Exact Solution of a Yang-Baxter Spin-1/2 Chain Model and Quantum Entanglement

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(Dated: November 16, 2008)

Entanglement is believed to be crucial in macroscopic physical systems for understanding the collective quantum phenomena such as quantum phase transitions. We start from and solve exactly a novel Yang-Baxter spin-1/2 chain model with inhomogeneous and anisotropic short-range interactions. For the ground state, we show the behavior of neighboring entanglement in the parameter space and find that the inhomogeneous coupling strengths affect entanglement in a distinctive way from the homogeneous case, but this would not affect the coincidence between entanglement and quantum criticality.

PACS numbers: 03.67.-a 05.30.-d 03.65.Ud

I. INTRODUCTION

Entanglement was conventionally considered to be a quirk of microscopic objects and has been recognized to be ubiquitous and so robust that it promises applications in the quantum communication and computation like technologies [1]. In the last few years, there was an increasing interest in entanglement in macroscopic physical systems [2, 3]. Entanglement may lead to further insight into condensed matter physics. For example, in statistical mechanics, given that quantum phase transitions (QPTs) occur at absolute zero and are driven by quantum fluctuations, entanglement may provide additional correlations for QPTs [4, 5] that have no classical counterpart. In return, materials and experience built up over the years in condensed matter are helping in finding new protocols for quantum computation and communication.

Studying entanglement of the ground state in macroscopic physical systems is crucial to understand a large variety of collective quantum phenomena. For a one-dimensional spin-1/2 XY chain with short-range interactions

\[ H_{XY} = -\sum_n \left( \frac{1+\gamma}{2} \sigma_n^x \sigma_{n+1}^x + \frac{1-\gamma}{2} \sigma_n^y \sigma_{n+1}^y + \lambda \sigma_n^z \right), \]

the entangled degree (ED) between any two nearest-neighbor particles keeps the same for the translational symmetry, and its derivative is capable to fulfill the role of an order parameter to characterize QPT at the critical point \( \lambda = 1 \) [4, 5, 6]. Potential as it is, we should ask whether such an observation is universal enough to assure all correspondences between entanglement and QPT. For example, in Ref. [6] it demonstrates a long-distance entanglement appearing for values of the microscopic parameters which do not coincide with known quantum critical points. In addition, if the short-range interactions are not homogeneous, e.g., a dual chain, ED between two nearest-neighbor particles would generally not keep in accordance for different sets of chains. At this case, questions arise on what ED is and whether it well coincides with critical points.

For self-contained and later use, let us recall the Yang-Baxter approach for entangled states with two qubits [7]. The unitary \( \hat{R}(\theta, \phi) \) matrix in this approach, taking \( \hat{R}(\theta) = \sin \theta + \cos \theta \hat{M}(\phi) \) with the generalized four-dimensional imaginary unit \( \hat{M} (M^2 = -1) \), is used to produce entangled states when acting on direct-product states and EDs of the resulting states are simply \( |\sin 2\theta| \). Supposing that \( \theta \) is time-independent and \( \phi \) is time-dependent, we can get a Hamiltonian through \( \dot{H}(\theta, \phi) = i\hbar (\partial \hat{R}/\partial t)\hat{R}^\dagger \) (see Eq. [2]), which only governs the evolution of entanglement varying with parameter \( \theta \). At the case of \( \theta = \pi/2 \), \( \hat{R} \) corresponds to an identity operation with no entanglement at all and \( H \) thus vanishes. Such a peculiar behavior of \( H \) actually creates a nonanalytical point of the ground state energy with respect to \( \theta \) and this should be reflected by some properties of its ground state such as the geometric phase (GP). When extended to an infinite lattice, the possibilities are richer and the vanishing point may correspond to a QPT.

The purpose of this paper is twofold: one is that we solve exactly a novel Yang-Baxter spin-1/2 chain model with alternating coupling strengths by means of the Jordan-Wigner transformation and GP of the ground state is examined for QPT; the other concerns the consequence of entanglement between two local nearest-neighbor particles of the chain, based on which we check whether entanglement under inhomogeneous coupling strengths can well characterize critical phenomena. This article is organized as follows. In Sec. III, we introduce and exactly solve an inhomogeneous Yang-Baxter spin-1/2 chain model. Based on the solution, we investigate the quantum criticality by analyzing GP of the ground state, and study the effect of inhomogeneity on entanglement between different nearest-neighbor sites and next-nearest-neighbor sites in Sec. IV. At last, Sec. V is
II. THE YANG-BAXTER SPIN-1/2 CHAIN MODEL AND EXACT DIAGONALIZATION

The Yang-Baxter equation was originated from solving the δ-function interaction model by Yang \[1\] and the statistical models by Baxter \[11\], and was then introduced to solve many quantum integrable models by Faddeev and Leningrad Scholars \[12\]. It plays a fundamental role in the theories of 1+1 and 2+1 dimensional integrable quantum systems, including lattice statistical models and nonlinear field theory. For example, Yang’s \( \hat{R} \)-matrix in YBE for the \( n \)th and \((n + 1)\)th particles is \( \hat{R}(u)_{n,n+1} = 1 + u \mathcal{P}_{n,n+1} \) (\( u \) is a spectral parameter, i.e., one-dimensional momentum and \( \mathcal{P} \) is permutation satisfying \( \mathcal{P}^2 = 1 \)); it yields the XXX chain model through \( H_{n,n+1} \sim \partial \hat{R}/\partial u \big|_{u=0} \), when \( \mathcal{P} \) takes its four-dimensional representation of \( \mathcal{P}_{n,n+1} = \frac{1}{2}(1 + \sum_i \sigma_i \cdot \sigma_{n+1}) \) with \( \sigma \) being the Pauli matrix. Considering the form of \( \hat{R}(\theta_n) \) in Sec. \( \mathcal{I} \) it has a two-body interacting Hamiltonian \( \mathcal{H} \):

\[
H_{n,n+1} = -\hbar \omega \cos \theta_n \left[ \cos \theta_n \left( S_n^z + S_{n+1}^z \right) + \sin \theta_n \left( e^{i\phi} S_n^+ S_{n+1}^+ + e^{-i\phi} S_n^- S_{n+1}^- \right) \right], \tag{2}
\]

where \( S^\pm = S^x \pm iS^y \) with \( S^{x,y,z} = \sigma^{x,y,z}/2 \), and \( \phi \) is the flux dependent of time \( t \) and it takes \( \phi(t) = \omega t \), denoting procession angle of spins around the \( z \) direction in a rotating magnetic field. For many particles, we should sum all of them as \( H = \sum_n H_{n,n+1} \) and if all of \( \theta_n \) are taken to be the same, it would correspond to a homogeneous chain, otherwise it would correspond to an inhomogeneous one.

From Eq. \( \mathcal{I} \), the family of Hamiltonians that is parameterized by \( \phi \) is clearly isospectral, and, therefore, the critical behavior is independent of \( \phi \). In fact, we can see that the spin raising-raising or lowering-lowering structure in Eq. \( \mathcal{I} \) allows a rotation for each spin around \( z \)-axis and such a rotation transformation can be employed to adjust the value of phase factors in Eq. \( \mathcal{I} \), e.g.,

\[
\mathcal{H} = g(\phi/2)H g^\dagger(\phi/2) \quad \text{and} \quad g(\phi) = \prod_{j=1}^N e^{-i\sigma_j^x \phi/2} \quad \text{giving} \quad g(\phi/2) S_n^+ g^\dagger(\phi/2) = e^{-i\phi/2} S_n^+ \quad \text{and} \quad g(\phi/2) S_n^- g^\dagger(\phi/2) = e^{i\phi/2} S_n^-.
\]

Then the Hamiltonian is reduced to

\[
\mathcal{H} = -\frac{1}{2} \hbar \omega \sum_n \cos \theta_n \left[ \sin \theta_n (\sigma_n^x \sigma_n^x + \sigma_n^y \sigma_n^y) + \cos \theta_n (\sigma_n^z + \sigma_n^z) \right].
\]

Comparing \( \mathcal{H} \) with the XY chain in Eq. \( \mathcal{I} \), one sees that the structure of dominant two-body interaction in \( \mathcal{H} \) is exactly that in \( H_{XY} \) yet under \( \gamma, \lambda \gg 1 \) limit. Like \( H_{XY} \), there is a global \( \mathbb{Z}_2 \) symmetry for \( H \) that keeps it invariant under a unitary transformation \( \prod_n \sigma_n^z \). In the following, we will see that the ground state does not break such a symmetry.

Noting the fact that it can define these operators:

\[
J_n^z = \frac{1}{2} (S_n^z + S_{n+1}^z), \quad J_n^+ = \frac{1}{2} (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) \quad \text{and} \quad J_n^- = \frac{1}{2} (S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+) \quad \text{that satisfy the angular momentum commutation relation, we see that} \quad J_n \quad \text{actually only occupies a subspace spanned by} \quad | \uparrow \uparrow \rangle_{n,n+1} \quad \text{and} \quad | \downarrow \downarrow \rangle_{n,n+1} \quad \text{that belongs to a} \quad j = 1/2 \quad \text{angular momentum representation. Thus we can write the Hamiltonian into an effective NMR-like form} \quad H_{n,n+1} = -\mathcal{E}_n(t) \cdot \mathbf{J}_n, \quad \text{where the magnetic field is} \quad \mathcal{E}_n(t) = 2\hbar \omega \cos \theta_n (\sin \theta_n \cos \phi(t) - \sin \phi(t) \cos \theta_n). \quad \text{Its}
\]
eigenvalues are readily given by \( E_{n+1}^\pm = \pm \hbar \omega \cos \theta_n \) and eigenstates in accordance are \( | E^\pm \rangle = \cos \frac{4\theta_n}{| \phi |} | \uparrow \uparrow \rangle \pm \sin \frac{4\theta_n}{| \phi |} | \downarrow \downarrow \rangle \), both EDs of which are \( | \sin \theta_n | \).

In the vicinity of \( \theta_n = \pi/2 \), we can set \( \cos \theta_n = \delta \) and see that it keeps the forms of the eigenstates \( | E^\pm (\delta) \rangle \) and hence EDs even when \( \delta \to 0 \).

Now, let us extend Eq. \( \mathcal{I} \) to an inhomogeneous chain which approaches infinite when the particle number takes to be arbitrarily large. For simplicity, we confine bonds between any pair of odd-even numbered nearest-neighbor sites to be the same and characterized by parameter \( \theta_1 \) and that between any pair of even-odd numbered nearest-neighbor sites to be the same and characterized by \( \theta_2 \) (see Fig. \( \mathcal{I} \)). By requiring the periodical boundary condition, there are totally \( 2N \) sites and the Hamiltonian can be written as

\[
H = -\sum_{n=1}^{N} (B_1 \cdot J_{2n-1} + B_2 \cdot J_{2n}), \tag{3}
\]

which can be interpreted simply as two sets of spins in an external field with different coupling strengths along \( z \)-axis. The composite qubit \( \mathbf{J}_n \) satisfies \( [\mathbf{J}_1, \mathbf{J}_j] = 0 \) for \( |i-j| \geq 2 \). At the same time, the property of \( H \) zero interaction at zero field—provides a critical phenomenon at \( \theta_1 = \theta_2 = \pi/2 \) and is similar but not exactly the same to the on-site exchange interactions \[13\] and superexchange interactions \[14\] with ultracold atoms in optical lattices, which would vanish as the optical field is taken off. Here we will focus more on the entangled aspect of these interactions by using the Hamiltonian Eq. \( \mathcal{I} \), which has a closed relation with entangled states. As for this, it is interesting to ask what ED is when extending to an infinite chain model with two-body interactions having the Hamiltonian equation \( \mathcal{I} \): the parameters \( \theta_n \) on all solid dark lines and \( \theta_2 \) on all dashed red lines describe two different coupling strengths; each ellipse including solid and dashed ones represents a two particle composite qubit with the angular momentum \( \mathbf{J}_1 \).

FIG. 1: A chain model with two-body interactions having the Hamiltonian equation \( \mathcal{I} \): the parameters \( \theta_n \) on all solid dark lines and \( \theta_2 \) on all dashed red lines describe two different coupling strengths; each ellipse including solid and dashed ones represents a two particle composite qubit with the angular momentum \( \mathbf{J}_1 \).

\[ \theta_1 \quad \theta_2 \]
From Eq. (7), it can be seen the ground state is invariant
where the reduced momentum \( k = -M, \ldots, M \) with \( M = (N - 1)/2 \) for \( N \) odd and fermion operators \( (a_k^{\dagger}, a_k) \) anticommute with each other. Thus the Eq. (3) can be written into

\[
H = -\frac{1}{2} \hbar \omega \sum_k \varepsilon_k^\pm (\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k - 1).
\]

The eigenspectra contain two bands of quasiparticle excitations: \( \varepsilon_k^\pm = \pm \sqrt{|\xi_k| + \Delta^2} \). The transformed fermion operators \( \alpha_k = u_k e^{i\phi/2} a_k^\dagger + v_k e^{-i\phi/2} a_k \) and \( \beta_k = \bar{u}_k e^{i\phi/2} a_k^\dagger + \bar{v}_k e^{-i\phi/2} a_k \), where \( \bar{u}_k = -u_k = (\Delta + \varepsilon_k^\pm)/(2\varepsilon_k^\pm (\Delta + \varepsilon_k^\pm))^{1/2} \) and \( \bar{v}_k = v_k = -\xi_k/[2\varepsilon_k^\pm (\Delta + \varepsilon_k^\pm)]^{1/2} \) for different bands \( \varepsilon_k^\pm \). For these coefficients, there is \( \bar{u}_k \bar{u}_k^\dagger + \bar{v}_k \bar{v}_k^\dagger = 0 \).

The ground state \( |g\rangle \) of \( H \) is the vacuum of the fermionic modes, satisfying \( \alpha_k |g\rangle = 0 \) and \( \beta_k |g\rangle = 0 \) for all \( k \). Generally it is hard to write the ground state obviously into a spin superposed state, but for our model there is a fact that the Néel state—\( |\Psi^1\rangle = \otimes N |\uparrow\rangle \)—just corresponds to the zero energy eigenstate of \( H \). Take \( |\Psi^1\rangle \) for example: it has \( \alpha_k |\Psi^1\rangle = 0 \) and it is identical to \( |\Psi^1\rangle = \prod_k \beta_k^\dagger |g\rangle \), which inversely gives an expression for the ground state \( |g\rangle = \prod_k |\Psi^1\rangle \), i.e.,

\[
|g\rangle = \prod_k \{ \sum_{m=1}^N e^{-i2\pi m/2N} \bar{v}_k e^{-i\phi/2} \prod_{l<2m-1} \sigma_l^z S_{2m-1}^- + \bar{u}_k e^{i\phi/2} \prod_{l=2m-1} \sigma_l^z S_{2m-1}^+ \} |\uparrow\rangle \otimes N \}.
\]

which would return to the biparticle case (i.e., \(|E^-\rangle\)) if one takes \( N = 1 \) and \( \theta_2 = \pi/2 \). When \( \theta_1 \neq \pi/2 \) and \( \theta_2 = \pi/2 \), we can see that Eq. (3) becomes to describe \( N \) isolated dimers, which has an exact ground state, \( \prod_m (\cos \frac{\theta_1}{2} |\uparrow\rangle |\uparrow\rangle \otimes N + \sin \frac{\theta_1}{2} e^{-i\phi} |\downarrow\rangle |\downarrow\rangle \otimes N) \).

From Eq. (7), it can be seen the ground state is invariant under the global \( Z_2 \) transformation and so it keeps the same symmetry as the Hamiltonian. Alternatively, the ground state can also be expressed by

\[
|g\rangle = \prod_k (\bar{u}_k e^{i\phi/2} |0\rangle \langle 0| + \bar{v}_k e^{-i\phi/2} |1\rangle \langle 1|),
\]

where \( |0\rangle_{N_k} \) and \( |1\rangle_{N_k} \) are the vacuum and single excitation of the \( k \)-th mode, \( a_k^{\dagger, c} \), respectively.

\[\text{III. QUANTUM CRITICALITY AND ENTANGLEMENT}\]

QPT occurs at a point in the external parameter space, where there can be a level-crossing and excited levels become the ground state, creating a point of nonanalyticity of the ground state energy as a function of external parameters \([13]\). With the Hamiltonian Eq. (6) in consideration, we take \( \theta_{1,2} \) as those external parameters. Obviously, at the point of \( \theta_1 = \theta_2 = \pi/2 \) all energy levels cross and hence it is a critical point, but it is different from the conventional QPT by having a vanishing Hamiltonian and for convenience of discussion, we might as well call it a QPT. Recently, GP of the ground state \([16,17]\) and ED between nearest-neighbor particles \([4,5]\) for a homogeneous Heisenberg XY chain were proposed to characterize the criticality of QPT. In this section, we investigate GP and ED for our novel inhomogeneous chain, analyze their behaviors as the parameters \( \theta_{1,2} \) vary, and further discuss their nonanalytical property in the proximity of QPT.

\[\text{A. Quantum Criticality Characterized by Geometric Phase}\]

GP of the ground state, accumulated by varying the angle \( \phi \) from 0 to \( 2\pi \), is described by \( \beta_g = \frac{1}{N} \int_{0}^{2\pi} \langle g | i \partial_\varphi | g \rangle d\varphi \), and by utilizing Eq. (8) it is

\[
\beta_g^\pm = -\frac{\pi}{N} \sum_k (|\bar{u}_k|^2 - |\bar{v}_k|^2) = -\frac{\pi}{N} \sum_k \Delta / \varepsilon_k^\pm, \tag{9}
\]

with \( \beta_g^+ = -\beta_g^- \). The term \( \beta_k = -\pi \Delta / \varepsilon_k^\pm \) is a geometric phase for the \( k \)-th mode, and represents the area in the parameter space enclosed by the loop determined by \( (\theta_1, \theta_2, \phi) \). One can see that when we turn off the coupling between dimers by setting \( \theta_2 = \pi/2 \), GP would return to the biparticle dimer case with \( \beta_g = \pi (1 - \cos \theta_1) \).

To study quantum criticality, we are interested in the thermodynamic limit when the spin lattice number \( N \to \infty \). In this case the summation \( \frac{1}{N} \sum_{k=-M}^{M} \) can be replaced by the integral \( \frac{1}{2} \int_{0}^{2\pi} d\varphi \) with \( \varphi = 2\pi k/N \); GP in
the thermodynamic limit is given by

$$\beta_g = -\int_0^\pi d\varphi \Delta / \varepsilon_\varphi^\pm,$$  \hspace{1cm} (10)

where the energy spectra $\varepsilon_\varphi^\pm = \pm \sqrt{\xi_\varphi^2 + \Delta^2}$ with $|\xi_\varphi|^2 = \sin^2 2\theta_1 + \sin^2 2\theta_2 - 2 \sin 2\theta_1 \sin 2\theta_2 \cos \varphi$.

To see the quantum criticality obviously, we plot GP $\beta_g$ and its derivatives $\partial \beta / \partial \theta_2$, $\partial^2 \beta / \partial \theta_1 \partial \theta_2$ in the parameter $(\theta_1, \theta_2)$ space, shown in Fig. 2. It can be seen, from Fig. 2(a), that there is a conical intersection at the point $\theta_1 = \theta_2 = \pi/2$, which indicates a nonanalytical point there. The nonanalytical property at the critical point can be seen obviously from the diagram of GP derivative [see Fig. 2(c)]. However, as we pointed above, such a QPT point is trivial, since at the point the whole Hamiltonian vanishes and hence it appears to be exotic there. If fixing one parameter, say $\theta_1$, it would correspond to the uniparameter case and we should check whether there are other critical phenomena as varying $\theta_2$. The derivative of GP with $\theta_2$ is plotted in Fig. 2(b), from which we can see, except for the above critical point and its vicinity, it is analytic everywhere. So there is no additional critical point.

B. Entanglement of the Ground State

In this section, we confine our interest at entanglement between nearest-neighbor sites in the chain, given long-distance entanglement decays rapidly with the distance (see below). To describe entanglement, we use the concurrence $18$ of a bipartite state, related to the “entanglement of formation” $19$, to define ED of a state. The concurrence for the state of the $i$th and $j$th particles is defined as

$$C(i, j) = \max\{r_1 - r_2 - r_3 - r_4, 0\},$$  \hspace{1cm} (11)

where $r_1, r_2, r_3, r_4$ are the square roots of the eigenvalues of the product matrix $R = \rho(i, j)\rho(i, j)$ in descending order; $\rho(i, j)$ is the density matrix of the $i$th and $j$th spin-1/2 particles and the spin flipped matrix is defined as $\tilde{\rho}(i, j) = \sigma^y \otimes \sigma^y \rho(i, j)\sigma^y \otimes \sigma^y$. If it is a pure state, e.g., $|E^\pm\rangle$, the density matrix $\rho(n, n+1) = |E^-\rangle\langle E^-|$ and the concurrence quantifying entanglement is $C(n, n+1) = |\sin \theta_n|$. If it is a bipartite state in a multiparticle system, $\rho(i, j)$ would represent a bipartite mixed state reduced from the multiparticle density matrix $\rho$.

For the chain in consideration, translation invariance of dual lattices implies that $C(2m, 2m+1) = C_e(1), C(2m-1, 2m) = C_e(1)$ and $C(2m-1, 2m+1) = C(2)$ for all $m$. The concurrence will be evaluated as a function of the relative position $|i - j|$ between the $i$th and $j$th spins and parameters $\theta_1, 2$. All information needed is contained in the reduced density matrix $\rho(i, j)$ obtained from the ground-state wavefunction after all the spins except those at positions $i$ and $j$ have been traced out. The resulting $\rho(i, j)$ represents a mixed state of a bipartite system. The structure of the reduced density matrix is obtained by exploiting symmetries of the chain. The nonzero entries of $\rho(i, j)$ can then be related to the various correlation functions $20, 21, 22$ as

$$\rho(i, j) = \left( I + \langle \sigma_i^z \sigma_j^z \otimes 1 \rangle + \langle \sigma_i^y \sigma_j^y \rangle + \langle \sigma_i^z \sigma_j^x \rangle + \langle \sigma_i^y \sigma_j^y \rangle \right) / 4.$$  \hspace{1cm} (12)

Correlation functions under the ground state can be evaluated by using the fermionic representation and the simple identity $1 - 2a_i^\dagger a_m = (a_i^\dagger)^2 + 4$. For each pair of fermion operators $(a_i, a_i^\dagger)$, we can further define two Majorana fermion operators $(A, B)$: $A_n = a_n^\dagger + a_n$ and $B_n = i(a_n - a_n^\dagger)$ with $A^\dagger = A$ and $B^\dagger = B$. Exploring them, we can write the Pauli matrices as:

$$\sigma_n^x = \prod_{l<n} \langle (i)A_lB_l \rangle A_n, \quad \sigma_n^y = \prod_{l<n} \langle (i)A_lB_l \rangle B_n,$$  \hspace{1cm} (13)

and $\sigma_n^z = \langle (i)A_nB_n \rangle$. A two-body correlation function, say $\langle \sigma_m^x \sigma_n^y \rangle$, under the ground state, is

$$\langle \sigma_m^x \sigma_n^y \rangle = -i \left\{ B_m \prod_{l=m+1}^{n-1} \langle (i)A_lB_l \rangle A_n \right\} \langle (i)B_m \rangle A_{m+1} \cdots A_{n-1} (i)B_{n-1})A_n.$$  \hspace{1cm} (13)

Since the expectation values are with respect to a free Fermi theory, the expression on the right-hand side can be evaluated by the Wick’s theorem $15, 23$, which relates it to a sum over products of expectation values of pairs of operators, i.e., $\langle A_lA_m \rangle$, $\langle B_lB_m \rangle$, and $\langle B_lA_m \rangle$. The evaluation of average values of these pairs is displayed in Appendix A. In order to see the macroscopic property of entanglement, we define two $k$-independent
functions:
\[ \mathcal{F}(n-m) = \frac{1}{N} \sum_{k} e^{i \frac{2\pi}{N}(n-m)(|\bar{u}_k|^2 - |\bar{v}_k|^2)}, \]
\[ \mathcal{G}(m-n) = \frac{1}{N} \sum_{k} e^{-i \frac{2\pi}{N}(n-m)2\bar{u}_k\bar{v}_k}, \] (14)

which have summed all frequencies in the momentum space to be the form in the position representation. We can see, \( \mathcal{F}(0) \) is nothing but the one proportional to GP in Eq. \( \mathcal{G} \). In this respect, we may well say \( \mathcal{F}, \mathcal{G} \) are macroscopically quantities, which under the thermodynamical limit \( N \to \infty \) can be calculated still by making the replacement \( \frac{1}{N} \sum_{k} \to \frac{1}{2} \int_{0}^{\pi} d\varphi. \)

Next, we would focus on entanglements between the nearest-neighbor sites. In principle, the numerical results on the concurrence of such two-site density state can be performed readily according to its definition introduced above, but before that, we find the concurrence depends only on the above two \( k \)-independent functions \( \mathcal{F}(n-m) \) and \( \mathcal{G}(m-n) \). As an illustration, we give out the expressions of ED in the form of concurrence between odd-even and even-odd neighboring sites, respectively, by

\[ C_e(1) = \max \{0,|\mathcal{G}(0)| - \frac{1}{2}[\mathcal{F}(0)^2 + \mathcal{G}(0)^2 - 1]\}, \]
\[ C_o(1) = \max \{0,|\mathcal{G}(1)| - \frac{1}{2}[\mathcal{F}(1)^2 + \mathcal{G}(1)^2 - 1]\}. \] (15)

Their varying trends in the parameter space are displayed in Fig. 3(a) associated with contours in 3(b). Note that although we plot merely the concurrence of even-odd neighboring sites in Fig. 3 that of odd-even neighboring sites can be immediately gotten by noticing the symmetry: \( C_o(\theta_1 \leftrightarrow \theta_2) = C_e. \)

Fig. 3(a) shows that the maximum of \( C_e(1) \) (or \( C_o(1) \)) approaches but cannot reach one (i.e., the intrinsic maximal value of ED) because of the vanishing Hamiltonian at the value. At \( \theta_1 = \pi/2 \) even-odd pairs become decoupled from the rest and the behavior of \( C_e \) for \( \theta_2 \to \pi/2 \) is the same as in the biparticle case. Whereas, the difference refers to the minimum of \( C_e(1) \) that relates to disentangled states with vanishing ED and from Fig. 3(b) we can see that in the parameter space it occupies a considerable regime enclosed by the dashed red lines for disentangled states. Thereby, at the interface of the entangled and disentangled states it will correspond to the unsmoothed part of ED mainly due to the unsmoothed definition of the concurrence [see Eq. (11)] and the inhomogeneous interaction strength in the chain, which would as well imply the nonanalytical behavior for derivatives of ED with respect to \( \theta_1, \theta_2 \). In contrast, at the homogeneous case of \( C_e = C_o \) achieved along the diagonal line of either \( \theta_1 = \theta_2 \) or \( \theta_1 + \theta_2 = \pi \) in Fig. 3[b], ED has only one unsmoothened point which corresponds to the critical point appropriately.

Fig. 3(c) and (d) show respectively the first and second derivatives of ED with respect to parameters \( \theta_1, \theta_2 \). The dominating divergence at the central region is well in agreement to that appeared in the derivatives of GP and thus indicates QPT. Except this, it does not diverge at other points, exhibiting instead just a finite discontinuity at the border between separable and pairwise entangled sectors. This type of non-analytic behavior is quite distinct from that at the critical point and stems just from the definition of concurrence. In addition, the divergence includes both upward and downward directions and this reflects the increasing and decreasing trends of ED in the vicinity of the nonanalytical region.

As for two next-nearest-neighbor sites and other farther neighboring sites, ED should decay rapidly with the distance (generally even more rapidly than standard correlations) for the short-ranged interaction. To illustrate it, our numerical result demonstrates that the next-nearest-neighbor concurrence \( C(2) \) vanishes for the whole chain. As a result, it is sufficient for us to only take the nearest-neighbor biparticle entanglement into account on this chain, while for multiparticle entanglement it may has a connection with the so called topological quantum phase transition (e.g., [24]) but not discussed here.

IV. CONCLUSION AND DISCUSSION

To summarize, we have demonstrated an exact solution to a particular spin-1/2 chain model with alternating nearest-neighbor coupling strengths and have analyzed the influence of inhomogeneous interaction on the ground state through GP and ED approaches. By evaluating GP of the ground state, we display its behavior at the parameter space, from which a critical point could
be determined through the divergent derivative of GP. After that, via examining the biparticle entanglement by virtue of concurrence, we also show the tendency of ED with respect to parameters and find that ED and its derivatives can determine the critical point as well as GP does at the inhomogeneous case. Although ED has an unsmoothed definition at the border of separable and pairwise entangled sectors, it does not exactly affect the nearest-neighbor concurrence to detect the critical point, exhibiting instead a clear signature of it in its derivative as seen in Fig. 3(c).

As remarked earlier, the specific parametrization of the Hamiltonian has an intimate relation with ED at the biparticle case and when extending it to an infinite lattice, the result is interesting: for homogeneous coupling strengths, ED has suppressed values with its maximum far less than one, keeping equal for every pair of nearest-neighbor sites; for inhomogeneous coupling strengths, ED appears to have different values between even-odd numbered and odd-even numbered nearest-neighbor sites, from which a very high ED is available (see Fig. 3). In a way, the property might apply to other inhomogeneous lattice models as a manifestation of general principles. Also, the analysis of the inhomogeneous entanglement for a condensed matter system is possibly of great importance for creating ideal entanglement resources in quantum information processing.

Acknowledgments

We thank J. L. Chen for helpful discussions. This work was supported by NSF of China (Grants No. 10575053 and No. 10605013) and LuiHui Center for Applied Mathematics through the joint project of Nankai and Tianjin Universities.

APPENDIX A: CALCULATION OF EXPECTATION VALUES OF PAIRS OF OPERATORS

In determining the expectation values of pairs of Majorana operators under the ground state, we have used the representation \( \{\alpha_k, \beta_k\} \) and the definition of the ground state \( \alpha_k|g\rangle = \beta_k|g\rangle = 0 \). If we define two independent real functions, i.e., Eq. (13) by

\[
\mathcal{F}(|n - m|) = \frac{1}{N} \sum_k e^{i\frac{2\pi}{N}(n - m)k} (|\bar{u}_k|^2 - |\bar{v}_k|^2) = \frac{1}{N} \sum_k \cos\left(\frac{2\pi}{N}k(n - m)|\Delta/\epsilon_k^\pm\right),
\]

which are obtained under the thermodynamical limit \( N \to \infty \) by making the replacement \( \frac{1}{N} \sum_k \to \frac{1}{\pi} \int_0^\pi d\varphi \), then the average values of Majorana operator pairs can be written as

\[
\langle A_{2n, A_{2m}} \rangle = \langle A_{2n-1, A_{2m-1}} \rangle = \delta_{n,m},
\]

\[
\langle B_{2n, B_{2m}} \rangle = \langle B_{2n-1, B_{2m-1}} \rangle = \delta_{n,m},
\]

\[
\langle A_{2n}(-iB_{2m}) \rangle = \langle A_{2n-1}(-iB_{2m-1}) \rangle = \mathcal{F}(|n - m|),
\]

\[
\langle A_{2n}A_{2m} \rangle = \langle (-iB_{2n})(-iB_{2m}) \rangle = i \sin \varphi \langle A_{2n} \rangle \langle A_{2m} \rangle,
\]

\[
\langle A_{2n}(-iB_{2m-1}) \rangle = \langle (-iB_{2n})(-iB_{2m-1}) \rangle = \cos \varphi \langle A_{2n} \rangle \langle A_{2m} \rangle.
\]

From these average values, we can calculate all correlation functions by using Wick theorem. For the nearest-neighbor case of \( \rho(2m - 1, 2m) \), we have

\[
\langle \sigma_{2m-1}^x \sigma_{2m}^x \rangle = \langle (-iB_{2m})A_{2m} \rangle = -\cos \varphi \langle A_{2m} \rangle,
\]

\[
\langle \sigma_{2m-1}^y \sigma_{2m}^y \rangle = -\langle A_{2m-1}(-iB_{2m}) \rangle = \cos \varphi \langle A_{2m} \rangle,
\]

\[
\langle \sigma_{2m-1}^x \sigma_{2m}^y \rangle = \langle \sigma_{2m-1}^y \sigma_{2m}^x \rangle = \sin \varphi \langle A_{2m} \rangle.
\]

For the nearest-neighbor case of \( \rho(2m, 2m + 1) \), we have

\[
\langle \sigma_{2m}^x \sigma_{2m+1}^x \rangle = \langle (-iB_{2m})A_{2m+1} \rangle = \cos \varphi \langle A_{2m+1} \rangle,
\]

\[
\langle \sigma_{2m}^y \sigma_{2m+1}^y \rangle = -\langle A_{2m}(-iB_{2m+1}) \rangle = -\cos \varphi \langle A_{2m+1} \rangle,
\]

\[
\langle \sigma_{2m}^x \sigma_{2m+1}^y \rangle = \langle \sigma_{2m}^y \sigma_{2m+1}^x \rangle = -\sin \varphi \langle A_{2m+1} \rangle.
\]

At last, for the next-nearest-neighbor case of \( \rho(2m - 1, 2m + 2) \), we have

\[
\langle \sigma_{2m-2}^x \sigma_{2m+1}^x \rangle = \langle (-iB_{2m-1})A_{2m}(-iB_{2m})A_{2m+1} \rangle = -\mathcal{G}(0)\mathcal{G}(1) - \mathcal{F}(0)\mathcal{F}(1),
\]

\[
\langle \sigma_{2m-2}^y \sigma_{2m+1}^y \rangle = -\langle A_{2m-1}A_{2m}(-iB_{2m+1}) \rangle = -\mathcal{G}(0)\mathcal{G}(1) - \mathcal{F}(0)\mathcal{F}(1),
\]

\[
\langle \sigma_{2m-2}^x \sigma_{2m+1}^y \rangle = \langle \sigma_{2m-2}^y \sigma_{2m+1}^x \rangle = 0.
\]

\[
\langle \sigma_{2m-2}^x \sigma_{2m+1}^x \rangle = \langle A_{2m-1}(-iB_{2m-1})A_{2m+1}(-iB_{2m+1}) \rangle = \mathcal{F}(0)^2 + \mathcal{G}(1)^2.
\]

[1] M. A. Nielsen and I. Chuang, Quantum Computation and Quantum Communication (Cambridge University Press, Cambridge, England, 2000).

[2] V. Vedral, Nature 453, 1004 (2008)

[3] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. 80, 517 (2008).
[4] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature 416, 608 (2002).
[5] T. J. Osborne and M. A. Nielsen, Phys. Rev. A 66, 032110 (2002).
[6] P. W. Anderson, Phys. Rev. 112, 1900 (1958).
[7] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
[8] L. Campos Venuti, C. Degli Esposti Boschi, and M. Roncaglia, Phys. Rev. Lett. 96, 247206 (2006).
[9] J. L. Chen, K. Xue, and M. L. Ge, Phys. Rev. A 76 042324 (2007).
[10] C. N. Yang, Phys. Rev. Lett. 19, 1312 (1967), Phys. Rev. 168, 1920 (1968).
[11] R. J. Baxter, Exactly Solved Models in Statistical Mechanics (Academic Press, London, 1982).
[12] E. K. Sklyanim, Zap. Nauchn. Semin. LOMI 95, 55 (1980); L. D. Faddeev, Integrable Models in 1 + 1 Dimensional QFT, Les Houches Lectures, (Elsevier, Amsterdam, 1984), pp.536-608; P. P. Kulish and E. K. Sklyanim, in Integral Quantum Field Theories, edited by J. Hietarinta and C. Montonen, Lecture Notes in Physics Vol. 151 (Springer, Berlin, 1982), pp. 61-119.
[13] M. Anderlini et al., Nature 448, 452 (2007).
[14] S. Trotzky, et al., Science 319, 295 (2008).
[15] S. Sachdev, Quantum Phase Transitions (Cambridge University Press, Cambridge, England, 1999).
[16] A. C. M. Carollo and J. K. Pachos, Phys. Rev. Lett. 95, 157203 (2005).
[17] S. L. Zhu, Phys. Rev. Lett. 96, 077206 (2006).
[18] W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
[19] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A 54, 3824 (1996).
[20] P. Pfeuty, Ann. Phys. 57, 79 (1970).
[21] E. Barouch and B. M. McCoy, Phys. Rev. A 3, 786 (1971).
[22] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. 60, 407 (1961).
[23] X. G. Wen, Quantum Field Theory of Many-Body Systems (Oxford University Press, Oxford, 2004).
[24] A. Hamma, R. Ionicioiu, and P. Zanardi, Phys. Lett. A 337, 22 (2005).