PHYSICAL REVIEW B **83**, 060414(R) (2011)

Connecting distant ends of one-dimensional critical systems by a sine-square deformation

Toshiya Hikihara[1,*] and Tomotoshi Nishino[2]
[1]*Department of Physics, Hokkaido University, Sapporo 060-0810, Japan*
[2]*Department of Physics, Graduate School of Science, Kobe University, Kobe 657-8501, Japan*
(Received 8 December 2010; published 28 February 2011)

We study one-dimensional quantum critical spin systems with sine-square deformation, in which the energy scale in the Hamiltonian at position x is modified by the function $f_x = \sin^2[\frac{\pi}{L}(x-\frac{1}{2})]$, where L is the length of the system. By investigating the entanglement entropy, spin correlation functions, and wave-function overlap, we show that the sine-square deformation changes the topology of the geometrical connection of the ground state drastically: Although the system apparently has open edges, the sine-square deformation links those ends and realizes the periodic ground state at the level of the wave function. Our results propose a method to control the topology of quantum states by energy-scale deformation.

DOI: 10.1103/PhysRevB.83.060414 PACS number(s): 75.10.Pq, 75.10.Jm, 75.40.Mg

Introduction. Topology is one of the most fundamental concepts in physics. It rules the connectivity of local elements of the system and governs how physical objects—particles, excitations, and information—propagate. Normally, the topology of a system is fixed once the spatial geometry of elements is given. The search for other paths to control of topology of the system is a challenging problem.

In a finite system, a boundary condition determines the topology of the geometrical connection of quantum state and crucially affects the properties of the system. If the system has open edges, they usually induce boundary oscillations such as Friedel oscillations. While the boundary oscillation contains important information such as the Fermi momentum, it is often regarded as an obstacle to mask the bulk properties. One simple way to remove it is to employ the periodic boundary condition, however, there has also been another attempt, called the smooth boundary condition, to suppress the boundary effects by turning off the energy scale of local Hamiltonians smoothly around the open edges.[1,2] The latter has proven to be useful when the open system is favored, for instance, for efficiency of numerical methods such as the density-matrix renormalization-group (DMRG) method.

Recently, a scheme of the smooth boundary condition, which we call the sine-square deformation (SSD), has been proposed as an efficient way to suppress finite-size and open-boundary effects.[3] In a system with SSD, the energy scale in the Hamiltonian is modified according to the function

$$f_x = \sin^2\left[\frac{\pi}{L}\left(x-\frac{1}{2}\right)\right], \tag{1}$$

where x is the position of the local term and L is the length of the system. In Ref. 3, Gendiar *et al.* applied the SSD to a one-dimensional (1D) free fermion system with open boundaries. They then showed that the SSD removed boundary effects successfully and resulted in position-independent one-point functions such as the bond strength and particle density in the ground state. Since the spatial profiles of these quantities were *almost completely* flat, the observation raised a natural question of what happened in the ground state of the system with SSD. This is indeed the motivation of the present study.

In this paper, we study the SSD in several 1D quantum spin systems. Using the DMRG and exact diagonalization methods, we study numerically the entanglement entropy (EE), correlation functions, and wave-function overlap in systems with SSD. We then show that the ground state of a critical system with SSD is equivalent to that of a uniform periodic system; the SSD drastically changes the topology of the critical ground state, from an open chain to a periodic ring. The result opens the possibility of controlling the topology of quantum states by the energy-scale deformation even in the case where the geometrical shape of the system is fixed.

Sine-square deformation. The SSD introduces a spatial modulation of energy scale by applying the rescaling factor f_x [Eq. (1)] to the local Hamiltonian at position x. For example, the model Hamiltonian of the spin-1/2 antiferromagnetic XXZ chain with SSD is given by

$$\mathcal{H}_{XXZ} = J\sum_{j=1}^{L-1} f_{j+\frac{1}{2}}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right) - h\sum_{j=1}^{L} f_j S_j^z, \tag{2}$$

where we have introduced the magnetic field h, which induces magnetization M per spin.[4] Hereafter, we consider the case of even L unless otherwise specified. The energy scale of the local Hamiltonians thus decreases smoothly closer to the boundaries and eventually vanishes at the open ends, as shown in Fig. 1(a).[5]

Figure 1(b) shows the DMRG data for the bond strength $\langle S_j^x S_{j+1}^x\rangle$ in the ground state of the XXZ chain, Eq. (2), with and without SSD. The data clearly show that the SSD almost completely eliminates the Friedel oscillation seen in the uniform open chain.[3] We will demonstrate below that the SSD is not only an efficient measure to suppress the boundary effects but also a device to drastically change the topology of the ground-state wave function.

Entanglement entropy. We first investigate EE in the ground state of 1D systems with SSD. We consider EE for a subsystem Ω of the left l spins,

$$\mathcal{S}(l) = -\mathrm{Tr}_\Omega[\rho(l)\ln\rho(l)], \tag{3}$$

where $\rho(l)$ is the reduced density matrix for Ω. For 1D critical uniform systems, EE is known to take a universal

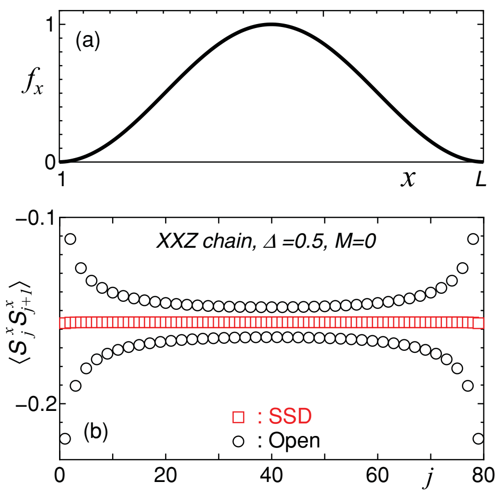

FIG. 1. (Color online) (a) Rescaling function f_x of the SSD. (b) Bond strength $\langle S^x_j S^x_{j+1} \rangle$ for the XXZ chain, Eq. (2), with $L = 80$ and $(\Delta, M) = (0.5, 0)$. Squares and circles represent the data for the chain with SSD and the uniform open chain, respectively.

form,[6–8]

$$\mathcal{S}(l) = s \ln[g(l)] + \text{const.}, \quad (4)$$

where $g(l) = \frac{L}{\pi} \sin(\frac{\pi l}{L})$. The slope s is determined by the boundary condition; $s = c/3$ for the periodic system, while $s = c/6$ for the system with open boundaries, where c is the central charge. Namely, the slope s divided by $c/6$ gives the number of "cuts" of the 1D critical state between the subsystem Ω and the environment $\bar{\Omega}$.

Figures 2(a) and 2(b) show DMRG data for EE in an XXZ chain with SSD [Eq. (2)]. EE in uniform open chains is also shown for comparison. Remarkably, EE in systems with SSD has slope $s = c/3$, which is twice as large as that in uniform open systems. This means that the ground state of the system with SSD has two cuts between the left and the right subsystems, Ω and $\bar{\Omega}$, although the lattice seemingly has only one cut. In addition, the boundary oscillation, which is pronounced in the uniform systems, is removed by the SSD. The results suggest that, although the system apparently possesses open edges, the SSD connects the open ends of the ground state effectively and the state becomes *periodic*, having two cuts between Ω and $\bar{\Omega}$.

We have also examined EE in the other models, the antiferromagnetic J_1-J_2 chain and two-leg ladder systems under a magnetic field. The Hamiltonians are given by

$$\mathcal{H}_{J_1-J_2} = \sum_{j=1}^{L-1} \sum_{n=1,2} J_n f_{j+\frac{n}{2}} \mathbf{S}_j \cdot \mathbf{S}_{j+n} - h \sum_{j=1}^{L} f_j S^z_j, \quad (5)$$

$$\mathcal{H}_{\text{lad}} = J_\parallel \sum_{j=1}^{L-1} \sum_{n=1,2} f_{j+\frac{1}{2}} \mathbf{S}_{n,j} \cdot \mathbf{S}_{n,j+1} + J_\perp \sum_{j=1}^{L} f_j \mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j} - h \sum_{j=1}^{L} f_j (S^z_{1,j} + S^z_{2,j}). \quad (6)$$

In Figs. 2(c)–2(e), we present DMRG results for EE of left l sites/rungs for subsystem Ω [see Fig. 2(f)]. The models in Figs. 2(c) and 2(e) are in critical phases with $c = 1$, while the model in Fig. 2(d) has $c = 2$.[9–13] It is again found that the slope of EE is doubled by the SSD. We note that, for the J_1-J_2 chain with large J_2/J_1, sizable boundary oscillations are observed in EE and one-point functions (not shown), even in the system with SSD. This is presumably attributed to an effective boundary field that cannot be eliminated completely by the SSD in Eq. (5).[14] However, we emphasize that, even in that case, the doubled slope of EE is observed, which suggests that the SSD also works for those models to lead to a topology

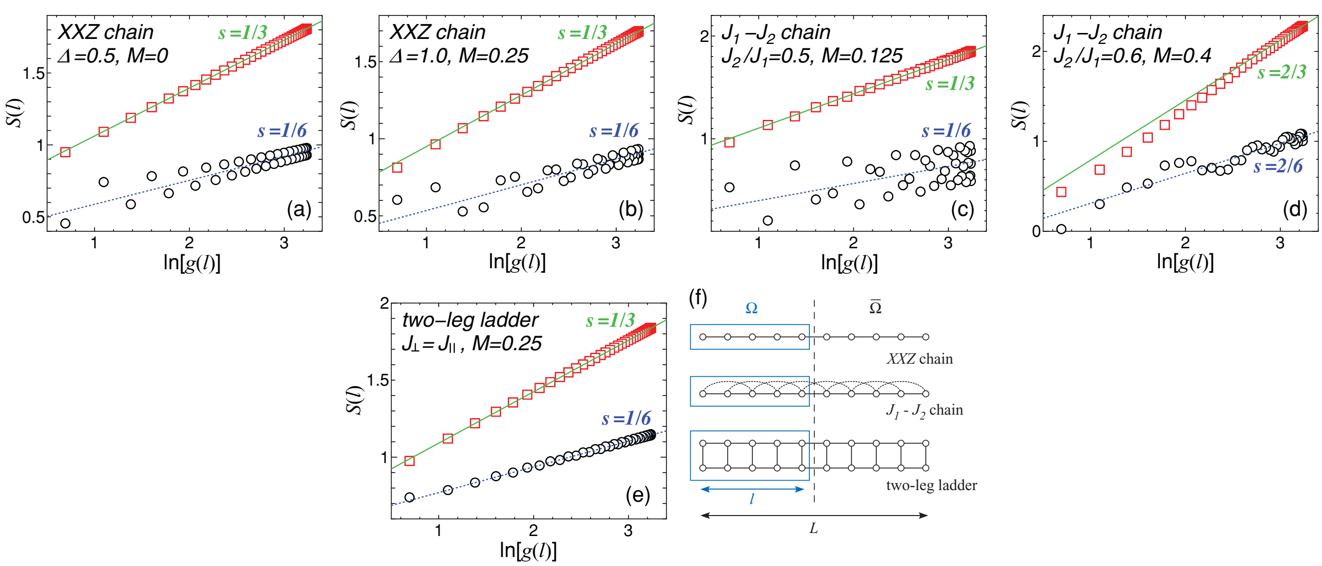

FIG. 2. (Color online) Entanglement entropy $\mathcal{S}(l)$ as a function of $g(l) = (L/\pi)\sin(\pi l/L)$ for $L = 80$ and (a) an XXZ chain with $(\Delta, M) = (0.5, 0)$, (b) an XXZ chain with $(\Delta, M) = (1.0, 0.25)$, (c) a J_1-J_2 chain with $(J_2/J_1, M) = (0.5, 0.125)$, (d) a J_1-J_2 chain with $(J_2/J_1, M) = (0.6, 0.4)$, and (e) a two-leg ladder with $(J_\perp/J_\parallel, M) = (1.0, 0.25)$. (a–c, e) Central charge $c = 1$; (d) $c = 2$. Squares and circles represent data for the open system with SSD and the uniform open system, respectively. Solid and dotted lines show the slopes of $c/3$ and $c/6$, respectively. (f) Shape of subsystem Ω for which $\mathcal{S}(l)$ is calculated.

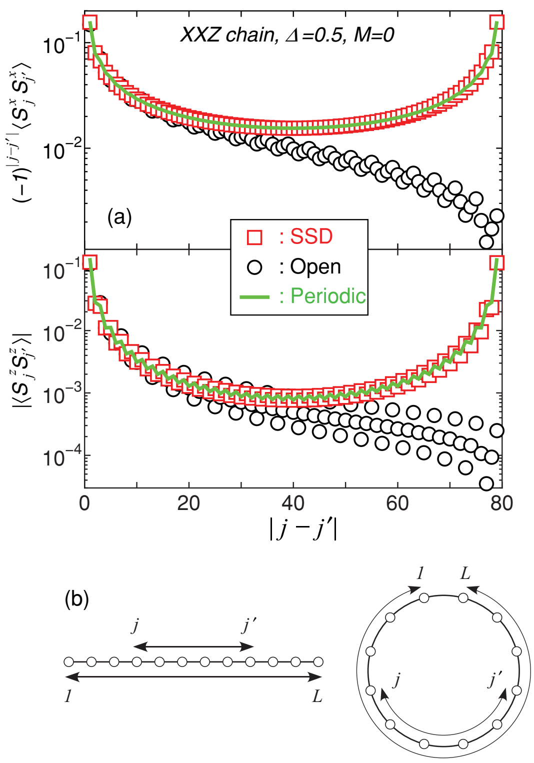

FIG. 3. (Color online) (a) Spin correlation functions $\langle S^\alpha_j S^\alpha_{j'}\rangle$ ($\alpha = x,z$) in an XXZ chain for $L = 80$ and $(\Delta, M) = (0.5,0)$ as a function of the distance $|j - j'|$, where sites (j, j') are selected as $j = L/2 - [r/2]$ and $j' = L/2 + [(r + 1)/2]$. Squares and circles represent DMRG data for an open chain with SSD and a uniform open chain, respectively, while lines show the analytic result for a uniform periodic chain. (b) Schematic showing the relation between pairs (j, j') in the open chain with SSD and those in the periodic chain.

change of the ground state. We thus conclude that the change in slope of EE is not peculiar to a specific model but a general outcome of the SSD when applied to a critical model.

Correlation functions. We next investigate two-spin correlation functions. Here, we consider a spin-1/2 XXZ chain in the critical regime, for which the asymptotic forms of the correlation functions are known to be

$$\langle S^x_0 S^x_r\rangle = A^x_0 \frac{(-1)^r}{r^\eta} - A^x_1 \frac{\cos(Qr)}{r^{\eta+1/\eta}} + \cdots, \quad (7)$$

$$\langle S^z_0 S^z_r\rangle - M^2 = -\frac{1}{4\pi^2\eta r^2} + A^z_1 \frac{(-1)^r \cos(Qr)}{r^{1/\eta}} + \cdots, \quad (8)$$

where $Q = 2\pi M$. The exponent η and the amplitudes A^x_0, A^x_1, and A^z_1 were obtained as a function of Δ and M.[11,15–17] Figure 3 shows DMRG results for ground-state correlation functions in an XXZ chain, Eq. (2), with SSD. We also plot DMRG data for a uniform open chain as well as the analytic result for a uniform periodic chain; the latter is obtained by replacing r in Eqs. (7) and (8) with $\frac{L}{\pi}\sin(\frac{\pi|j-j'|}{L})$. As shown in Fig. 3, the results for the open chain with SSD agree almost completely with those for the periodic chain.

Figure 4(a) shows the ground-state correlation function $\langle \mathbf{S}_j \cdot \mathbf{S}_{j'}\rangle$ in a small system calculated by exact diagonalization. Data are plotted as a function of position j and "distance" $r = \min(|j - j'|, L - |j - j'|)$ [see Fig. 4(b)]. We again observe

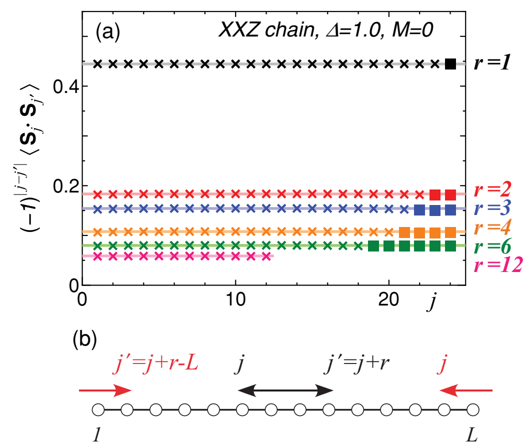

FIG. 4. (Color online) (a) Spin correlation function $(-1)^r\langle \mathbf{S}_j \cdot \mathbf{S}_{j'}\rangle$, with $j' = j + r$ (mod L), in an XXZ chain for $L = 24$ and $(\Delta, M) = (1.0,0)$ as a function of j and r. Symbols show data for an open chain with SSD: crosses represent correlations between sites j and $j' = j + r$ (pairs "within" the chain), while squares represent those between j and $j' = j + r - L$ (pairs "across" the edges). Lines show values of correlations in the uniform periodic chain. (b) Schematic showing the two sites (j, j') at a "distance" r.

that the correlations in the open chain with SSD are in excellent agreement with those in the uniform periodic chain; The results are independent of position j, and more remarkably, the correlations between sites j and $j' = j + r - L$, which are located at the distance r *across* the open ends, have the same value as those in the periodic chain.[18] We have observed the same phenomena as shown in Figs. 3 and 4 for several parameter sets of (Δ, M). The results indicate that correlation functions, and presumably all observables, in the ground state of systems with SSD become equal to those in uniform periodic systems.

We note that for the two-leg ladder with zero magnetization, $M = 0$, which has an energy gap above the singlet ground state, the spin correlation decays exponentially even in systems with SSD and no recovery of the correlation between edge spins is observed. This suggests that the SSD does not work for spin-gapped systems.

Wave functions. Finally, we discuss the overlap of ground-state wave functions. Using the exact diagonalization method, we calculated the ground-state wave function $|\mathbf{v}_{\rm SSD}\rangle$ of an XXZ chain, Eq. (2), with SSD for $L \leqslant 24$ and several sets of (Δ, M), and compared it with the ground-state wave function $|\mathbf{v}_{\rm PBC}\rangle$ of the uniform periodic chain. We then found that the overlap of those ground-state wave functions is very close to unity; the deviation from unity is at most $|1 - \langle \mathbf{v}_{\rm SSD}|\mathbf{v}_{\rm PBC}\rangle| \lesssim 10^{-3}$ and exactly 0 within the numerical accuracy of 10^{-14} for the XX case ($\Delta = 0$). The result indicates that the ground states $|\mathbf{v}_{\rm SSD}\rangle$ and $|\mathbf{v}_{\rm PBC}\rangle$ are equivalent at the level of the wave function.[18]

We note that the equivalence of the ground-state wave functions is not trivial even in the case of an XX chain [Eq. (2) with $\Delta = 0$]. Through the Jordan-Wigner transformation, the XX chain is mapped onto the free fermion system and the one-particle eigenstates of the periodic chain are simple plane waves. In contrast, the Hamiltonian of an open chain with SSD is not translationally invariant and its one-particle eigenstates are distinct from plane waves. Nevertheless, when and only when the fermions are filled up to the Fermi level, the Slater determinants of the two ground states become equivalent. This means that the excitation spectrum and dynamics of the system with SSD are in general different from those of the periodic system.

Concluding remarks. In summary, we have studied the SSD applied to 1D critical spin systems. From numerical analyses of the EE, correlation functions, and wave-function overlap, we have shown that the ground state of an open system with SSD is equivalent to that of a uniform periodic system.

We note that our finding that the SSD realizes the periodic ground state is not restricted to a specific model but is a generic feature of the SSD. We have found a change in the slope of the EE for several spin systems, and suppression of boundary effects by the SSD has also been observed in free and interacting fermion systems.[3,19] The only condition required is that the system is critical. This may suggest that the result can be understood in a theory applicable to general critical systems, such as the conformal-field theory. Investigating the effects of the SSD on low-energy excited states would reveal clues about the mechanism of the SSD.

The results of the present study offer a scheme to modify and further control the topology of quantum states by energy-scale deformation, even under the condition that the spatial shape of the system is fixed. The approach might be applicable to real systems such as ultracold atoms, for which spatial modulation of interatomic interactions has been demonstrated.[20] The search for an energy-scale deformation to yield other topological changes in the ground state is another interesting problem.

Acknowledgments. We thank Shunsuke Furukawa, Akira Furusaki, Andrej Gendiar, Hosho Katsura, and Tsutomu Momoi for stimulating discussions. T.H. was supported in part by the MEXT and JSPS, Japan, through Grant Nos. 21740277 and 22014016.

*Corresponding author: hikihara@phys.sci.hokudai.ac.jp

[1] M. Vekić and S. R. White, Phys. Rev. Lett. **71**, 4283 (1993).

[2] M. Vekić and S. R. White, Phys. Rev. B **53**, 14552 (1996).

[3] A. Gendiar, R. Krcmar, and T. Nishino, Prog. Theor. Phys. **122**, 953 (2009); **123**, 393 (2010).

[4] Unlike the usual uniform systems, the Zeeman term in the Hamiltonian with SSD does not commute with the exchange term and the relation between the field h and the ground-state magnetization M is not trivial. In our calculation, we use the value of $h(M)$ obtained from the Bethe ansatz or the DMRG analysis for the corresponding uniform systems as an approximation of the field to realize the ground state with M in the system with SSD.

[5] To be precise, applying SSD to a periodic chain with only nearest-neighbor interactions leads to the same Hamiltonian, Eq. (2), since $f_{L+\frac{1}{2}} = 0$. In this paper, we call model (2) the "open" chain with SSD, as it apparently has open ends.

[6] C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. B **424**, 443 (1994).

[7] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).

[8] P. Calabrese and J. Cardy, J. Stat. Mech. Theory Exp. (2004) P06002.

[9] R. Chitra and T. Giamarchi, Phys. Rev. B **55**, 5816 (1997).

[10] A. Furusaki and S.-C. Zhang, Phys. Rev. B **60**, 1175 (1999).

[11] T. Hikihara and A. Furusaki, Phys. Rev. B **63**, 134438 (2001).

[12] K. Okunishi and T. Tonegawa, J. Phys. Soc. Jpn. **72**, 479 (2003).

[13] T. Hikihara, T. Momoi, A. Furusaki, and H. Kawamura, Phys. Rev. B **81**, 224433 (2010).

[14] The reason the SSD fails to eliminate boundary oscillations in the J_1-J_2 chain can be understood if one considers a system with $J_1 = 0$, which consists of two Heisenberg chains placed with a shift of a half-lattice spacing. In this case, we should apply the SSD to each chain as in Eq. (2). This suggests that for finite J_2/J_1, one must modify the form of the SSD around open edges from Eq. (5). Finding the correct form is left for future studies.

[15] N. M. Bogoliubov, A. G. Izergin, and V. E. Korepin, Nucl. Phys. B **275**, 687 (1986).

[16] S. Lukyanov and V. Terras, Nucl. Phys. B **654**, 323 (2003).

[17] T. Hikihara and A. Furusaki, Phys. Rev. B **69**, 064427 (2004).

[18] For odd L, we calculated the spin correlation functions and wave-function overlap and found that the ground state of an open XXZ chain with SSD is equivalent to that of an XXZ chain under the *antiperiodic* boundary condition: The edge spins are connected via an exchange coupling $J[-(S_L^x S_1^x + S_L^y S_1^y) + \Delta S_L^z S_1^z]$ with the sign change of the transverse part, which picks up the π phase of the antiferromagnetic interaction.

[19] A. Gendiar, M. Daniska, Y. Lee, and T. Nishino, e-print arXiv:1012.1472.

[20] R. Yamazaki, S. Taie, S. Sugawa, and Y. Takahashi, Phys. Rev. Lett. **105**, 050405 (2010).