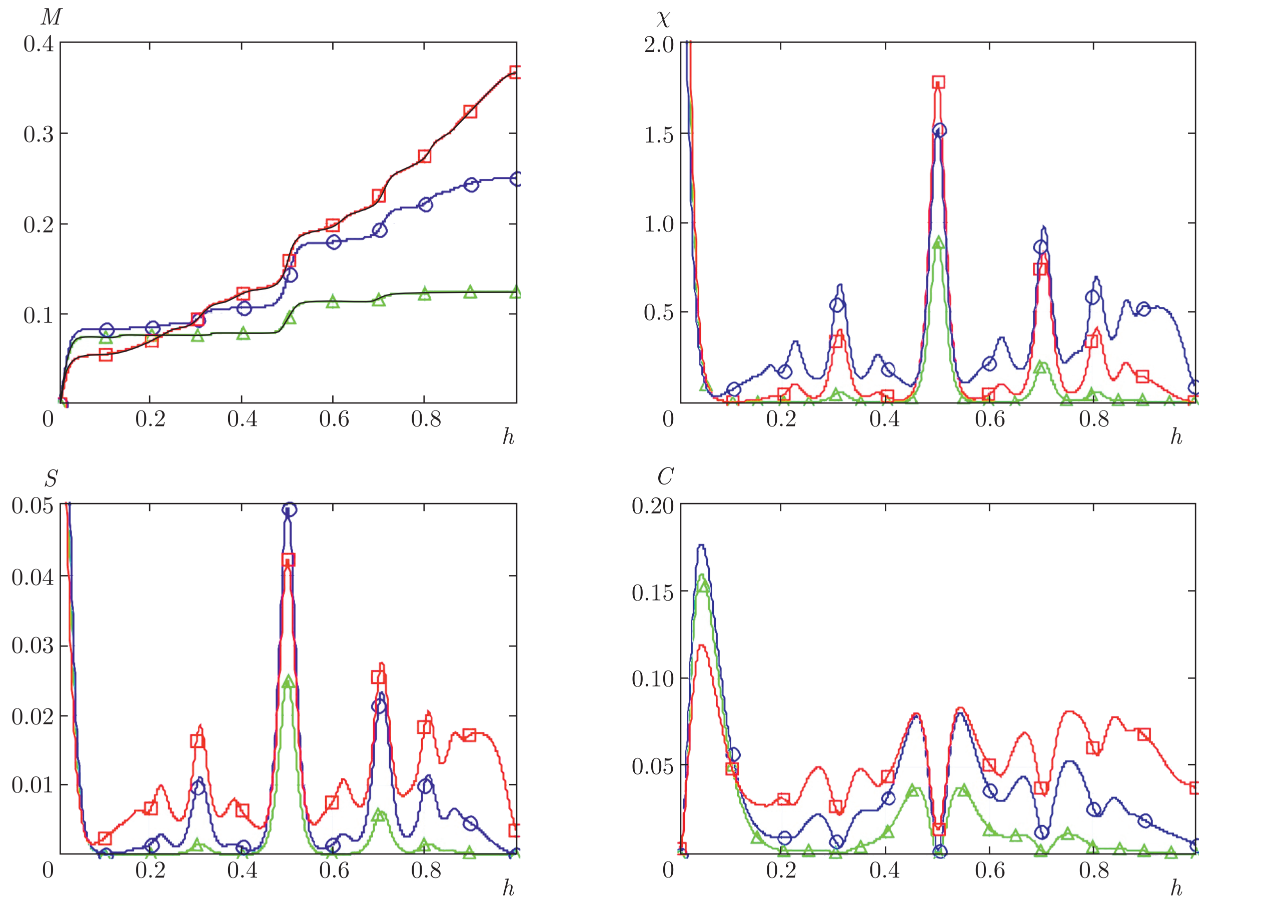

Fig. 1. Field dependences of the magnetization M, the susceptibility along the field χ, the entropy S, and the specific heat C of a dilute XX chain at $T = 0.1$J for $p = 0.25$ ($\triangle$), 0.5 ($\circ$), and 0.75 ($\square$). The sums in Eqs. (8)–(11) are limited by $L = 20$ terms

i. e., for the fields

$$h \approx \cos\frac{\pi}{k} \equiv h_k, \quad k = 2, 3, 4, 5, 6, \ldots,$$

$$h_k = 0, \frac{1}{2}, \frac{\sqrt{2}}{2}, \frac{\sqrt{5}+1}{4}, \frac{\sqrt{3}}{2}, \ldots$$

we use Eq. (14) with $l > k-2 \geq 1$, $l+1 = km+n$ with integer $m \geq 1$ and $n \geq 0$ to obtain

$$2M \approx (1-p)^2 \left\{ \sum_{l=1}^{k-2} p^l l + \sum_{m=1}^{\infty} p^{km-1} \times \right.$$
$$\left. \times \sum_{n=0}^{k-1} p^n \left[m(k-2)+n-1+\delta_{n,0}\left(1+\operatorname{sign}(h-h_k)\right)\right] \right\}.$$

Performing the summations, near h_k, we obtain the expression (also valid for $k = 2$)

$$2M \approx p\frac{1-p^{k-2}}{1-p^k} + \operatorname{sign}(h-h_k)\nu_k(p), \qquad (16)$$

where $\nu_k(p)$ is the number of magnetic clusters (per site) whose site numbers are integer multiples of k,

$$\nu_k(p) = p^{k-1}\frac{(1-p)^2}{1-p^k}. \qquad (17)$$

As $p \to 1$, Eq. (16) gives the magnetization of the pure chain at h_k because $M = (k-2)/2k$ in conformity with Eq. (15).

For lowest k values, we have

$$k = 2, \quad h_2 = 0, \quad 2M \approx \operatorname{sign}(h)p\frac{1-p}{1+p},$$

$$k = 3, \quad h_3 = \frac{1}{2},$$

$$2M \approx \frac{p}{1+p+p^2}\left[1 + \operatorname{sign}\left(h - \frac{1}{2}\right)p(1-p)\right],$$

$$k = 4, \quad h_4 = \frac{\sqrt{2}}{2},$$

$$2M \approx \frac{p}{1+p^2}\left[1 + \operatorname{sign}\left(h - \frac{\sqrt{2}}{2}\right)p^2\frac{1-p}{1+p}\right].$$

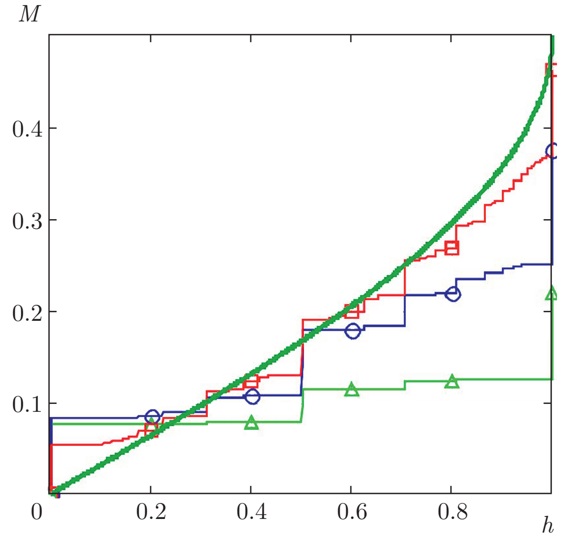

Fig. 2. Field dependences of the magnetization of a dilute XX chain at $T = 0$ for $p = 0.25$ ($\triangle$), 0.5 ($\circ$), and 0.75 ($\square$), and 1 (thick solid line). The sum in Eq. (14) is limited by $L = 20$ terms

As $T \to 0$, S, χ, and C tend to zero for irrational values of $g_F(h)$. However, when the field tends to a rational value $q_F(h)$ linearly in $T \to 0$, i. e.,

$$h = \cos\left(\pi \frac{m}{k}\right) + \frac{2\alpha T}{J},$$

with some constant α and an irreducible fraction m/k, then S, $T\chi$, and C stay finite:

$$S = \nu_k(p)\left[\ln(2\cosh\alpha) - \alpha\tanh\alpha\right], \quad T\chi = \frac{\nu_k(p)}{4\cosh^2\alpha},$$

$$C = \nu_k(p)\frac{\alpha^2}{\cosh^2\alpha}.$$

Here, $\nu_k(p)$ is given by Eq. (17).

Thus, the dependences of thermodynamic quantities on h and T are represented by surfaces with a number of wrinkles at low T as Fig. 3 shows.

3. CORRELATION FUNCTIONS

The static paired correlation functions of spins define the intensity of magnetic diffraction of neutrons on magnetic materials, and therefore knowing them is important for experimentally identifying a model that gives the correct description of a real magnet. We consider the average two-point correlators

$$C_r^\alpha = \frac{1}{4}\left\langle\left\langle\sigma_n^\alpha\sigma_{n+r}^\alpha\right\rangle_T\right\rangle_p, \quad \alpha = x, y, z.$$

For these correlators, there are two possibilities to be nonzero in the dilute chain: either sites n and $n+r$ both belong to the same magnetic cluster or they belong to different clusters. Hence, for $r \geq 3$, we have

$$\begin{aligned} C_r^\alpha &= \frac{1}{4}\sum_{l=r+1}^{\infty} w_l \sum_{n=1}^{l-r}\left\langle\sigma_n^\alpha\sigma_{n+r}^\alpha\right\rangle_{T,l} + \\ &+ \frac{1}{4}\sum_{n=1}^{r-2}\sum_{l=n}^{\infty} w_l\left\langle\sigma_n^\alpha\right\rangle_{T,l}\sum_{n'=1}^{r-1-n}\sum_{l'=n'}^{\infty} w_{l'}\left\langle\sigma_{n'}^\alpha\right\rangle_{T,l'} = \\ &= \sum_{l=r+1}^{\infty} w_l \sum_{n=1}^{l-r} C_{l,n,r}^\alpha + \delta_{\alpha,z}\sum_{n=1}^{r-2}\sum_{l=n}^{\infty} w_l M_{l,n} \times \\ &\times \sum_{n'=1}^{r-1-n}\sum_{l'=n'}^{\infty} w_{l'} M_{l',n'}, \end{aligned} \quad (18)$$

$$w_l = (1-p)^2 p^l, \quad M_{l,n} = \frac{1}{2}\left\langle\sigma_n^z\right\rangle_{T,l},$$

$$C_{l,n,r}^\alpha = \frac{1}{4}\left\langle\sigma_n^\alpha\sigma_{n+r}^\alpha\right\rangle_{T,l}.$$

Here, $\langle\ldots\rangle_{T,l}$ is the Gibbs average for a pure magnetic cluster with l sites and w_l is the probability that a given site belongs to such a cluster. We note that due to the symmetry between two cluster edges,

$$M_{l,n} = M_{l,l-n+1}, \quad C_{l,n,r}^\alpha = C_{l,l-n-r+1,r}^\alpha.$$

For $r = 2$, there is just one empty site between different clusters, whence

$$\begin{aligned} C_2^\alpha &= \frac{1}{4}\left\langle\left\langle\sigma_i^\alpha\sigma_{i+2}^\alpha\right\rangle_T\right\rangle_p = \sum_{l=3}^{\infty} w_l \times \\ &\times \sum_{n=1}^{l-2} C_{l,n,2}^\alpha + \delta_{\alpha,z}(1-p)^{-1}\left(\sum_{l=1}^{\infty} w_l M_{l,1}\right)^2 \end{aligned} \quad (19)$$

and for $r = 1$, there is no contribution from different clusters,

$$C_1^\alpha = \frac{1}{4}\left\langle\left\langle\sigma_i^\alpha\sigma_{i+1}^\alpha\right\rangle_T\right\rangle_p = \sum_{l=2}^{\infty} w_l \sum_{n=1}^{l-1} C_{l,n,1}^\alpha. \quad (20)$$

For the local magnetizations $M_{l,n}$ and correlators $C_{l,n,r}^\alpha$ in finite clusters, we obtain

$$\begin{aligned} M_{l,n} &= \frac{1}{2}\left\langle\sigma_n^z\right\rangle_{T,l} = \left\langle a_n^+ a_n\right\rangle_{T,l} - \frac{1}{2} = \\ &= \frac{1}{l+1}\sum_{k=1}^{l}\tanh u_{k,l}\sin^2\left(\pi\frac{kn}{l+1}\right), \end{aligned} \quad (21)$$

$$C_{l,n,r}^z = \frac{1}{4}\left\langle\sigma_n^z\sigma_{n+r}^z\right\rangle_{T,l} = M_{l,n}M_{l,n+r} - D_{l,n,r}^2, \quad r \neq 0, \quad (22)$$

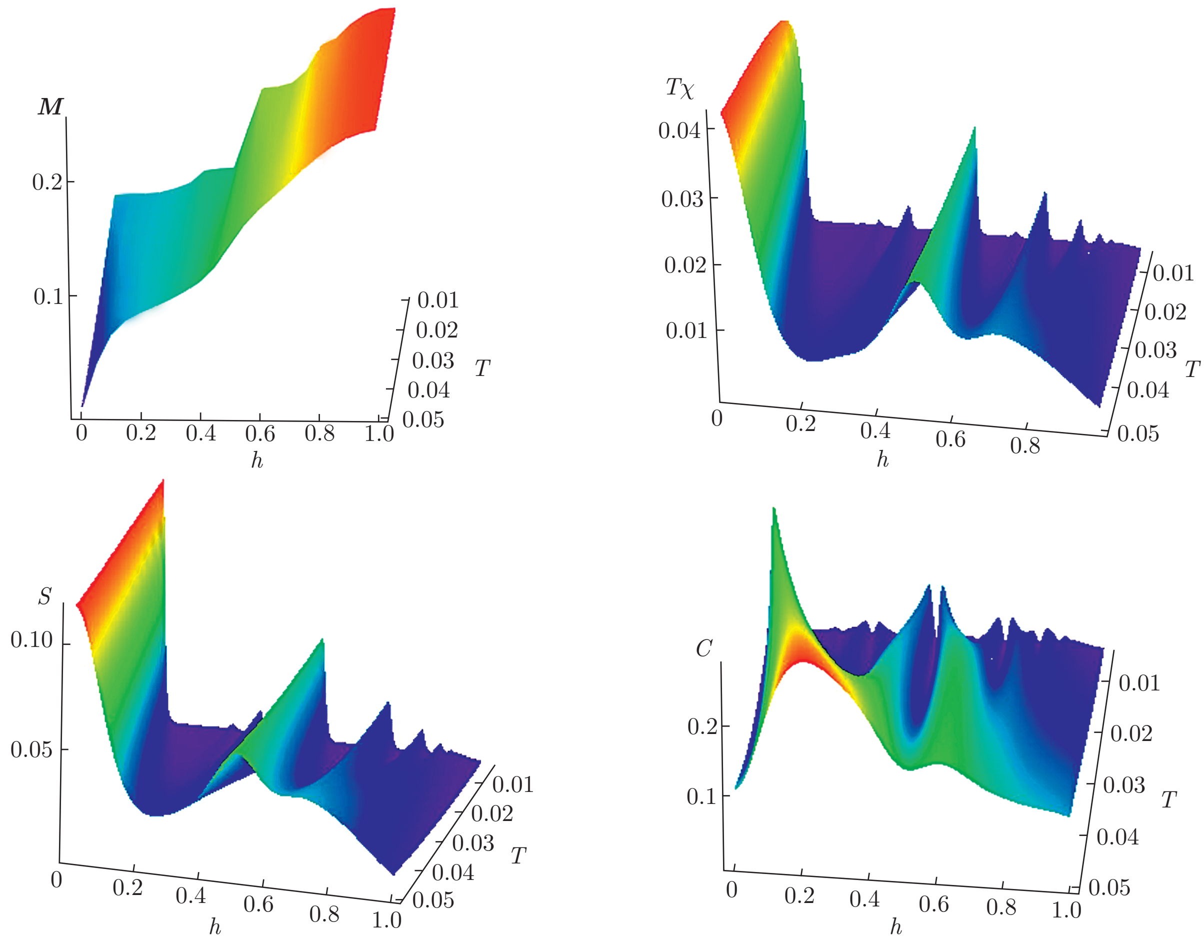

Fig. 3. The dependences of thermodynamic quantities on $h < 1$ and $T \ll J$ for the chain with $p = 0.5$. The sums in Eqs. (8)–(11) are limited by $L = 20$ terms

$$D_{l,n,r} \equiv \left\langle a_n^+ a_{n+r} \right\rangle_{T,l} = \frac{1}{l+1} \sum_{k=1}^{l} \tanh u_{k,l} \sin \frac{\pi k n}{l+1} \times \\ \times \sin \frac{\pi k(n+r)}{l+1}, \quad r \neq 0, \quad D_{l,n,0} = M_{l,n} + \frac{1}{2}. \quad (23)$$

The expression for $C^x_{l,n,r} = C^y_{l,n,r} \equiv C^\perp_{l,n,r}$ is more cumbersome: it involves the determinant of an $r \times r$ matrix [1], which in our notations is

$$C^\perp_{l,n,r} = \frac{1}{4} \times \\ \times \begin{vmatrix} G_{l,n,1} & G_{l,n,2} & \dots & G_{l,n,r} \\ G_{l,n+1,0} & G_{l,n+1,1} & \dots & G_{l,n+1,r-1} \\ \vdots & \vdots & \ddots & \vdots \\ G_{l,n+r-1,2-r} & G_{l,n+r-1,3-r} & \dots & G_{l,n+r-1,1} \end{vmatrix}, \\ G_{l,n,r} = 2D_{l,n,r} - \delta_{r,0}. \quad (24)$$

Equations (18)–(24) allow obtaining the average correlators with any prescribed precision.

Equations (18)–(20) can be simplified in the case of weak dilution, $1 - p \ll 1$, when major contributions come from large clusters with $l \gg 1$, and we can therefore set

$$M_{l,n} \approx M_\infty \equiv \lim_{n,l\to\infty} M_{l,n} = \\ = \int_0^\pi \frac{d\vartheta}{2\pi} \tanh \frac{J}{2T}(h - \cos\vartheta), \quad (25)$$

$$C^\alpha_{l,n,r} \approx C^\alpha_{\infty,r} \equiv \lim_{n,l\to\infty} C^\alpha_{l,n,r}, \quad C^z_{\infty,r} = M^2_\infty - D^2_{\infty,r}, \\ r \neq 0, \\ D_{\infty,r} \equiv \lim_{n,l\to\infty} D_{l,n,r} = \int_0^\pi \frac{d\vartheta}{2\pi} \cos(\vartheta r) \times \\ \times \tanh \frac{J}{2T}(h - \cos\vartheta), \quad r \neq 0, \quad (26) \\ D_{\infty,0} = M_\infty + \frac{1}{2},$$

$$C^{\perp}_{\infty,r} = \frac{1}{4}\begin{vmatrix} G_1 & G_2 & \dots & G_r \\ G_0 & G_1 & \dots & G_{r-1} \\ \vdots & \vdots & \ddots & \vdots \\ G_{2-r} & G_{3-r} & \dots & G_1 \end{vmatrix}, \tag{27}$$

$$G_r = 2D_{\infty,r} - \delta_{r,0},$$

to obtain

$$C^{\alpha}_r \approx p^{r+1}C^{\alpha}_{\infty,r} + \delta_{\alpha,z}M^2_{\infty}p^2\left[1-(r-1)p^{r-2} + \right. \\ \left. + (r-2)p^{r-1}\right], \quad r > 2, \tag{28}$$

$$C^{\alpha}_2 \approx p^3 C^{\alpha}_{\infty,2} + \delta_{\alpha,z}M^2_{\infty}p^2(1-p), \\ C^{\alpha}_1 \approx p^2 C^{\alpha}_{\infty,1}. \tag{29}$$

Thus, in the case of weak dilution, the correlations are determined essentially by those of the pure infinite chain. At $T=0$, Eqs. (25) and (26) again give simple known expressions [2–4]

$$M_{\infty} = \frac{1}{2} - q_F, \quad D_{\infty,r} = -\frac{\sin \pi q_F r}{\pi r}, \quad r \neq 0,$$

which allow finding $C^z_{\infty,r} = M^2_{\infty} - D^2_{\infty,r}$ [4] and the asymptotic form of $C^{\perp}_{\infty,r}$ at $h=0$ [8–10]:

$$C^{\perp}_{\infty,r} \approx c(-1)^r/\sqrt{r}\,, \quad c = 0.147088.$$

Our numerical simulations show that in finite fields,

$$C^{\perp}_{\infty,r} \approx A(h)(-1)^r/\sqrt{r}, \quad A(h) = c(1-h^2)^{1/4}, \\ r \to \infty.$$

Thus, in the weak dilution regime, the power-law asymptotic behavior of $C^{\perp}_r$ is modified by the exponential prefactor p^{r+1}, while

$$C^z_r \approx p^2 M^2_{\infty}\left[1-(1-p)rp^{r-2}\right]$$

at large r.

In general, at $T=0$, we can perform summation in Eqs. (21) and (23) with the result

$$M_{l,n} = \frac{1}{2(l+1)}\left[f(l, m^F_l, 2n) + l - 2m^F_l + \right. \\ \left. + \delta_{m^F_l, q_F(l+1)}(1-\cos 2\pi q_F n)\right], \tag{30}$$

$$D_{l,n,r} = \frac{1}{2(l+1)}\left[f(l, m^F_l, 2n+r) - f(l, m^F_l, r) + \right. \\ \left. + \delta_{m^F_l, q_F(l+1)}\left[\cos \pi q_F r - \cos \pi q_F(2n+r)\right]\right], \tag{31}$$

$$r \neq 0, \quad D_{l,n,0} = M_{l,n} + \frac{1}{2},$$

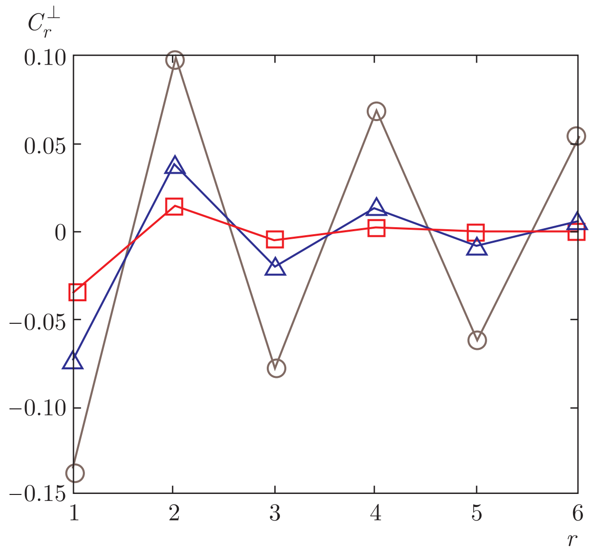

Fig. 4. $C^{\perp}_r$ at $T=0$ and $h=0.5$ for $p=0.5$ (□), 0.75 (△), and 1 (○). The l-sums are truncated at $L=15$

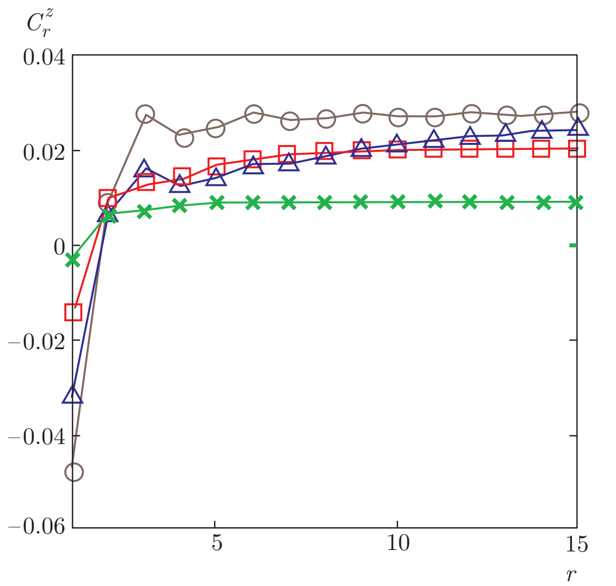

Fig. 5. C^z_r at $T=0$ and $h=0.5$ for $p=0.25$ (×), 0.5 ((□), 0.75 (△), and 1 (○). The l-sums are truncated at $L=30$

$$f(l,m,r) = \sin\frac{\pi r(2m+1)}{2(l+1)} \Big/ \sin\frac{\pi r}{2(l+1)}. \tag{32}$$

These compact expressions make it possible to obtain the averaged correlators at $T=0$ numerically with reasonable precision. Figures 4 and 5 show the distance dependence of the correlators $C^{\perp}_r$ and C^z_r at $T=0$ and $h=0.5$. These figures are obtained by truncating the l-sums in Eqs. (18)–(20) at $L=15$ for $C^{\perp}_r$ and at $L=30$ for C^z_r. The relative error ε that we have by dropping

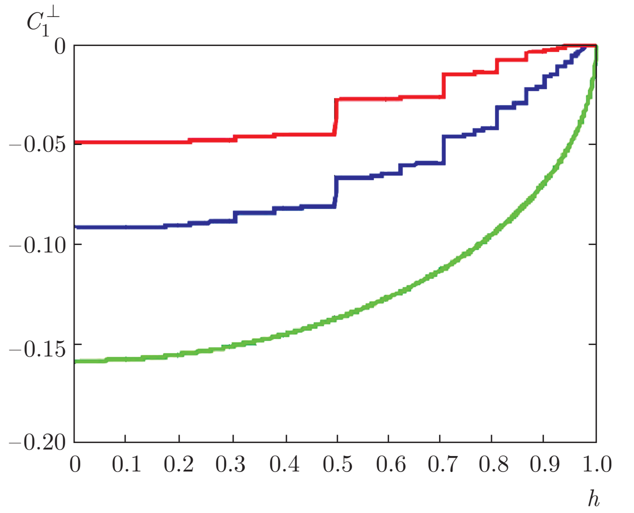

Fig. 6. The field dependences of $C_1^\perp$ for $p = 0.5$, 0.75, 1 (from top down). The l-sums are truncated at $L = 15$

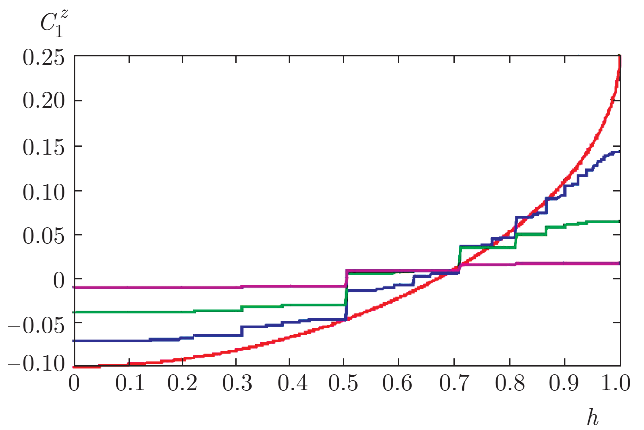

Fig. 7. The field dependences of C_1^z for $p = 1$, 0.75, 0.5, and 0.25 (from top down in the r.h.s. of the figure). The l-sums are truncated at $L = 30$

the terms with $l > L > r$ in these equations can be estimated as in Eq. (13):

$$\varepsilon \approx p^{L-r}\frac{L(1-p)+1}{r(1-p)+1}.$$

We can see that under dilution, the oscillations repidly die out in $C_r^\perp$ at large r owing to the exponentially small probability (less than p^r) to find magnetic clusters larger than r. Similarly, C_r^z rapidly tends to a constant proportional to $p^2 M_\infty^2$.

Figures 6 and 7 show the numerical results for the field dependences of nearest-neighbor correlators at $T = 0$ exhibiting the jumps at rational q_F values. These data are compared with correlators of the pure chain

$$C_{\infty,1}^\perp = -\frac{\sqrt{1-h^2}}{2\pi}, \quad C_{\infty,1}^z = M_\infty^2 - \frac{1-h^2}{\pi^2}.$$

We note that $|C_1^\perp|$ steadily diminishes with diminishing p, but $|C_1^z|$ can be greater in the dilute chain than in the pure one. The latter effect correlates with that found for the magnetization (cf. Fig. 2).

4. CONCLUSIONS

The present results show that the dilute isotropic XY chain in a transverse magnetic field is a rare macroscopic object where the signatures of numerous quantum phase transitions can be observed in macroscopic experiments at low T. Actually, with due precision, one can find arbitrarily large number of quantum transitions in every finite field interval at $h < 1$. Moreover, these transitions allow an exact analytic description of its mechanism as the change of the ground state (level crossing) under variation of the external field. The continuous level crossing is an inherent property of many other quantum phases with permanent criticality — the gapless (algebraic) spin-liquid states that have been shown to exist in quantum spin chains [12], ladders [13], and planar models [14, 15]. The dilution of such chains and ladders would result in a discretization of their spectra, thus inducing quantum jumps under the variation of couplings and the field similar to those of XX chain. In the gapless phases of planar models, such jumps could also exist, but should be much smaller owing to the great variety of possible magnetic clusters.

The present results can be used for some practical aids. For example, if one suspects that some crystal with an uncoupled chains of magnetic ions of spin 1/2 in its structure can be described by the XX model, it suffices to dilute these chains to verify the appearance of highly nonlinear behavior of the ordinary thermodynamic parameters (cf. Fig. 3). Also, the dilution of such crystals can be used to enhance their magnetization and longitudinal correlations due to peculiar quantum finite-size effects (see Figs. 2 and 7).

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