# Low-Energy Properties of Aperiodic Quantum Spin Chains

André P. Vieira*
*Instituto de Física da Universidade de São Paulo, Caixa Postal 66318, 05315-970, São Paulo, Brazil*
(Received 30 November 2003; published 22 February 2005)

We investigate the low-energy properties of antiferromagnetic quantum *XXZ* spin chains with couplings following two-letter aperiodic sequences, by an adaptation of the Ma-Dasgupta-Hu renormalization-group method. For a given aperiodic sequence, we argue that, in the easy-plane anisotropy regime, intermediate between the *XX* and Heisenberg limits, the general scaling form of the thermodynamic properties is essentially given by the exactly known *XX* behavior, providing a classification of the effects of aperiodicity on *XXZ* chains. As representative illustrations, we present analytical and numerical results for the low-temperature thermodynamics and the ground-state correlations for couplings following the Fibonacci quasiperiodic structure and a binary Rudin-Shapiro sequence, whose geometrical fluctuations are similar to those induced by randomness.

DOI: 10.1103/PhysRevLett.94.077201 PACS numbers: 75.10.Jm, 75.50.Kj

At low temperatures, the interplay between lack of translational invariance and quantum fluctuations in low-dimensional strongly correlated electron systems may induce novel phases with peculiar behavior. In particular, randomness in quantum spin chains may lead, for instance, to Griffiths phases [1], large-spin formation [2], and random-singlet phases [3]. On the other hand, studies on the influence of deterministic but aperiodic elements on similar systems (see, e.g., [4–9]), inspired by the experimental discovery of quasicrystals, have revealed strong effects on dynamical and thermodynamic properties, but far less is known concerning the precise nature of the underlying ground-state phases.

Prototypical models for those studies are spin-1/2 antiferromagnetic (AFM) *XXZ* chains described by the Hamiltonian

$$H = \sum_i J_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z), \qquad (1)$$

where all $J_i > 0$ and the $S_i$ are spin operators. Random-bond versions of these systems have been much studied by a real-space renormalization-group (RG) method introduced [10] by Ma, Dasgupta and Hu (MDH) for the Heisenberg chain ($\Delta = 1$) and more recently extended by Fisher [1,3], who gave evidence that the method becomes asymptotically exact at low energies. The idea is to decimate the spin pairs coupled by the strongest bonds (those with the largest gaps between the local ground state and the first excited multiplet), forming singlets and inducing weak effective couplings between neighboring spins, thereby reducing the energy scale. For *XXZ* chains in the regime $-1/2 < \Delta \leq 1$, the method predicts the ground state to be a random-singlet phase, consisting of arbitrarily distant spins forming rare, strongly correlated singlet pairs [3]. Here we employ the MDH method to investigate the low-energy properties of aperiodic chains.

Two-letter aperiodic sequences (AS's) can be generated by an inflation rule such as $a \to ab$, $b \to a$, which produces the Fibonacci sequence *abaababa*.... Associating with each $a$ a coupling $J_a$ and with each $b$ a coupling $J_b$, we can build an aperiodic quantum spin chain. In the *XX* limit ($\Delta = 0$), the low-temperature thermodynamic behavior can be qualitatively determined for any AS by an exact RG method [6]. The effects of aperiodicity depend on topological properties of the AS. If the fraction of letters $a$ (or $b$) at odd positions is different from that at even positions (i.e., if there is average dimerization), then a finite gap opens between the global ground state and the first excited states, and the chain becomes noncritical. Otherwise, the scaling of the lowest gaps can be classified according to the wandering exponent $\omega$ measuring the geometric fluctuations $g$ related to nonoverlapping pairs of letters [6], which vary with the system size $N$ as $g \sim N^{\omega}$. If $\omega < 0$, aperiodicity has no effect on the long-distance, low-temperature properties, and the system behaves as in the uniform case, with a finite susceptibility at $T = 0$. If $\omega = 0$, as in the Fibonacci sequence, aperiodicity is marginal and may lead to nonuniversal power-law scaling behavior of thermodynamic properties. If $\omega > 0$, aperiodicity is relevant in the RG sense, affecting the $T = 0$ critical behavior and leading to exponential scaling of the lowest gaps ($\Lambda$) at long distances $r$, of the form $\Lambda \sim \exp(-r^{\omega})$. In particular, for sequences with $\omega = 1/2$, geometric fluctuations mimic those induced by randomness, and the scaling behavior is similar to the one characterizing the random-singlet phase [3]. No analogous results exist for general *XXZ* chains, although bosonization and density-matrix RG (DMRG) calculations on the Heisenberg chain indicate that Fibonacci couplings should be relevant [7–9]. We argue below that, for a given AS, low-temperature properties of all chains in the regime $0 \leq \Delta \leq 1$ should follow essentially the *XX* scaling form. Moreover, we also obtain information on ground-state correlation functions.

In order to apply the MDH method to aperiodic chains, we must remember that now there are many spin blocks with the same gap at a given energy scale. Also, those blocks may consist of more than two spins, in which case effective spins would form upon renormalization. The strategy is to sweep through the lattice until all blocks with the same gap have been renormalized, leading to new effective couplings (and possibly spins). Then we search for the next largest gap, which again corresponds to many blocks. When all possible original blocks have been considered, there remain some unrenormalized spins, possibly along with effective ones, defining new blocks which form a second generation of the lattice. The process is then iterated, leading to the renormalization of the spatial distribution of effective blocks along the generations; for small enough coupling ratios (which are indeed required for the MDH method to work), *this distribution will be the same for all* $0 \le \Delta \le 1$. Because of the self-similarity inherent to AS's generated by inflation rules, the effective couplings take a finite number of values, and it is natural that the block distribution reaches a periodic attractor (usually a fixed point) after a few lattice sweeps. By studying recursion relations for the effective couplings, we can obtain analytical results. As the RG proceeds, the coupling ratio usually gets smaller, suggesting that the method becomes asymptotically exact. This picture holds for marginal ($\omega = 0$) and relevant ($\omega > 0$) aperiodicity; for irrelevant AS's, such as the Thue-Morse sequence ($a \to ab$, $b \to ba$), the coupling ratio approaches unity as the RG proceeds, and the method eventually breaks down. As representative examples, we consider the marginal case of Fibonacci couplings and the relevant case of a binary Rudin-Shapiro sequence. Full details of the calculations, as well as application to other AS's, will be reported elsewhere [11].

The blocks to be renormalized consist of $n$ spins connected by equal bonds $J_0$, and coupled to the rest of the chain by weaker bonds $J_l$ and $J_r$. The ground state (GS) for blocks with an even number of spins is a singlet, and at low energies we can eliminate the whole block, along with $J_l$ and $J_r$, leaving an effective AFM bond $J'$ coupling the two spins closer to the block and given by second-order perturbation theory as $J' = \gamma_n J_l J_r / J_0$, with $\Delta$-dependent coefficients $\gamma_n$. A block with an odd number of spins has a doublet as its GS; at low energies, it can be replaced by an effective spin connected to its nearest neighbors by AFM effective bonds $J'_{l,r} = \gamma_n J_{l,r}$ whose values are calculated by first-order perturbation theory. In general, the anisotropy parameters are also renormalized and become site dependent; for $n$ even, the effective anisotropy is $\Delta' = \delta_n(\Delta_0)\Delta_l\Delta_r$, while for $n$ odd $\Delta'_{l,r} = \delta_n(\Delta_0)\Delta_{l,r}$, with $|\delta_n(\Delta)| < 1$ for $0 \le \Delta < 1$ and $\delta_n(1) = 1$. Thus, for $0 < \Delta < 1$ the $\Delta_i$ flow to the $XX$ fixed point (all $\Delta_i = 0$), ultimately reproducing the corresponding scaling behavior, while for the Heisenberg chain all $\Delta_i$ remain equal to unity. So, we focus here on the Heisenberg and $XX$ limits, and postpone examples for intermediate cases to a future publication [11].

First we apply the method to chains with Fibonacci couplings. This is the simplest example of the quasiperiodic precious-mean sequences with marginal fluctuations [6]. A few bonds closer to the left end of the original chain, along with induced effective couplings, are shown in Fig. 1 for $J_a < J_b$ [12]. Only singlets are formed by the RG process, producing two different effective couplings,

$$J'_a = \gamma_2^2 J_a^3 / J_b^2 \quad \text{and} \quad J'_b = \gamma_2 J_a^2 / J_b.$$

The bare coupling ratio is $\rho = J_a/J_b$, its renormalized value being $\rho' = \gamma_2 \rho$. In each generation $j$, all decimated blocks have the same size $r_j$ and gap $\Lambda_j$ (proportional to the effective $J_b$ bonds). The recursion relations for $\rho$ and $\Lambda$ are given by

$$\rho_{j+1} = \gamma_2 \rho_j \quad \text{and} \quad \Lambda_{j+1} = \gamma_2 \rho_j^2 \Lambda_j.$$

The distance between spins forming a singlet in the $j$th generation defines a characteristic length $r_j$, corresponding to the Fibonacci numbers $r_j = 1, 3, 13, 55, \ldots$; for $j \gg 1$ the ratio $r_{j+1}/r_j$ approaches $\phi^3$, where $\phi = (1 + \sqrt{5})/2$ is the golden mean. So we have $r_j \sim r_0 \phi^{3j}$, where $r_0$ is a constant, and by solving the recursion relations we obtain the dynamic scaling behavior,

$$\Lambda_j \sim r_j^{-\zeta} e^{-\mu \ln^2 (r_j/r_0)}, \tag{2}$$

with $\zeta = -2/3 \ln\rho / \ln\phi$ and $\mu = -\ln\gamma_2 / 9\ln^2\phi$. For the Heisenberg chain $\gamma_2 = 1/2$, and Eq. (2) describes a weakly exponential scaling, but not of the form $\Lambda \sim \exp(-r^\omega)$ found for the $XX$ chain with relevant aperiodicity ($\omega > 0$) and used to fit the DMRG data for the Fibonacci Heisenberg chain [7,8]. For the $XX$ chain $\gamma_2 = 1$, so that $\mu = 0$ and we can identify $\zeta$ with a dynamical critical exponent $z$, whose value depends on the coupling ratio, leading to nonuniversal scaling behavior, characteristic of strictly marginal operators [13]. This nonuniversality should hold in the anisotropy regime $0 < \Delta < 1$ with a "bare" value of $\rho$ defined at a crossover scale. Note that we can view the Heisenberg scaling form ($\mu \neq 0$) as a marginally relevant ($\omega \to 0^+$) case.

The susceptibility $\chi(T)$ can be estimated [3] by assuming that, at energy scale $\Lambda_j \sim T$, only unrenormalized spins are magnetically active (and essentially free), singlet pairs being effectively frozen. Thus, if $n_j \sim r_j^{-1}$ is the number of surviving spins in the $j$th generation, $\chi(T \sim \Lambda_j) \sim n_{j+1}/\Lambda_j$. As shown in Fig. 2(a), $\chi(T)$ estimated for the Fibonacci $XX$ chain from the MDH method agrees very well with results from free-fermion [14] numerical diagonalization (ND) of finite chains, even for $\rho = 1/4$.

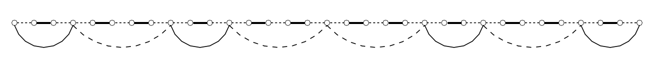

FIG. 1. Left end of the Fibonacci $XXZ$ chain. Dashed (solid) lines represent $J_a$ ($J_b$) bonds. An effective coupling $J'_b$ is induced between spins separated by only one singlet pair, while $J'_a$ connects spins separated by two singlet pairs. Apart from a few bonds close to the chain ends, the effective couplings also form a Fibonacci sequence.

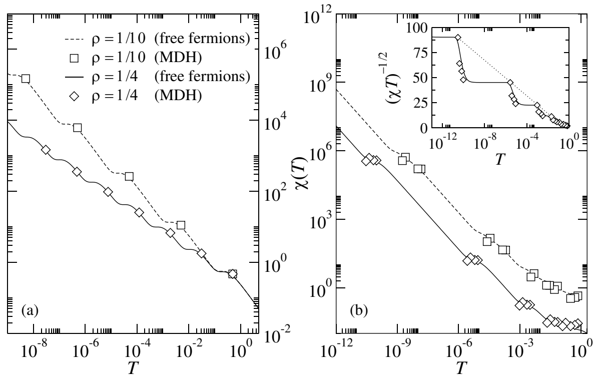

FIG. 2. Behavior of $\chi(T)$ for aperiodic $XX$ chains, obtained from the MDH method (symbols) and from numerical diagonalization on chains with $10^4$–$10^5$ sites (curves), for two values of $\rho = J_a/J_b$. (a) Fibonacci couplings. The slope of the curves depends on $\rho$, reflecting the marginal character of the aperiodicity. (b) Rudin-Shapiro couplings. The inset plots the inverse square root of $T\chi(T)$ versus $T$ (in log scale) with $\rho = 1/4$, showing that for points corresponding to the smallest gaps in each generation the random-singlet phase result $\chi(T) \sim 1/T\ln^2 T$ is reproduced (dotted line).

As all singlets formed at the $j$th generation have size $r_j$ and the block distribution is fixed, the average GS correlation between spins separated by a distance $r_j$ is

$$C^{\alpha\alpha}(r_j) \equiv \overline{\langle S_i^\alpha S_{i+r_j}^\alpha \rangle} = \tfrac{1}{2}|c_0|(n_j - n_{j+1}) = \sigma |c_0| r_j^{-1}, \quad (3)$$

where $\sigma$ is a constant, $\alpha = x, y, z$, and $c_0$ is the GS correlation between the two spins in a singlet, given by $c_0 = -1/4$ for the Heisenberg chain and for both $\alpha = x$ and $\alpha = z$ in the $XX$ chain. We point out that these should be the dominant correlations, and spins separated by distances other than $r_j$ are predicted to be only weakly correlated. This can be checked for the $XX$ chain by calculating GS correlations via the free-fermion method. Results for chains with $\rho \lesssim 1/4$ (see [11]) reveal very good agreement with Eq. (3). As correlations in the uniform $XX$ chain [14] decay as $C^{xx}(r) \sim r^{-1/2}$ and $C^{zz}(r) \sim r^{-2}$, dominant $xx$ ($zz$) correlations in the Fibonacci chain are weaker (stronger) than in the uniform chain.

Relevant aperiodicity is characterized by strong geometric fluctuations, and is usually induced by sequences with blocks having two or more neighboring strong bonds. Furthermore, after the first lattice sweep, more than two values of effective couplings may be produced. However, they all derive from the original pair of couplings $J_a$ and $J_b$, so that, in the presence of a periodic attractor, it is generally possible to write recursion relations for an effective coupling ratio and gap having the forms [11]

$$\rho_{j+1} = c\rho_j^k \quad \text{and} \quad \Lambda_{j+1} = \lambda \rho_j^\ell \Lambda_j, \quad (4)$$

where $c$ and $\lambda$ are $\Delta$-dependent nonuniversal constants, and $\ell$ (a rational number) and $k$ (an integer) relate to the number of singlets involved in determining the effective couplings. We assume $k \geq 2$, $k = 1$ corresponding to marginal behavior, as in the Fibonacci case [15]. If a characteristic length scale takes the form $r_j = r_0\tau^j$, with a rescaling factor $\tau$, solving the recursion relations leads to a dynamic scaling described by

$$\Lambda_j \sim r_j^{-\zeta} \exp(-\mu r_j^\omega) \sim \exp(-\mu r_j^\omega), \quad (5)$$

with $\zeta$ and $\mu$ nonuniversal constants and $\omega = \ln k/\ln\tau$. Note that $\omega$ has *precisely the same form* as the exact result [6] obtained for the $XX$ chain with aperiodic couplings not inducing average dimerization. Moreover, $\omega$ depends only on the topology of the sequence and on its self-similar properties, but not on the anisotropy; so, for a given AS, the scaling form in Eq. (5) should be valid for any $XXZ$ chain in the regime $0 \leq \Delta \leq 1$, with the same exponent $\omega$.

As an example, we consider couplings following the binary Rudin-Shapiro (RS) sequence, whose inflation rule for letter pairs is $aa \to aaab$, $ab \to aaba$, $ba \to bbab$ and $bb \to bbba$. This generates blocks having between two and five spins. Figure 3 shows a few bonds closer to the left end of the chain for the first three generations of the lattice. Blocks with more than three spins are eliminated in the first sweep and do not appear in later generations. Both two- and three-spin blocks are present in the fixed-point block distribution (already reached at the second generation), and a hierarchy of effective spins is produced, as depicted in Fig. 3. At the $j$th generation, three-spin blocks have size $r_j = 2\times 4^{j-1}$ (so that $\tau = 4$), while two-spin blocks have size $r_j/2$. The first lattice sweep generates effective couplings $\tilde{J}_i$ having eight different values, but three of them are enough to write recursion relations,

$$\tilde{J}_a' = \gamma_2^2\gamma_3 \tilde{J}_c \tilde{J}_a^2/\tilde{J}_b^2, \qquad \tilde{J}_b' = \gamma_3 \tilde{J}_c,$$
$$\text{and} \quad \tilde{J}_c' = \gamma_2\gamma_3 \tilde{J}_a \tilde{J}_c/\tilde{J}_b.$$

The gap in a given generation is proportional to the effective $\tilde{J}_b$; defining $\rho = \tilde{J}_a/\tilde{J}_b$ and eliminating $\tilde{J}_c$ gives

$$\rho_{j+1} = \gamma_2^2 \rho_j^2 \quad \text{and} \quad \Lambda_{j+1} = \gamma_3^3 \rho_j^{1/2} \Lambda_j,$$

which correspond to the forms in Eq. (4) with $k = 2$ and $\ell = 1/2$. So we obtain, for the whole regime $0 \leq \Delta \leq 1$, the dynamical scaling form in Eq. (5) with an exponent $\omega = 1/2$, as predicted for the $XX$ chain, reproducing the result for the random-singlet phase. In Fig. 2(b) we plot $\chi(T)$ for the $XX$ chain calculated from both ND and the MDH method, again obtaining very good agreement.

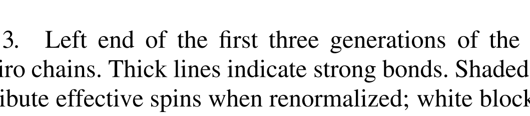

FIG. 3. Left end of the first three generations of the Rudin-Shapiro chains. Thick lines indicate strong bonds. Shaded blocks contribute effective spins when renormalized; white blocks form singlets.

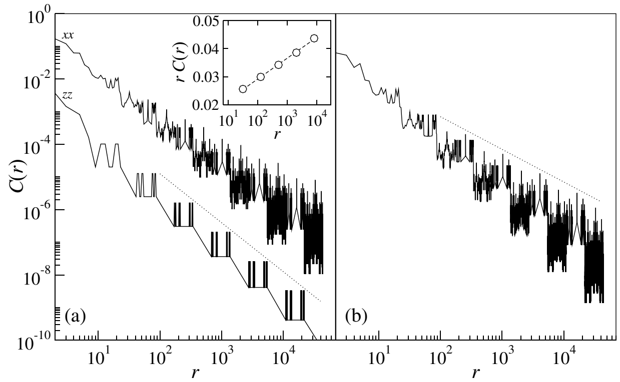


FIG. 4. GS correlations for chains with RS couplings, obtained from extrapolation of numerical MDH results for chains with $2^{16}$ to $2^{20}$ sites. (a) $C^{xx}(r)$ (upper solid curve) and $C^{zz}(r)$ (lower solid curve) for the $XX$ chain. The dotted curve is proportional to $r^{-3/2}$. (Curves offset for clarity.) Inset: dominant $C^{xx}$ correlations, fitted by a law of the form $rC^{xx}(r) = y_0 + y_1 \ln r$ (dashed curve). (b) $C(r)$ for the Heisenberg chain (solid curve). The dotted curve is proportional to $1/r$.

For chains with RS couplings, effective-spin formation from three-spin blocks determines the dominant GS correlations. These blocks stem from both original three-spin (and some five-spin) blocks and unrenormalized spins. An effective spin represents all spins in the original block via Clebsch-Gordan coefficients, allowing us to calculate correlations between any two spins whose effective spins end up in the same block at some stage of the RG process. Because of the hierarchical structure seen in Fig. 3, for each block renormalized at the $j$th generation the correlation between its end spins connects a number of order $2^j$ original spin pairs separated by the same distance $r_j$ (the size of the block), yielding a contribution $g_j$ to the average correlation in the Heisenberg chain and $C^{xx}(r_j)$ in the $XX$ chain given by a geometric series in $2\gamma_3^2$. For the Heisenberg chain $2\gamma_3^2 = 8/9 < 1$, and thus

$$C(r_j) \sim g_j n_j = \sigma |c_0| r_j^{-1}, \tag{6}$$

where $c_0$ is the correlation between end spins in a three-spin block and $n_j = \sigma/r_j$ is the fraction of such blocks in the $j$th generation. For the $XX$ chain $2\gamma_3^2 = 1$, so that $C^{xx}(r_j)$ carries a logarithmic correction,

$$C^{xx}(r_j) \sim g_j n_j = |c_0|(y_0 + y_1 \ln r_j) r_j^{-1}, \tag{7}$$

where $y_0$ and $y_1$ are constants. The $zz$ correlation between end spins in a three-spin block is zero, so that the dominant correlations correspond to spin pairs (connected through one of the effective end spins and the middle spin) at distances $r'_j = 4^{j-1} \pm 4^{j-2} \pm 4^{j-3} \pm \cdots \pm 1$, with average $\langle r'_j \rangle = 4^{j-1}$, and are given by $g'_j \sim 1/2^{j-1}$. We then have

$$C^{zz}(r'_j) \sim g'_j n_j = \sigma' |c'_0| \langle r'_j \rangle^{-3/2}. \tag{8}$$

Equations (7) and (8) should be contrasted with the random-singlet isotropic result $C(r) \sim r^{-2}$, indicating a clear distinction between the ground-state phases induced by disorder and aperiodicity, even in the presence of similar geometric fluctuations. This is related to the inflation symmetry of the AS's, which is absent in the random-bond case (or in aperiodic systems with random perturbations [16]). Its effects are exemplified by the fractal structure of the GS correlations visible in Fig. 4, which displays results from numerical implementations of the MDH method for both $XX$ and Heisenberg chains, showing conformance to the scaling forms in Eqs. (6)–(8).

In summary, we have used the Ma-Dasgupta-Hu method to investigate numerically and analytically the low-energy properties of aperiodic antiferromagnetic $XXZ$ chains. From a general scaling argument, we suggest that the effects of binary aperiodicity on the whole anisotropy regime from the $XX$ to the Heisenberg limits can be classified based on the same wandering exponent ($\omega$) which is know exactly to govern the scaling behavior of aperiodic $XX$ chains. We have also shown that ground-state correlations are dominated by characteristic distances related to the rescaling factor of the sequences.

This work has been supported by the Brazilian agencies CAPES and FAPESP. The author is indebted to T. A. S. Haddad for fruitful conversations.

*Note added.*—While this Letter was under review, some of the results for the Fibonacci chain were published in a Letter by K. Hida [17].

*Electronic address: apvieira@if.usp.br

[1] D. S. Fisher, Phys. Rev. Lett. **69**, 534 (1992); Phys. Rev. B **51**, 6411 (1995).
[2] E. Westerberg, A. Furusaki, M. Sigrist, and P. A. Lee, Phys. Rev. Lett. **75**, 4302 (1995); Phys. Rev. B **55**, 12 578 (1997).
[3] D. S. Fisher, Phys. Rev. B **50**, 3799 (1994).
[4] J. M. Luck and T. M. Nieuwenhuizen, Europhys. Lett. **2**, 257 (1986).
[5] J. M. Luck,J. Stat. Phys. **72**, 417 (1993).
[6] J. Hermisson,J. Phys. A **33**, 57 (2000).
[7] K. Hida, J. Phys. Soc. Jpn. **68**, 3177 (1999).
[8] K. Hida, Phys. Rev. Lett. **86**, 1331 (2001).
[9] J. Vidal, D. Mouhanna, and T. Giamarchi, Phys. Rev. Lett. **83**, 3908 (1999); Phys. Rev. B **65**, 014201 (2002).
[10] S.-K. Ma, C. Dasgupta, and C.-K. Hu, Phys. Rev. Lett. **43**, 1434 (1979); C. Dasgupta and S.-K. Ma, Phys. Rev. B **22**, 1305 (1980).
[11] A. P. Vieira, Phys. Rev. B (to be published).
[12] If $J_a > J_b$, effective spins form in the first lattice sweep, producing a Fibonacci chain with the roles of weak and strong bonds interchanged, and we are back to Fig. 1.
[13] We can check that $z = \zeta$ corresponds to the asymptotic form of the exact $XX$ expression [4,6] for $\rho \ll 1$.
[14] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[15] Solving Eq. (4) with $k = 1$ leads to the scaling form in Eq. (2), irrespective of $\ell$.
[16] M. Arlego, Phys. Rev. B **66**, 052419 (2002).
[17] K. Hida, Phys. Rev. Lett. **93**, 037205 (2004).