XY model on the circle: Diagonalization, spectrum, and forerunners of the quantum phase transition

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We exactly diagonalize the finite-size *XY* model with periodic boundary conditions and analytically determine the ground-state energy. We show that there are two types of Bogoliubov fermions, singles and pairs, whose dispersion relations have a completely arbitrary gauge-dependent sign. It follows that the ground state can be determined by a competition between the vacuum states (with a suitable gauge) of two parity sectors. We finally exhibit some points in finite-size systems that forerun criticality. They are associated to single Bogoliubov fermions and to the level crossings between physical and unphysical states. In the thermodynamic limit, they approach the ground state and build up singularities at logarithmic rates.

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I. INTRODUCTION

The analysis of one-dimensional spin chains is a useful approach to the modeling of quantum computers [1]. This class of systems has been thoroughly investigated in the thermodynamic limit [2–4]; however, experimental and theoretical difficulties impose strong bounds on the realization of large scale systems and this has boosted a high interest in finite-size systems [5–8]. The investigation of the last few years has focused on entanglement [9,10] in diverse finite-size models by means of direct diagonalization [11–18]. These studies were boosted by the recent discovery that entanglement can detect the presence of quantum phase transitions [19–25].

In this paper, we exactly diagonalize the *XY* model with periodic boundary conditions, describing a one-dimensional chain of spins with nearest-neighbor coupling, in a constant and uniform magnetic field. The *XY* model is a class of Hamiltonians distinguished by a different value of the anisotropy coefficient, which introduces a different coupling between the x and the y components of the spins (in particular, the isotropic case, corresponding to the case in which the anisotropy coefficient vanishes, is known as *XX* model).

Our aim is to perform a theoretical investigation and propose a strategy to look at the diagonalization of the *XY* spin model. As for infinite chains [4], the diagonalization procedure is divided in three steps: the Jordan-Wigner transformation, a deformed Fourier transform (generalizing the discrete Fourier transform), and a gauge-dependent Bogoliubov transformation. After the Jordan-Wigner transformation, the Hamiltonian, expressed as a quadratic form of annihilation and creation operators of spinless fermions, is characterized by the presence of a boundary term [2] whose contribution, which scales like $O(1/N)$, cannot be neglected for finite-size systems. However, this boundary term vanishes in Fourier space if the discrete Fourier transform is deformed with a local gauge coefficient, depending on the parity of the spins antiparallel to the magnetic field. This technique was introduced in [26]; however, we will follow a different approach that can be easily generalized to different boundary conditions and show that the deformation of the discrete Fourier transform comes out quite naturally as the result of a modular equation on its phases. After the Fourier transform, there emerge two classes of fermions, paired and single ones [4,26]. In particular, in the *XX* model there are only single fermions. The last step of the diagonalization procedure is the unitary Bogoliubov transformation given by a continuous rotation for fermion pairs and by a discrete one for single fermions.

In this paper, we exploit the simple fact that the Bogoliubov unitary transformation is gauge dependent, since it is given by two possible continuous rotations for fermion pairs and by either the identity or the charge-conjugation operator for single fermions. As a consequence, the sign of the dispersion relation is completely arbitrary, apart from the constraint that fermions belonging to the same pair have the same sign.

It seems that this feature, quite surprisingly, has been neglected in the large literature on finite-size spin models. Of course, by its very definition, a gauge freedom does not change the physical results. However, it paves the way to a deeper comprehension of physical phenomena.

From the gauge freedom of the Bogoliubov transformation, it follows that a possible expression for the diagonalized Hamiltonian is such that for successive intervals of the magnetic field, the vacuum energies of the two parity sectors alternatively coincide with the ground state and the first-excited level. We will exhibit this mechanism of "competition" between vacua.

Finally, we also present a way of looking at quantum phase transitions for this class of one-dimensional spin models. We will show that finite-size systems exhibit the "forerunners" of the points of quantum phase transition of the thermodynamic systems. They are associated to single Bogoliubov fermions and arise at the level crossings between physical and unphysical states. In fact, at the values of the magnetic field corresponding to the forerunners, the second derivative of the ground-state energy scales as $-\log N$, building up a singularity in the thermodynamical limit $N\to\infty$. Since in the XX model all Bogoliubov fermions are single, one reobtains the well-known result that in the thermodynamic limit, the anisotropic case presents two discrete quantum phase transitions whereas the isotropic or XX model is characterized by a continuous one.

II. XY HAMILTONIAN

We consider N spins on a circle with nearest-neighbor interaction in the xy plane and with a constant and uniform magnetic field along the z axis. The Hilbert space is $\mathcal{H}=\otimes_{i\in\mathbb{Z}_N}\mathfrak{H}_i$, where $\mathfrak{H}_i\cong\mathbb{C}^2$ is the Hilbert space of a single spin and $\mathbb{Z}_N$, labeling the positions on the circle, is the ring of integers mod N with the standard modular addition and multiplication. The XY Hamiltonian is given by

$$H_\gamma(g)=-J\sum_{i\in\mathbb{Z}_N}\left[g\sigma_i^z+\left(\frac{1+\gamma}{2}\right)\sigma_i^x\sigma_{i+1}^x+\left(\frac{1-\gamma}{2}\right)\sigma_i^y\sigma_{i+1}^y\right], \tag{1}$$

with

$$\sigma_i^l=\mathbb{1}\otimes\mathbb{1}\otimes\cdots\otimes\sigma^l\otimes\cdots\otimes\mathbb{1},\quad i\in\mathbb{Z}_N,\quad l\in\{x,y,z\}, \tag{2}$$

where σ^l acts on the ith spin and may be represented by the Pauli matrices. $J>0$ is a constant with dimensions of energy and $g\in\mathbb{R}$ and $\gamma\in[0,1]$ are two dimensionless parameters. g is the magnetic field and γ the degree of anisotropy in the xy plane, varying from 0 (XX or isotropic model) to 1 (Ising model). As is well known, in the thermodynamic limit, the diagonalization of the XY Hamiltonian is achieved by means of three transformations: the Jordan-Wigner (JW), Fourier, and Bogoliubov (BGV) transformations. We will first analyze in detail how the topology of the circle will induce a deformation on these transformations in finite-size chains.

A. Jordan-Wigner and deformed Fourier transformations

In this section, we set up the notation and recall some known results that we will need in the following. First of all, we will see that after applying the Jordan-Wigner transformation to the Hamiltonian, it will appear a boundary term proportional to the parity operator of the number of spins down in the system [2]. Fortunately, this operator commutes with the Hamiltonian and therefore one can separately diagonalize its projections on the eigenspace of even and odd parities [4,26,27]. The diagonalization procedure is given by a discrete Fourier transform; however, in case of finite-size systems, one has to take into account the presence of the boundary term and in order to get rid of it, one has to deform the standard Fourier transform by means of a local gauge phase [4,26]. We will obtain the above correct phase deformation by solving a modular equation based on the translational invariance of the model. This approach has the advantage of being suitable to generalizations to different boundary conditions.

The Jordan-Wigner transformation is based on the observation that there exists a unitary mapping

$$\mathcal{U}:(\mathbb{C}^2)^{\otimes N}\to\mathcal{F}_-(\mathbb{C}^N) \tag{3}$$

between the Hilbert space of a system of N spins $\mathcal{H}\cong(\mathbb{C}^2)^{\otimes N}$ and the fermion Fock space $\mathcal{F}_-(\mathbb{C}^N)$ of spinless fermions on N sites. Here,

$$\mathcal{F}_-(\mathfrak{H})=Q_-\bigoplus_{n\geq 0}\mathfrak{H}^n, \tag{4}$$

where $\mathfrak{H}^n=\mathfrak{H}^{\otimes n}$ for $n\geq 1$, $\mathfrak{H}^0=\mathbb{C}$, and Q_- is the projection onto the subspace of antisymmetric wave functions [28]. In order to simplify the notation, in the following we will use the above isomorphism and will identify the two spaces $\mathcal{H}\cong\mathcal{F}_-(\mathbb{C}^N)$ without making any longer mention to $\mathcal{U}$. By virtue of this identification, we can consider the canonical annihilation JW fermion operators [29]

$$c_i=\left(\prod_{j\in\mathbb{Z}_N,j<i}\sigma_j^z\right)\sigma_i^-=e^{i\pi\boldsymbol{n}_{i\downarrow}}\sigma_i^-,\quad\forall\quad i\in\mathbb{Z}_N, \tag{5}$$

where $\sigma_i^-=(\sigma_i^x-i\sigma_i^y)/2$ and $\boldsymbol{n}_{i\downarrow}$ is the operator counting the number of holes (or spins down) to the left of i

$$\boldsymbol{n}_{i\downarrow}=\sum_{j\in\mathbb{Z}_N,j<i}(1-c_j^\dagger c_j). \tag{6}$$

Note that the above definitions rely upon the following (arbitrary) ordering of $\mathbb{Z}_N$: $[0]<[1]<\cdots<[N-1]$, where $[k]=k+N\mathbb{Z}$. In particular, if the choice of the successive elements can be considered natural and is well adapted to the Hamiltonian (1), the choice of the first element [0] is totally arbitrary and is related to the choice of a privileged point of the circle.

The JW operators anticommute both on site and on different sites whereas the Pauli operators anticommute only on the same site. From Eq. (5), one sees that the term in the Hamiltonian describing the coupling between spins [0] and $[N-1]=[-1]$, when written in terms of the JW operators, is characterized by an operator phase at variance with the other coupling terms. This introduces some difficulties in the diagonalization of the Hamiltonian because its expression written in terms of the fermionic operators is characterized by the presence of a boundary term

$$\begin{aligned}H_\gamma(g)=-J\Bigg\{&\sum_{j\in\mathbb{Z}_N}[g(1-2c_jc_j^\dagger)+c_jc_{j+1}^\dagger+c_{j+1}c_j^\dagger+\gamma(c_jc_{j+1}\\&+c_{j+1}^\dagger c_j^\dagger)]-(e^{i\pi\boldsymbol{n}_\downarrow}+1)[(c_{[-1]}c_{[0]}^\dagger+c_{[0]}c_{[-1]}^\dagger)\\&+\gamma(c_{[-1]}c_{[0]}+c_{[0]}^\dagger c_{[-1]}^\dagger)]\Bigg\},\end{aligned} \tag{7}$$

where the number operator,

$$\boldsymbol{n}_\downarrow=\sum_{j\in\mathbb{Z}_N}(1-c_j^\dagger c_j), \tag{8}$$

counts the total number of spins down in the chain. In the thermodynamic limit, the boundary term can be neglected since it introduces corrections of order $1/N$; the problem is then reduced to the diagonalization of the so-called "c-cyclic" Hamiltonian [2] and can be easily achieved by means of a discrete Fourier transform.

Since we are interested in finite-size systems, with finite N, the boundary term cannot be neglected [4,26]. The main difficulty introduced by the boundary term in the Hamiltonian (7) is that it breaks the periodicity of the JW operators due to the arbitrary dependence of the phase $e^{i\pi \boldsymbol{n}_{i\downarrow}}$ on the ordering of the spins on the circle. However, Eq. (7) can be simplified by noting that the parity of the number of spins down,

$$\mathcal{P} = e^{i\pi \boldsymbol{n}_\downarrow}, \tag{9}$$

is conserved, $[\mathcal{P}, H_\gamma]=0$, although not so the spin-down number operator $\boldsymbol{n}_\downarrow$ itself. Its spectral decomposition is

$$\mathcal{P} = \sum_{\varrho=\pm 1} \varrho P_\varrho = P_+ - P_-. \tag{10}$$

Therefore, the Hamiltonian can be decomposed as [27]

$$H_\gamma = P_+ H_\gamma P_+ + P_- H_\gamma P_- = H_\gamma^{(+)} + H_\gamma^{(-)} \tag{11}$$

and the analysis can be separately performed in each parity sector, where $\mathcal{P}$ acts as a superselection charge.

In each sector, the *XY* Hamiltonian can be diagonalized by deforming the discrete Fourier transform by means of a local gauge α_j,

$$c_j = \frac{1}{\sqrt{N}} \sum_{k\in\mathbb{Z}_N} \exp\left(\frac{2\pi i}{N}(kj+\alpha_j)\right)\hat{c}_k, \quad j \in \mathbb{Z}_N. \tag{12}$$

This deformation preserves the anticommutation relations of $\hat{c}_k$ and $\hat{c}_k^\dagger$ in the Fourier space. The local gauge can be determined by imposing that the Fourier transforms of all terms in the sum of Eq. (7) have the same form. One gets, $\forall\ j \in \mathbb{Z}_N$,

$$\exp\left[\frac{2\pi i}{N}(\alpha_j - \alpha_{j+1})\right] = \exp[i\pi(n_\downarrow + 1)] \times \exp\left\{\frac{2\pi i}{N}[\alpha_{[-1]} - \alpha_{[0]}]\right\}. \tag{13}$$

Therefore, the left-hand side, like the right-hand side, must not depend on j,

$$\alpha_{j+1} - \alpha_j = \alpha, \quad \forall\ j \in \mathbb{Z}_N, \tag{14}$$

with α solution to the equation

$$\exp(2\pi i\alpha) = \exp[i\pi(n_\downarrow + 1)], \tag{15}$$

and the phase α_0 associated to the first site completely free. The solutions in the two parity sectors are

$$\alpha \equiv \frac{1+\varrho}{4}(\text{mod } N) \equiv \begin{cases} 0(\text{mod } N) & \text{if } \varrho = -1(n_\downarrow \text{odd}) \\ \frac{1}{2}(\text{mod } N) & \text{if } \varrho = +1(n_\downarrow \text{even}). \end{cases} \tag{16}$$

In conclusion, by substituting the (sector-dependent) deformed Fourier transform

$$c_j = \frac{e^{(2\pi i/N)\alpha_0}}{\sqrt{N}} \sum_{k\in\mathbb{Z}_N} \exp\left(\frac{2\pi i j}{N}(k+\alpha)\right)\hat{c}_k, \quad j \in \mathbb{Z}_N \tag{17}$$

into Eq. (7), we obtain

$$H_\gamma^{(\varrho)}(g) = -J \sum_{k\in\mathbb{Z}_N} \left\{ g + 2\hat{c}_k\hat{c}_k^\dagger\left[\cos\left(2\pi\frac{\alpha+k}{N}\right) - g\right] + i\gamma \sin\left(2\pi\frac{\alpha+k}{N}\right)(e^{4\pi i\alpha_0/N}\hat{c}_{\bar{k}}\hat{c}_k + e^{-4\pi i\alpha_0/N}\hat{c}_k^\dagger\hat{c}_{\bar{k}}^\dagger)\right\}P_\varrho, \tag{18}$$

where $\forall\ k \in \mathbb{Z}_N$,

$$\bar{k} = -2\alpha - k + N\mathbb{Z}. \tag{19}$$

A comment is now in order. Note that, alternatively, one could have deformed, instead of the Fourier transform, the JW transformation in the following way:

$$c_j = e^{i\pi n_{j\downarrow}} e^{-2\pi i/N(j\alpha+\alpha_0)}\sigma_j^-, \quad \forall\ j \in \mathbb{Z}_N \tag{20}$$

and would have obtained the same results.

B. Bogoliubov transformation: Gauge freedom

This section deals with the last step of the diagonalization procedure given by the Bogoliubov transformation. For finite-size systems, one finds that there are two classes of fermions, characterized by a different kind of Bogoliubov transformation [26,30]. Here we show that the Bogoliubov transformation has a gauge freedom, a simple fact that to our knowledge has been unrecognized in the literature.

Consider the Hamiltonian (18). When $\gamma > 0$, the last term couples fermions with momenta k and $\bar{k}$. In fact, there are two types of fermions: the single and the coupled ones (fermion pairs). Their momenta k belong to the two sets

$$\mathcal{S}_\varrho = \{k \in \mathbb{Z}_N | k = \bar{k}\} = \left\{k \in \mathbb{Z}_N \middle| 2k = -\frac{1+\varrho}{2} + N\mathbb{Z}\right\}, \tag{21}$$

$$\mathcal{C}_\varrho = \mathbb{Z}_N \setminus \mathcal{S}_\varrho, \tag{22}$$

respectively. Note that the mapping $k \mapsto \bar{k}$ is an involution of $\mathbb{Z}_N$, i.e., $\bar{\bar{k}} = k$. Therefore it can be viewed as an action of the group $\mathbb{Z}_2$ on the space $\mathbb{Z}_N$. From this perspective, $\mathcal{S}_\varrho$ and $\mathcal{C}_\varrho$ are nothing but the sets of points belonging to one-element and two-element orbits of the above action, respectively. The terms in the Hamiltonian involving pairs $(k,\bar{k})$ of fermions, in fact, depend only on the orbit. The *XY* Hamiltonian can be written accordingly as

$$H_\gamma^{(\varrho)}(g) = 2J\left\{\sum_{k\in\mathcal{S}_\varrho}\left[\cos\left(2\pi\frac{\alpha+k}{N}\right) - g\right]\left(\hat{c}_k^\dagger\hat{c}_k - \frac{1}{2}\right) + \frac{1}{2}\sum_{k\in\mathcal{C}_\varrho} \boldsymbol{C}_k^\dagger h_\gamma(k)\boldsymbol{C}_k\right\}P_\varrho, \tag{23}$$

where $\boldsymbol{C}_k^\dagger = (e^{-2\pi i\alpha_0/N}\hat{c}_k^\dagger, e^{2\pi i\alpha_0/N}\hat{c}_{\bar{k}})$ and $h_\gamma(k)$ is a Hermitian operator on $\mathbb{C}^2$ given by

$$h_\gamma(k) = -\gamma \sin\left(2\pi\frac{\alpha+k}{N}\right)\sigma^y + \left[\cos\left(2\pi\frac{\alpha+k}{N}\right) - g\right]\sigma^z. \tag{24}$$

The factor 1/2 in front of the pair terms in Eq. (23) derives from the identity $C_{\bar{k}}^\dagger h_\gamma(\bar{k}) C_{\bar{k}} = C_k^\dagger h_\gamma(k) C_k$ that expresses the fact that the various terms depend only on the orbit they belong to.

Let us first focus on fermion pairs. For each $k \in \mathcal{C}_\varrho$, h_γ can be thought as a vector in the yz plane of the internal space of the pair and is diagonalized by a unitary rotation along x up to the z direction,

$$R_x(\theta_k) h_\gamma(k) R_x(\theta_k)^\dagger = \tilde{h}\sigma^z, \tag{25}$$

with $\tilde{h} \in \mathbb{R}$ and $R_x(\theta_k) = \exp(-i\frac{\theta_k}{2}\sigma^x)$. One obtains

$$\gamma \sin\frac{2\pi(\alpha+k)}{N}\cos\,\theta_k + \left[\cos\frac{2\pi(\alpha+k)}{N} - g\right]\sin\,\theta_k = 0. \tag{26}$$

Note that for each pair $(k,\bar{k})$, there are *two* possible solutions that differ by π,

$$\theta_k^s = \theta_k + s\pi, \quad \theta_{\bar{k}}^s = -\theta_k + s\pi, \quad s \in \{0,1\}, \tag{27}$$

where

$$\theta_k = \arctan\left(\frac{\gamma \sin\left(2\pi\frac{\alpha+k}{N}\right)}{g - \cos\left(2\pi\frac{\alpha+k}{N}\right)}\right) \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right], \tag{28}$$

and

$$\tilde{h} = \left[\cos\frac{2\pi(\alpha+k)}{N} - g\right]\cos\,\theta_k^s(1 + \tan^2\,\theta_k^s). \tag{29}$$

The unitary transformation $R_x(\theta_k^s)$ applied to C_k defines a new vector of fermion operators $B_{k,s}^\dagger = (b_k^\dagger, b_{\bar{k}}) = C_k^\dagger R_x(\theta_k^s)^\dagger$, for $k \in \mathcal{C}_\varrho$ and $s \in \{0,1\}$, where $B_{k,0}$ is related to $B_{k,1}$ by the relation

$$B_{k,1} = R_x(\pi) B_{k,0}, \quad k \in \mathcal{C}_\varrho \tag{30}$$

(see Fig. 1). The fermion operators b_k and $b_{\bar{k}}$ are the Bogoliubov operators and R_x is the Bogoliubov transformation for fermion pairs. By noting that $\cos\,\theta_k^s = (-1)^s(1+\tan^2\,\theta_k^s)^{-1/2}$, for each pair of momenta one gets

$$H_{\gamma,k}^{(\varrho)} = C_k^\dagger h_\gamma(k) C_k = (-1)^s \varepsilon_k^{(\varrho)}(g) B_{k,s}^\dagger \sigma^z B_{k,s},$$

$$k \in \mathcal{C}_\varrho, \quad s \in \{0,1\}, \tag{31}$$

where $\varepsilon_k^{(\varrho)}$ is the dispersion relation for fermion pairs

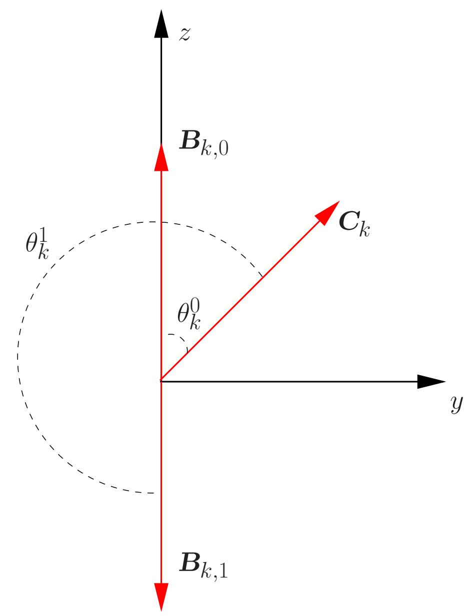

FIG. 1. (Color online) Bogoliubov rotation for fermion pairs.

$$\varepsilon_k^{(\varrho)}(g) = \mathrm{sgn}\left[\cos\frac{2\pi(\alpha+k)}{N} - g\right] \times \sqrt{\left[\cos\frac{2\pi(\alpha+k)}{N} - g\right]^2 + \gamma^2\sin^2\frac{2\pi(\alpha+k)}{N}}. \tag{32}$$

Here, $\mathrm{sgn}\,x = x/|x|$ for $x \neq 0$ and $\mathrm{sgn}\,0 = 0$. Note that the choice between the two possible angles θ_k^s affects the Bogoliubov vectors $B_{k,s}$ by exchanging particles with antiparticles, while the corresponding dispersion relation is affected by a sign $(-1)^s$. We stress that for each $k \in \mathcal{C}_\varrho$, the Bogoliubov rotation is defined independently of the other pairs and so the sign of the dispersion relation can be chosen in a completely arbitrary way, pair by pair. It is not difficult to show that the unitary operator on the Fock space $\mathcal{F}_-(\mathbb{C}^N)$, corresponding to a Bogoliubov rotation $R_x(\theta)$, reads

$$U_k(\theta) = \exp\left(-i\frac{\theta}{2}K_k\right), \quad K_k = \hat{c}_k^\dagger \hat{c}_{\bar{k}}^\dagger + \hat{c}_{\bar{k}}\hat{c}_k, \quad k \in \mathcal{C}_\varrho. \tag{33}$$

Its action on the Hamiltonian is

$$U_k(\theta_k^s) H_{\gamma,k}^{(\varrho)} U_k(\theta_k^s)^\dagger = (-1)^s \varepsilon_k^{(\varrho)}(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{\bar{k}}\hat{c}_{\bar{k}}^\dagger) \tag{34}$$

for $k \in \mathcal{C}_\varrho$. Observe that since K_k is quadratic with respect of creation and annihilation operators, it commutes with the parity operator (9),

$$\mathcal{P} = U_k(\theta)\mathcal{P}U_k^\dagger(\theta), \quad k \in \mathcal{C}_\varrho, \tag{35}$$

and this means that the Bogoliubov transformation for fermion pairs preserves the parity sector. Finally, according to (30), one gets the relation

$$U_k(\theta_k^1) = V_{k\bar{k}} U_k(\theta_k^0), \quad \text{with} \;\; V_{k\bar{k}} = U_k(\pi), \quad k \in \mathcal{C}_\varrho. \tag{36}$$

Note that the unitary operator $V_{k\bar{k}}$ can be decomposed in the form

$$V_{k\bar{k}} = S_{k\bar{k}} C_k C_{\bar{k}}, \tag{37}$$

where C_k and $S_{k\bar{k}}$ are, respectively, the charge-conjugation operator, $C_k \hat{c}_k C_k^\dagger = \hat{c}_k^\dagger$, and the swapping operator $S_{k\bar{k}} \hat{c}_k S_{k\bar{k}}^\dagger = -i\hat{c}_{\bar{k}}$, given by

$$C_k = \exp\left(i\frac{\pi}{2}(\hat{c}_k + \hat{c}_k^\dagger) \right), \tag{38}$$

$$S_{k\bar{k}} = \exp\left(i\frac{\pi}{2}(\hat{c}_k^\dagger \hat{c}_{\bar{k}} + \hat{c}_{\bar{k}}^\dagger \hat{c}_k) \right), \quad k \in \mathcal{C}_\varrho. \tag{39}$$

Consider now the case of single fermions, $k \in \mathcal{S}_\varrho$. The set $\mathcal{S}_\varrho$ depends both on the parity sector and on the parity of N. For N even one gets

$$\mathcal{S}_\varrho = \begin{cases} \left\{ [0], \left[\frac{N}{2} \right] \right\} & \text{if } \varrho = -1 \\ \{[0]\} & \text{if } \varrho = +1, \end{cases} \tag{40}$$

while for N odd,

$$\mathcal{S}_\varrho = \begin{cases} \{[0]\} & \text{if } \varrho = -1 \\ \left\{ \left[\frac{N-1}{2} \right] \right\} & \text{if } \varrho = +1. \end{cases} \tag{41}$$

It is convenient to look at single fermions as a degenerate case of Bogoliubov pairs. Indeed, Eq. (28) reduces to

$$\tan \theta_k = 0, \quad k \in \mathcal{S}_\varrho, \tag{42}$$

whose solutions are given by $\theta_k^s = s\pi$, with $s \in \{0,1\}$. Therefore, in this case we are free to choose between two possible unitary transformations: the identity and the charge conjugation,

$$U_k = (C_k)^0 = 1 \quad \text{or} \quad U_k = C_k, \quad k \in \mathcal{S}_\varrho. \tag{43}$$

Note that an important consequence of this gauge freedom is that the parity is *not* always preserved: if charge conjugation is chosen, two parity sectors are swapped by the Bogoliubov transformation

$$\mathcal{P} = -C_k \mathcal{P} C_k^\dagger. \tag{44}$$

Finally, note that for single fermions, the dispersion relation (32) reduces to

$$\varepsilon_k^{(\varrho)}(g) = \cos\left(2\pi \frac{\alpha + k}{N} \right) - g, \quad k \in \mathcal{S}_\varrho, \tag{45}$$

since $\sin[2\pi(\alpha+k)/N]=0$, when $k \in \mathcal{S}_\varrho$.

In conclusion, the total Bogoliubov transformation that diagonalizes the Hamiltonian (23) has the form

$$U_B(g,\gamma;\varrho,\boldsymbol{s}) = \prod_{k \in \mathcal{C}_\varrho/\mathbb{Z}_2} U_k(\theta_k)(V_{k\bar{k}})^{s_k} \prod_{j \in \mathcal{S}_\varrho} (C_j)^{s_j}, \tag{46}$$

where

$$\boldsymbol{s} = (s_k) \in \{0,1\}^N, \quad \text{with} \;\; s_k = s_{\bar{k}}, \tag{47}$$

and the restriction of the product to $\mathcal{C}_\varrho/\mathbb{Z}_2$ implies that, in the case of coupled fermions, one must consider only one element for each pair (orbit of $\mathbb{Z}_2$). Due to the constraint in Eq. (47), we infer that the Bogoliubov unitary transformation has a gauge freedom represented by the arbitrary choice of a binary vector of length $|\mathcal{S}_\varrho| + |\mathcal{C}_\varrho|/2$.

Note that the anticommutation relations are preserved by the Bogoliubov transformation, while the parity sectors are swapped according to

$$\mathcal{P} = (-1)^{|\boldsymbol{s}|_\varrho} U_B(g,\gamma;\varrho,\boldsymbol{s}) \mathcal{P} U_B(g,\gamma;\varrho,\boldsymbol{s})^\dagger, \tag{48}$$

where

$$|\boldsymbol{s}|_\varrho = |\boldsymbol{s}_{\mathcal{S}_\varrho}| = \sum_{k \in \mathcal{S}_\varrho} s_k. \tag{49}$$

Therefore, one obtains the final expression of the diagonalized Hamiltonian

$$\begin{aligned} \tilde{H}_\gamma^{(\varrho)}(g) &= U_B(g,\gamma;\varrho,\boldsymbol{s}) H_\gamma^{(\varrho)}(g) U_B(g,\gamma;\varrho,\boldsymbol{s})^\dagger \\ &= 2J \sum_{k \in \mathbb{Z}_N} (-1)^{s_k} \varepsilon_k^{(\varrho)}(g) \left(\hat{c}_k^\dagger \hat{c}_k - \frac{1}{2} \right) P_{\bar{\varrho}}, \end{aligned} \tag{50}$$

where $\bar{\varrho} = (-1)^{|\boldsymbol{s}|_\varrho} \varrho$, which depends on an arbitrary vector $\tilde{\boldsymbol{s}} \in \{0,1\}^{|\mathcal{S}_\varrho| + |\mathcal{C}_\varrho|/2}$ that generates $\boldsymbol{s}$ by the relation $s_k = s_{\bar{k}} = \tilde{s}_k$. Note that the physical part of $\tilde{H}_\gamma^{(\varrho)}$ acts on the sector of parity $\bar{\varrho}$.

C. *XY* ground state: Vacua competition

One can use the gauge freedom of the Bogoliubov transformation (46) in the following convenient way. Let $\boldsymbol{s} = \boldsymbol{s}(g)$ be a function of the intensity of the magnetic field g such that $(-1)^{s_k(g)} \varepsilon_k^{(\varrho)}(g) \geq 0$ for every $g \in \mathbb{R}$. From Eq. (32), this means that

$$(-1)^{s_k(g)} = \operatorname{sgn}\left[\cos \frac{2\pi(\alpha + k)}{N} - g \right], \tag{51}$$

that is

$$s_k(g) = \frac{1}{2} - \frac{1}{2} \operatorname{sgn}\left[\cos \frac{2\pi(\alpha + k)}{N} - g \right]. \tag{52}$$

Note that since $s_{\bar{k}}(g) = s_k(g)$, the above solution is consistent with the constraint (47) of $\boldsymbol{s}$. Therefore, the diagonalized expression of the *XY* Hamiltonian reads

$$H_\gamma^{(\varrho)}(g) = 2J \sum_{k \in \mathbb{Z}_N} |\varepsilon_k^{(\varrho)}(g)| \left(\hat{c}_k^\dagger \hat{c}_k - \frac{1}{2} \right) P_{\bar{\varrho}(g)}, \tag{53}$$

where $\bar{\varrho}(g) = (-1)^{|\boldsymbol{s}(g)|_\varrho} \varrho$. With this choice, in each parity sector, the lowest energy state is the one with zero fermions (*vacuum state*) whose energy density/J is given by

$$E_{\mathrm{vac}}^{(\varrho)}=-\frac{1}{N}\sum_{k\in\mathbb{Z}_N}\left\{\left[g-\cos\left(\frac{2\pi k}{N}+\frac{(1+\varrho)\pi}{4N}\right)\right]^2+\gamma^2\sin^2\left(\frac{2\pi k}{N}+\frac{(1+\varrho)\pi}{4N}\right)\right\}^{1/2}, \tag{54}$$

with $\varrho=\pm 1$. Note, however, that a condition must be satisfied: the Bogoliubov vacuum state is a physical state, *provided* it has the right parity $\bar{\varrho}(g)$. Were this is not the case, the projection $P_{\bar{\varrho}(g)}$ would automatically rule it out.

Let us look at the function $\bar{\varrho}(g)$ more closely. For N even, we have from Eqs. (40) and (52)

$$|s(g)|_{\varrho}=[s_{[0]}(g)+s_{[N/2]}(g)]\delta_{\varrho,-1}=\left[1+\frac{1}{2}\mathrm{sgn}(1-g)-\frac{1}{2}\mathrm{sgn}(1+g)\right]\delta_{\varrho,-1}, \tag{55}$$

where

$$\bar{\varrho}(g)=\mathrm{sgn}\left(1-\frac{1-\varrho}{2}g^2\right)\quad (N\ \text{even}). \tag{56}$$

For N odd, we have from Eqs. (41) and (52)

$$|s(g)|_{\varrho}=s_{[0]}(g)\delta_{\varrho,-1}+s_{[N-1/2]}(g)\delta_{\varrho,+1}=\frac{1}{2}-\frac{1}{2}\mathrm{sgn}(1-g)\delta_{\varrho,-1}+\frac{1}{2}\mathrm{sgn}(1+g)\delta_{\varrho,+1}, \tag{57}$$

where

$$\bar{\varrho}(g)=-\mathrm{sgn}(1+\varrho g)\quad (N\ \text{odd}). \tag{58}$$

Since the vacuum state has N holes, its parity is $(-1)^N$ and it is a physical state only if

$$\bar{\varrho}(g)=(-1)^N. \tag{59}$$

Equation (59) is satisfied for arbitrary ϱ when $g\in(-1,1)$, while it is true only for $\varrho=(-1)^N$ for $g<-1$ and $\varrho=+1$ for $g>1$. Therefore, for $g\in(-1,1)$, in the various regions of magnetic field g, the ground state is alternatively given by one of the two vacua with energy (54). We call this mechanism *vacua competition* between the two parity sectors (see Fig. 2).

For $g<-1$, the vacuum state with $\varrho=-1$ for N even ($\varrho=+1$ for N odd) is not physical because it has the wrong parity $\bar{\varrho}=\varrho=-(-1)^N$ and it is ruled out by the projection $P_{\bar{\varrho}}$. Analogously, for $g>1$ the vacuum state with $\varrho=-1$ for both N even and odd is ruled out. However, it is not difficult to prove that the energy of the unphysical vacuum when $|g|>1$ is always larger than the physical one. Therefore, as far as one is interested in the ground state, the ground state is the result of the vacua competition in the *whole* range $g\in\mathbb{R}$. Not so for the first-excited level, which is the energy of the "losing" vacuum only in the range $(-1,1)$, while outside it is the lowest one-fermion energy level above the losing vacuum.

More generally, from Eqs. (56) and (58), it easily follows that the whole spectrum is given for $g\in(-1,1)$ by the union of the spectra of eigenstates with an even number of Bogoliubov fermions $[\bar{\varrho}=(-1)^N]$ of both Hamiltonians $\tilde{H}_{\gamma}^{(\varrho)}$, with $\varrho=\pm 1$. On the other hand, outside the above interval,

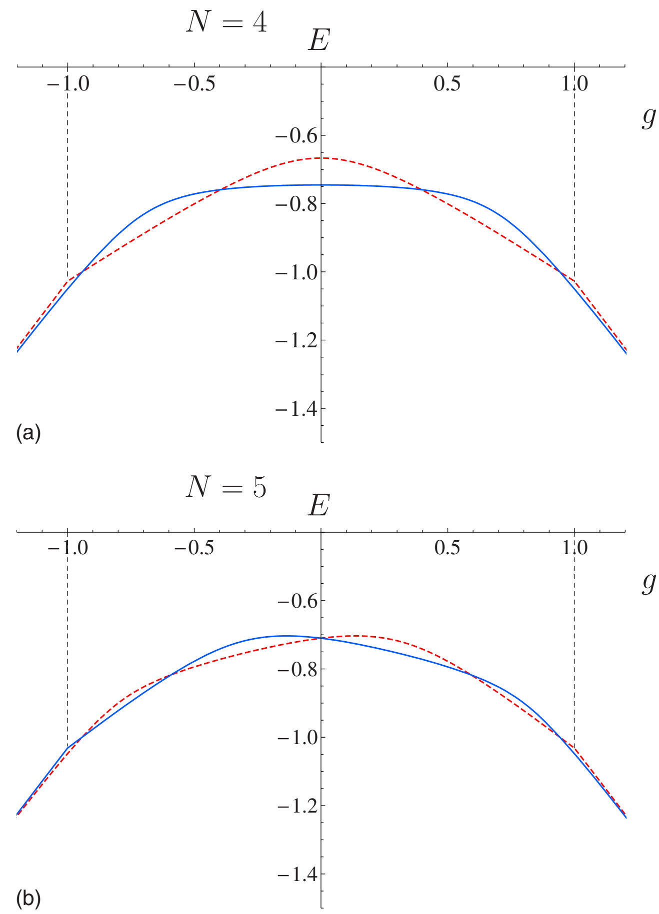

FIG. 2. (Color online) Vacua competition for $N=4$ and 5 spins: in both cases, the dashed line corresponds to $E_{\mathrm{vac}}^{(-)}$ and the solid one to $E_{\mathrm{vac}}^{(+)}$.

the spectrum is given by the eigenstates of $\tilde{H}_{\gamma}^{(\varrho)}(\tilde{H}_{\gamma}^{(-\varrho)})$ with an even (odd) number of Bogoliubov particles, where $\varrho=(-1)^N$ for $g<-1$ and $\varrho=+1$ for $g>1$. The intersection points between the vacua energy densities depend in general on the number of spins N; however, independently of N, the difference between the two energy densities,

$$E_{\mathrm{vac}}^{\mathrm{diff}}(g)=E_{\mathrm{vac}}^{(-)}-E_{\mathrm{vac}}^{(+)}=-\frac{1}{N}\sum_{m\in\mathbb{Z}_{2N}}(-1)^m\left\{\left[g-\cos\left(\frac{\pi m}{N}\right)\right]^2+\gamma^2\sin^2\left(\frac{\pi m}{N}\right)\right\}^{1/2}, \tag{60}$$

always vanishes at $g=\pm\sqrt{1-\gamma^2}$ (see Fig. 3). Indeed one has

$$E_{\mathrm{vac}}^{\mathrm{diff}}(\pm\sqrt{1-\gamma^2})=-\frac{1}{N}\sum_{k\in\mathbb{Z}_{2N}}(-1)^m\left[1\mp\sqrt{1-\gamma^2}\cos\left(\frac{\pi m}{N}\right)\right] \tag{61}$$

and

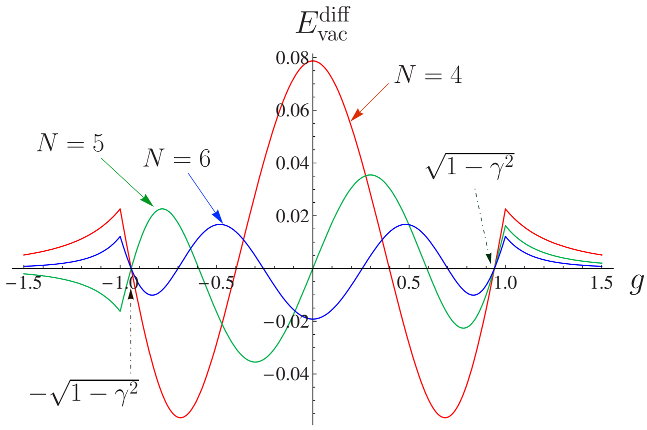

FIG. 3. (Color online) Difference between energy densities (in unit J) of the two vacua at $\gamma=\frac{1}{3}$ for $N=4,5,6$. For all N, $E_{\rm vac}^{\rm diff}$ vanishes at $g=\sqrt{1-\gamma^2}$.

$$\sum_{k\in\mathbb{Z}_{2N}}(-1)^m\cos\left(\frac{\pi m}{N}\right)=\mathrm{Re}\left(\frac{1-e^{i2\pi(N+1)}}{1-e^{i\pi(N+1)/N}}\right)=0. \quad (62)$$

From Fig. 3, one can also observe that for finite-size systems, the vacua intersection points present discontinuities of the first derivative, as will be explicitly shown in Sec. IV. In that section, we will also focus on the points $g=\pm 1$, which are two interesting values of the magnetic field for this class of Hamiltonians, since they will be shown to represent the *finite-size forerunners* of the quantum phase-transition points (in the thermodynamic limit). Finally, it is worth mentioning that an analogous description in terms of vacuum states belonging to different parity sectors can be found already in numerical investigations (see, for example, [31]). In fact, in these works, one is interested in the diagonalization of the chain Hamiltonian and is faced with the problem of resolving a phase ambiguity, which is nothing but the Bogoliubov gauge introduced here. For this reason, our results can be of interest also for numerical applications.

III. *XX* MODEL

In this section, we look at a particular case of the *XY* model: the *XX* model ($\gamma=0$) known as the isotropic model. In fact, as recently shown [32], the symmetry of this model enables one to reconstruct the spectrum of the system and in particular the expression of the ground state by following a direct approach. Thus, we will use it as a benchmark for the method here proposed.

Since $\gamma=0$, the interaction between nearest-neighbors spins along x and y axis is characterized by the same coefficient in the Hamiltonian (1),

$$H_{XX}(g)=H_{\gamma=0}(g)=-J\sum_{i\in\mathbb{Z}_N}\left[g\sigma_i^z+\frac{1}{2}\sigma_i^x\sigma_{i+1}^x+\frac{1}{2}\sigma_i^y\sigma_{i+1}^y\right]. \quad (63)$$

Equation (18) then reduces to

$$H_0^{(\varrho)}(g)=2J\sum_{k\in\mathbb{Z}_N}\left[\cos\left(2\pi\frac{\alpha+k}{N}\right)-g\right]\left(\hat{c}_k\hat{c}_k^\dagger-\frac{1}{2}\right)P_\varrho,$$

$$\alpha=\frac{1+\varrho}{4}. \quad (64)$$

From this follows that the Fourier-transformed *XX* Hamiltonian is already diagonal and the last term characterizing coupled fermions in Eq. (18) vanishes for all k. In other words, in the *XX* model, we are only dealing with single fermions, $\mathcal{S}_\varrho=\mathbb{Z}_N$, and the Bogoliubov transformation (46) reduces to

$$U_B(g;\varrho,\boldsymbol{s})=\prod_{k\in\mathbb{Z}_N}C_k^{s_k}, \quad (65)$$

where now $\boldsymbol{s}\in\{0,1\}^N$ is an *unconstrained* binary string of length N. This yields

$$\begin{aligned}\tilde{H}_0^{(\varrho)}(g)&=U_B(g;\varrho,\boldsymbol{s})H_0^{(\varrho)}(g)U_B(g;\varrho,\boldsymbol{s})^\dagger\\&=2J\sum_{k\in\mathbb{Z}_N}(-1)^{s_k}\left[\cos\left(2\pi\frac{\alpha+k}{N}\right)-g\right]\\&\quad\times\left(\hat{c}_k\hat{c}_k^\dagger-\frac{1}{2}\right)P_{\bar{\varrho}},\end{aligned} \quad (66)$$

with $\bar{\varrho}=(-1)^{|s|}\varrho$. In particular, if $s_k=0$, the Bogoliubov transformation associates JW fermions to Bogoliubov fermions, while if $s_k=1$, it transforms JW fermions into Bogoliubov antifermions or holes.

Energy spectrum

As already emphasized at the end of Sec. II B, the energy spectrum does not depend on the choice of the gauge $\boldsymbol{s}$ of the unitary Bogoliubov transformation. If $\boldsymbol{s}=0$, Eq. (66) becomes

$$\tilde{H}_0^{(\varrho)}=H_0^{(\varrho)}=2J\sum_{k\in\mathbb{Z}_N}\left[\cos\left(2\pi\frac{\alpha+k}{N}\right)-g\right]\left(\hat{c}_k^\dagger\hat{c}_k-\frac{1}{2}\right)P_\varrho. \quad (67)$$

The spectrum of the above Hamiltonian, and in particular its ground-state energy, has been studied in [32]. We quickly summarize the main results and show how they derive from vacua competition.

One can show that the general expression of the lowest energy levels in the different n-particle sectors does not depend on the parity of N. For n fermions, one gets

$$E_n^{\min}(g)=g\left(1-\frac{2n}{N}\right)-\frac{2}{N}\frac{\sin(n\pi/N)}{\sin(\pi/N)}. \quad (68)$$

In Fig. 4, we plot the lowest energy levels corresponding to $0\leq n\leq N$ for $N=8$ sites. The intersections of levels corresponding to n and $n+1$ fermions (starting from $n=0$) define the *points of level crossing* g_c, where an excited level and the ground state are interchanged. The analytic expression of the critical points is easily obtained by the condition $E_n^{\min}(g_c)=E_{n+1}^{\min}(g_c)$. We find

$$g_c(n)=\frac{\sin(n\pi/N)-\sin[(n+1)\pi/N]}{\sin(\pi/N)}, \quad (69)$$

for $0\leq n\leq N-1$. As a consequence, the ground-state energy density is

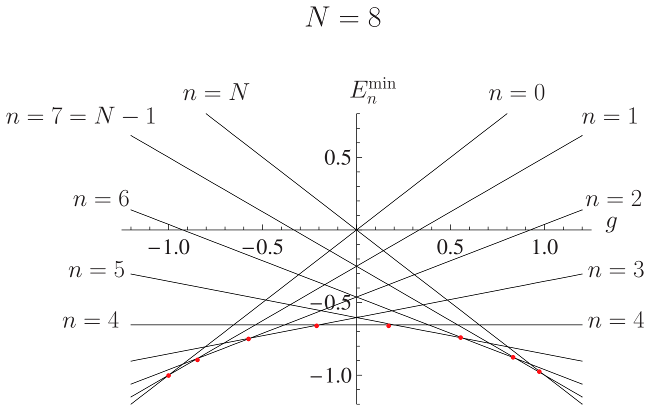

FIG. 4. (Color online) Lowest energy levels $E_n^{\min}(g)$ for different number of fermions n; the intersections between the energy levels corresponding to n and $n+1$ fermions (starting from $n=0$) are the points of level crossing (dots).

$$E_{\rm gs}(g) = g\left(1 - \frac{2n}{N}\right) - \frac{2}{N}\frac{\sin(n\pi/N)}{\sin(\pi/N)}, \quad 0 \le n \le N, \tag{70}$$

with $g \in (g_c(n-1), g_c(n))$ and where we stipulated that $g_c(-1) = -\infty$ and $g_c(N) = +\infty$. Thus, for $g \in (g_c(n-1), g_c(n))$, the ground state contains n JW fermions. Note that $g_c(0) = -1$ and $g_c(N-1) = +1$, independently of N.

We will now derive the ground-state energy density starting from the same choice of the Bogoliubov transform made for the XY model (53) that particularizes to

$$\tilde{H}_0^{(\varrho)}(g) = 2J\sum_{k\in\mathbb{Z}_N}\left|\cos\left(2\pi\frac{\alpha+k}{N}\right) - g\right|\left(\hat{c}_k^\dagger\hat{c}_k - \frac{1}{2}\right)P_{\bar{\varrho}(g)}, \tag{71}$$

with $\bar{\varrho}(g) = (-1)^{|s(g)|}\varrho$. The ground state is then the winner of the vacua competition between $E_{\rm vac}^{(-)}$ and $E_{\rm vac}^{(+)}$, where

$$E_{\rm vac}^{(\varrho)}(g) = -\frac{1}{N}\sum_{k\in\mathbb{Z}_N}\left|\cos\left(\frac{2\pi k}{N} + \frac{(1+\varrho)\pi}{4N}\right) - g\right| \tag{72}$$

(see Fig. 5). The points of level crossing (69) are given by those values of the magnetic field that satisfy the following equation:

$$E_{\rm vac}^{\rm diff}(g) = -\frac{1}{N}\sum_{k\in\mathbb{Z}_{2N}}(-1)^k\left|\cos\left(\frac{\pi k}{N}\right) - g\right| = 0. \tag{73}$$

Consider the regular polygon inscribed in a circle of unit radius in Fig. 6. It is a geometrical representation of the function $\cos(\frac{\pi k}{N})$ for $k \in \mathbb{Z}_N$. When $|g| > 1$, one immediately gets $E_{\rm vac}^{\rm diff}(g) = 0$, whereas for $|g| \le 1$, the key idea is to consider the N intervals on the x axis limited by the dashed vertical lines, represented in Fig. 6. For each interval one can write the explicit expression for the vacua difference (73). For example, when $g \in [\cos(\frac{\pi}{N}), 1]$, one gets

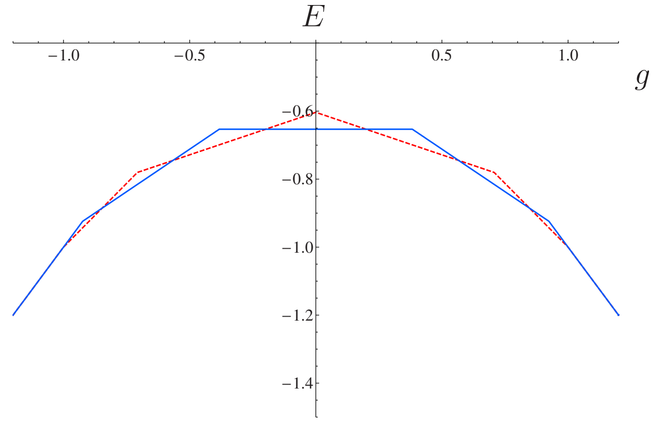

FIG. 5. (Color online) The ground-state energy density of the XX model ($N=8$) is given by the competition between the vacua energy densities $E_{\rm vac}^{(-)}$ (dashed line) and $E_{\rm vac}^{(+)}$ (solid line).

$$E_{\rm vac}^{\rm diff}(g) = -\frac{1}{N}\left\{(1-g) + \sum_{k\in\mathbb{Z}_{2N}, k\neq[0]}(-1)^k\left[g - \cos\left(\frac{\pi k}{N}\right)\right]\right\}$$
$$= -\frac{2}{N}(1-g), \tag{74}$$

from which follows that in this interval $E_{\rm vac}^{\rm diff}(g) = 0$ for $g = 1$. Similarly when $g \in [\cos\frac{(m+1)\pi}{N}, \cos\frac{m\pi}{N}]$, for $0 \le m \le N-1$, one gets that $E_{\rm vac}^{\rm diff}(g) = 0$ when

$$g = (-1)^m\left[1 + 2\sum_{k=1}^{m}\cos\left(\frac{\pi k}{N}\right)\right] = -g_c(m), \quad 0 \le m \le N-1, \tag{75}$$

where $g_c(m)$ are the points of level crossing (69) [for $n=0$, one gets $g=1$, in agreement with Eq. (73)]. By virtue of the symmetry $g_c(n) = -g_c(N-1-n)$, one immediately sees that the level crossing points have the same analytic expression of the intersection points between the two vacua for $n = N - 1 - m$.

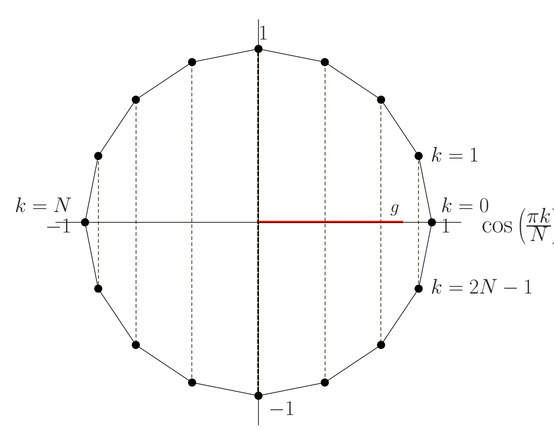

FIG. 6. (Color online) Geometrical representation of Eq. (73) when $N=8$; the thick red line is the magnetic field g.

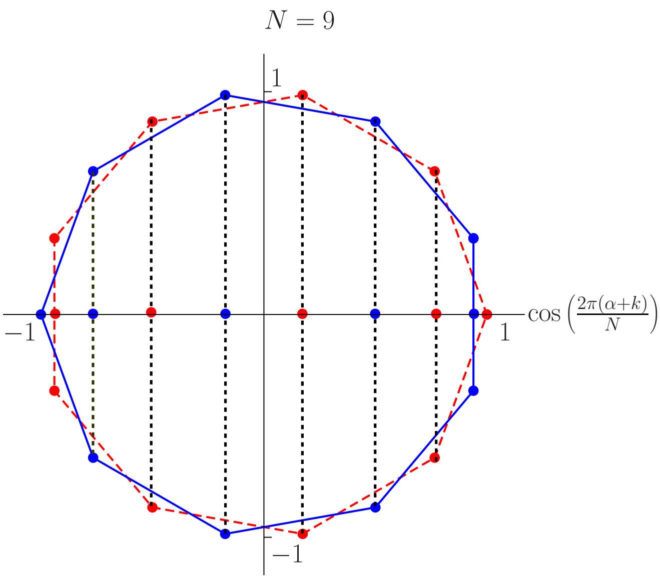

FIG. 7. (Color online) Geometrical description for $\cos(\frac{2\pi(\alpha+k)}{N})$ for $N=9$: the two polygons belong to the parity sectors $\alpha=0(\mathrm{mod}\ N)$ (dashed line) and $\alpha\equiv 1/2(\mathrm{mod}\ N)$ (solid line)

IV. THERMODYNAMIC LIMIT AND QUANTUM PHASE TRANSITIONS

In this final section, we exhibit an unexpected link with quantum phase transitions: the combination of the Bogoliubov gauge with the conservation of parity sectors uniquely determines the points where quantum phase transition will occur when the size of the system becomes infinite. These points correspond to single Bogoliubov fermions. In fact, while the gauge of Bogoliubov pairs does not affect parity, the gauge of single fermions does change it. Thus, it couples physical states with unphysical ones (with wrong parity). It is just at the level crossings of these states that quantum phase transitions will occur. Because of the different symmetries between the isotropic and the anisotropic cases, we will separately consider these two cases.

A. Quantum phase transitions in the *XY* model

In the anisotropic case, the forerunners of the points of quantum phase transition are characterized by the presence of large values of the second derivative of the ground-state energy density that is then amplified and gives rise to a singularity in the thermodynamic limit. As observed in Sec. II C, the first derivative of the ground-state energy evaluated at the intersection points between the two vacua is not continuous and for finite-size systems, the second derivatives diverge at these points; however we will show that these singularities vanish when $N\to\infty$. Consider, for example, the level crossing at $g=\sqrt{1-\gamma^2}$. The difference between the first derivatives of the two vacuum energies is given by the derivative of Eq. (60)

$$\frac{dE_{\mathrm{vac}}^{\mathrm{diff}}}{dg}(\sqrt{1-\gamma^2})=\frac{1}{N}\frac{\gamma^2}{\sqrt{1-\gamma^2}}\sum_{k\in\mathbb{Z}_N}\left[\frac{1}{1-\sqrt{1-\gamma^2}\cos\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)}-\frac{1}{1-\sqrt{1-\gamma^2}\cos\left(\frac{2\pi k}{N}\right)}\right]. \tag{76}$$

When the number of spins N is odd, for each $k\in\mathbb{Z}_N$, there is a given $\tilde{k}=k+\frac{N}{2}$ such that $\cos(\frac{2\pi k}{N})=-\cos(\frac{2\pi\tilde{k}}{N}+\frac{\pi}{N})$ (see Fig. 7) and the last equation becomes

$$\frac{dE_{\mathrm{vac}}^{\mathrm{diff}}}{dg}(\sqrt{1-\gamma^2})=\frac{1}{N}\frac{\gamma^2}{\sqrt{1-\gamma^2}}\left[\frac{2\sqrt{1-\gamma^2}}{\gamma^2}+4\sum_{k=1}^{(N-1)/2}\frac{\cos\left(\frac{2\pi k}{N}\right)\sqrt{1-\gamma^2}}{1-\cos\left(\frac{2\pi k}{N}\right)(1-\gamma^2)}\right]. \tag{77}$$

From the symmetries of the function $\cos(\frac{2\pi k}{N})$, one gets that the last expression is strictly greater than zero. From this, it follows that the second derivative of the vacua energy difference diverges for all finite N at $g=\sqrt{1-\gamma^2}$ and the same argument can be extended to all intersection points between the two vacua. The case of even N is analogous, as one can see by noting that the polygon corresponding to $\alpha\equiv\frac{1}{2}(\mathrm{mod}\ N)$ is rotated by an angle $\frac{\pi}{N}$ (or in other words, it associates to each momentum $k\mapsto\tilde{k}=k+\frac{N-1}{2}$).

Summarizing, for finite-size systems, the second derivative of the energy density of the ground state diverges at the intersection points of the two vacua. On the other hand, in the thermodynamic limit, this divergence is suppressed. Indeed, in the $N\to\infty$ limit, Eq. (76) becomes

$$\frac{dE_{\mathrm{vac}}^{\mathrm{diff}}}{dg}(\sqrt{1-\gamma^2})\sim\frac{\gamma^2}{2\pi\sqrt{1-\gamma^2}}\int_0^{2\pi}dx[f(x)-f(x+\pi/N)], \tag{78}$$

where $f(x)=1/(1-\sqrt{1-\gamma^2}\cos x)$. Expanding in Taylor series $f(x+\pi/N)$, one gets

$$\frac{dE_{\text{vac}}^{\text{diff}}}{dg}(\sqrt{1-\gamma^2}) \to \frac{\gamma^2}{\pi\sqrt{1-\gamma^2}} f'(0) = 0, \quad N \to \infty. \quad (79)$$

This means that the singularities of the second derivative of the ground state vanish in the thermodynamic limit; in other words, the forerunners of the quantum phase transition are *not* related to the finite-size level crossings of the ground state. In this section, we will show that they are related to the level crossings between the unphysical vacuum and the losing physical vacuum where single Bogoliubov fermions sit.

Consider the explicit expressions of the vacua energies corresponding to the four possible cases given by the parity of N and the two parity sectors:

(1) N even, $\varrho=-1$, $\mathcal{S}_\varrho=\{[0],[\frac{N}{2}]\}$,

$$E_{\text{vac}}^{(-)} = -\frac{1}{N}\left(\sum_{k\in\mathcal{C}_\varrho}\left\{\left[g-\cos\left(\frac{2\pi k}{N}\right)\right]^2+\gamma^2\sin^2\left(\frac{2\pi k}{N}\right)\right\}^{1/2}+|g-1|+|g+1|\right). \quad (80)$$

(2) N odd, $\varrho=-1$, $\mathcal{S}_\varrho=\{[0]\}$,

$$E_{\text{vac}}^{(-)} = -\frac{1}{N}\left(\sum_{k\in\mathcal{C}_\varrho}\left\{\left[g-\cos\left(\frac{2\pi k}{N}\right)\right]^2+\gamma^2\sin^2\left(\frac{2\pi k}{N}\right)\right\}^{1/2}+|g-1|\right). \quad (81)$$

(3) N even, $\varrho=+1$, $\mathcal{S}_\varrho=\varnothing$,

$$E_{\text{vac}}^{(+)} = -\frac{1}{N}\left(\sum_{k\in\mathbb{Z}_N}\left\{\left[g-\cos\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)\right]^2+\gamma^2\sin^2\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)\right\}^{1/2}\right). \quad (82)$$

(4) N odd, $\varrho=+1$, $\mathcal{S}_\varrho=\{[\frac{N-1}{2}]\}$,

$$E_{\text{vac}}^{(+)} = -\frac{1}{N}\left(\sum_{k\in\mathcal{C}_\varrho}\left\{\left[g-\cos\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)\right]^2+\gamma^2\sin^2\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)\right\}+|g+1|\right). \quad (83)$$

Observe that the absolute values in the previous expressions correspond to the cosines evaluated at single fermion momenta $\mathcal{S}_\varrho$. At these values of the magnetic field, the first derivative of energy is not continuous (see Fig. 2) and the second derivative has terms proportional to the Dirac delta functions $\delta(g\pm 1)$. However, remember that the vacuum in case (i) becomes unphysical as soon as $|g|>1$, so that at $g=\pm 1$, there is a level crossing between physical and unphysical states. The same phenomenon happens to the vacuum in case (ii) at $g=1$ and to the vacuum in case (iv) at $g=-1$. On the other hand, one can observe that for finite-size chains, for both even and odd N, the ground state is smooth at $g=\pm 1$. In other words, the ground state, which coincides with the winning vacuum state, does not have any singularities at these points. However, it can be shown that the second derivative of the ground-state energy at $g=\pm 1$ scales as $-\log N$. Consider, for example, the case of an even number of spins N. In this case, the ground state belongs to the parity sector with $\varrho=+1$ without singularities. Figure 8 displays $d^2E_{\text{vac}}^{(+)}/dg^2$ for $N=6,24,54$; at $g=\pm 1$, it scales like $-\log N$. Indeed when $g=1$, by deriving Eq. (54), one has

$$\frac{d^2E_{\text{vac}}^{(+)}}{d^2g}(1) = -\frac{\gamma^2}{N}\sum_{k\in\mathbb{Z}_N}\frac{\left[1+\cos\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)\right]^{3/2}}{\left|\sin\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)\right|} \times\frac{1}{\left[1+\gamma^2+\cos\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)(\gamma^2-1)\right]^{3/2}} \sim -\frac{1}{\gamma\pi}\log N \quad (84)$$

for $N\to\infty$ as shown in Fig. 9. The cases $g=-1$ and N even ($\varrho=+1$) and $g=\pm 1$ and N odd ($\varrho=\mp 1$) are analogous.

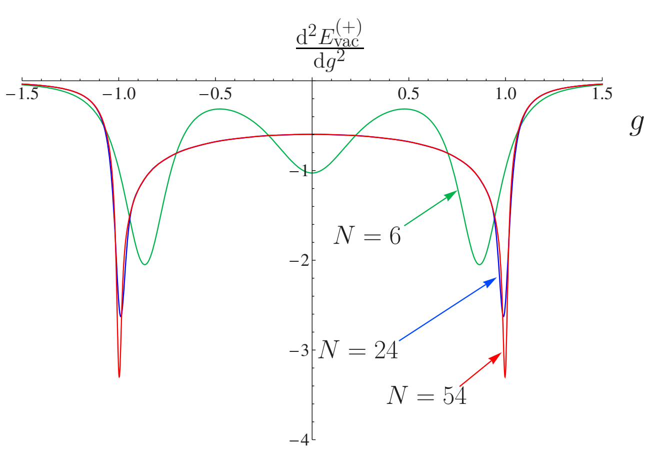

FIG. 8. (Color online) Second derivative of the vacuum energy density for even values of N in the parity sector $\varrho=+1$.

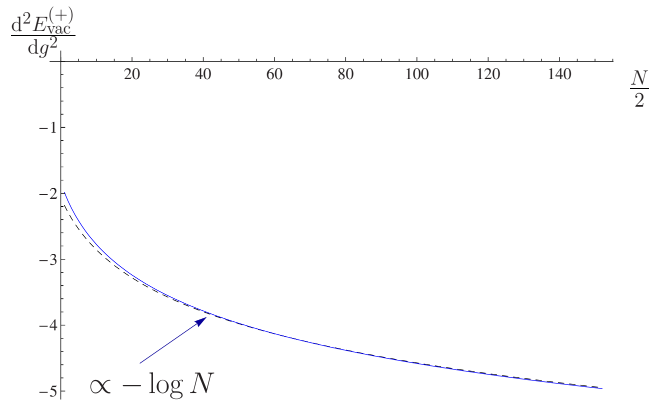

FIG. 9. (Color online) Second derivative of the vacuum energy density at $g=1$ in the parity sector $\varrho=+1$ for N even, from 18 to 320 (dashed line): it scales as $-\log N$ (solid line).

The quantum phase transition is forerun by the losing vacuum whose second derivative contains a Dirac delta function at the transition between physical and unphysical states. When N tends to infinity, as we will now show, the difference between the two vacua at $g=\pm 1$ tends to zero and quantum phase-transition forerunners approach the ground state, building up singularities at logarithmic rates. Indeed, at $g=\pm 1$ from Eq. (60), one has

$$E_{\mathrm{vac}}^{\mathrm{diff}}(\pm 1)=\frac{1}{N}\sum_{k\in\mathbb{Z}_N} f_{\pm}\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)-f_{\pm}\left(\frac{2\pi k}{N}\right), \qquad (85)$$

where $f_{\pm}(x)=\sqrt{(\pm 1-\cos x)^2+\gamma^2\sin^2 x}$. In the thermodynamic limit, by applying the same technique used in Eq. (78), Eq. (85) becomes

$$E_{\mathrm{vac}}^{\mathrm{diff}}(\pm 1)\sim -\frac{1}{2\pi}\int_0^{2\pi}\left[f\left(x+\frac{\pi}{N}\right)-f(x)\right]dx\sim\frac{\pi}{2N^2}\gamma,$$

$$N\to\infty, \qquad (86)$$

where we used the equality $f'_{\pm}(0)=-\gamma$ (see Fig. 10). In Fig. 11, we display the low energy part of the spectrum (thin lines) and the energy density of the two vacua (thick lines). At $g=\pm 1$, the ground state is the winning vacuum that has no singularities. The first-excited level coincides with the losing vacuum for $g\in(-1,1)$. Its second derivative diverges at $g=\pm 1$, forerunning the quantum phase transitions. Observe that they are at the transition between a physical state, which coincides with the first-excited level, and an unphysical state, which does not correspond to any physical level. For $|g|>1$, the losing vacuum is unphysical. Summarizing, we identify as forerunners of the quantum phase transition those points of the losing vacuum energy density whose second derivative diverges. These points are associated to single Bogoliubov fermions and belong to the crossing between the first-excited level and the unphysical vacuum for finite-size systems. When $N\to\infty$, they approach the ground state as N^{-2}.

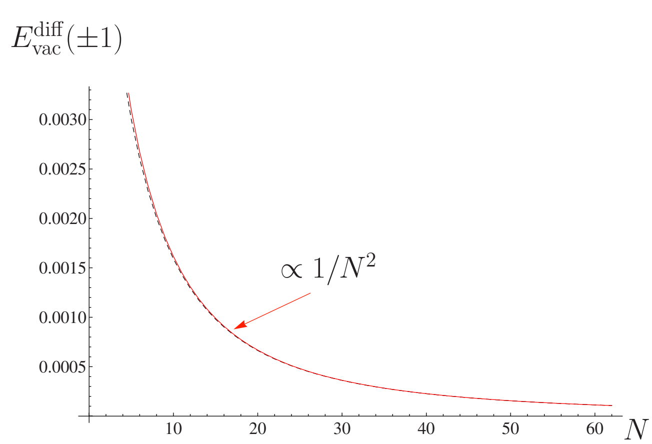

FIG. 10. (Color online) Difference between the two vacua energy densities at $g=\pm 1$: exact result (dotted line) and asymptotic approximation of order $1/N^2$ (solid line).

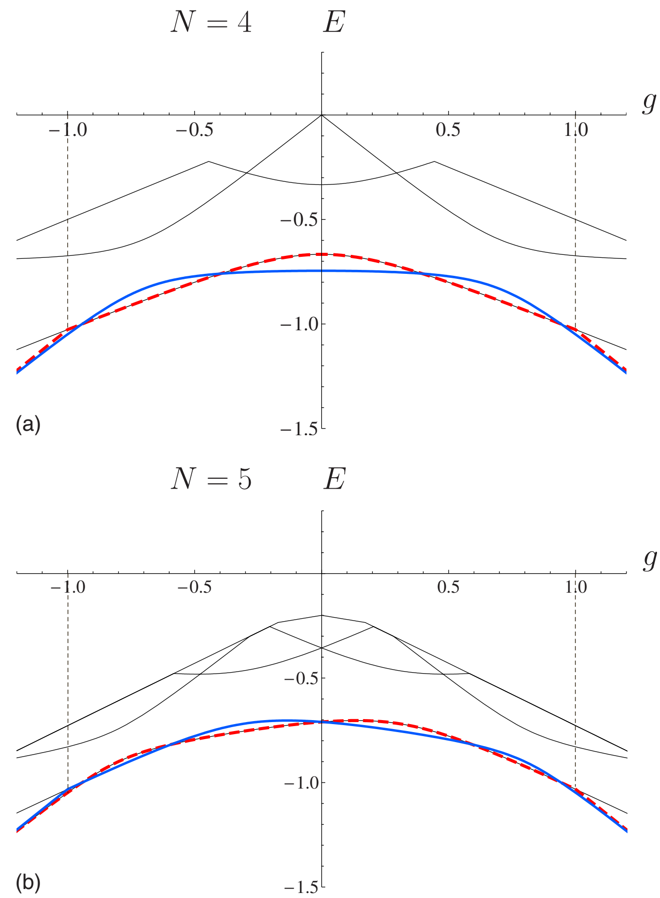

FIG. 11. (Color online) The thin lines represent the (numerically evaluated) lowest energy levels of the spectrum of the *XY* chain, respectively, with $N=4$ and $N=5$ spins; the thick solid and dashed lines refer to the two vacua energy densities, $E_{\mathrm{vac}}^{(-)}$ and $E_{\mathrm{vac}}^{(+)}$, respectively. These vacua alternatively coincide with the ground state and the first-excited state for $|g|\leq 1$. When $g=\pm 1$, one vacuum energy is the ground-state energy, while the other one does not correspond to any physical level. The transition points are the forerunners of the quantum phase transition.

B. Quantum phase transitions in the *XX* model

The isotropic *XX* model is very peculiar with respect to the above analysis because all Bogoliubov fermions are

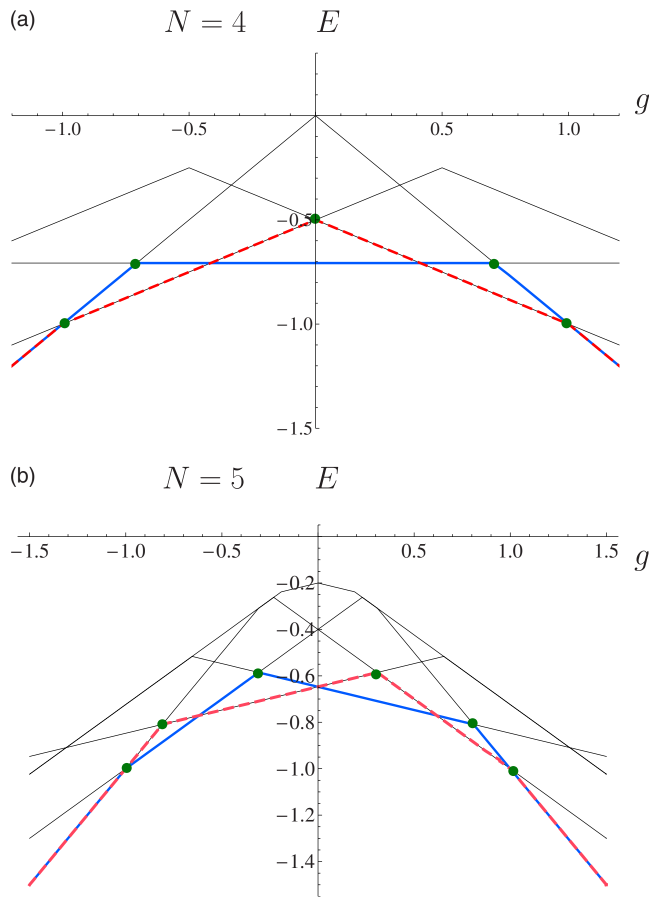

FIG. 12. (Color online) The thin lines represent the first four and five lowest energy levels of the spectrum of the *XX* chain, respectively, with $N=4$ and $N=5$ spins; the solid and dashed thick lines refer the two vacua energy densities in the parity sectors with $\varrho=-1$ and $\varrho=+1$, respectively. The forerunners of the (continuous) quantum phase-transition points are indicated with bold points; they are given by $g_k=\cos(\frac{2\pi k}{N})$, $k\in\mathbb{Z}_N$.

single and thus, by densely filling an interval in the $N\to\infty$ limit, are forerunning a continuous quantum phase transition. Therefore, here we are completely bypassing the usual way to detect such a phase transition that is to look at the scaling behavior of the correlation length.

As observed in Sec. III, the *XX* model ($\gamma=0$) is characterized by the only presence of single fermions and the absence of Bogoliubov pairs. As a result, all points $g=\cos(\frac{2\pi(\alpha+k)}{N})$ (in both parity sectors) with $k\in\mathbb{Z}_N$ can be considered quantum phase-transitions forerunners [see Eq. (72) and compare to Eqs. (80)–(83)]. Indeed, the second derivative of the vacua energy density contains a Dirac delta function at these points and, apart from $g=\pm1$, they all belong to the first-excited level such as in the *XY* model (see Fig. 12) (we will focus on $g=\pm1$ at the end of this section). In the thermodynamic limit, these points forerunning the quantum phase transition approach the ground state and become critical points. Consider, for example, $g_\ell=\cos(\frac{2\pi\ell}{N})\neq\pm1$. The energy difference between the vacua is now given by

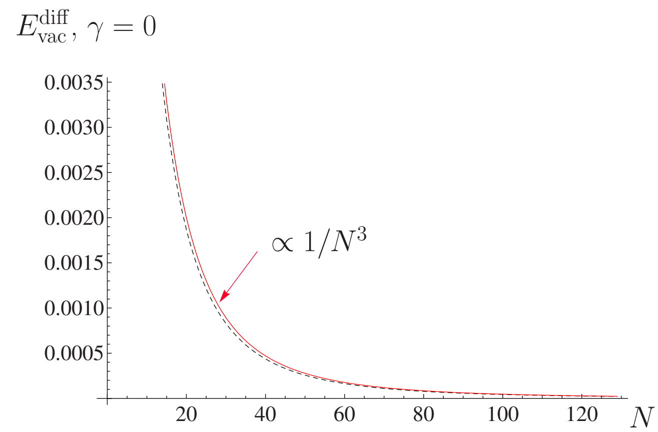

FIG. 13. (Color online) Difference between vacuum energies at $\ell=3$ vs N (dashed line) and its asymptotic approximation (solid line).

$$E_{\rm vac}^{\rm diff}(g_\ell)=-\frac{1}{N}\sum_{k\in\mathbb{Z}_N\setminus\{\ell\}}\left[\left|\cos\left(\frac{2\pi\ell}{N}\right)-\cos\left(\frac{2\pi k}{N}\right)\right|-\left|\cos\left(\frac{2\pi\ell}{N}\right)-\cos\left(\frac{2\pi k}{N}+\frac{\pi}{N}\right)\right|\right]+\frac{1}{N}\left|\cos\left(\frac{2\pi\ell}{N}\right)-\cos\left(\frac{2\pi\ell}{N}+\frac{\pi}{N}\right)\right|. \tag{87}$$

By using the same technique of the previous section, one gets

$$E_{\rm vac}^{\rm diff}(g_\ell)=\frac{1}{2\pi}\int_0^{2\pi}\left[\frac{\pi}{N}f_\ell'(x)+\left(\frac{\pi}{N}\right)^2\frac{f_\ell''(x)}{2!}+\left(\frac{\pi}{N}\right)^3\frac{f_\ell'''(x)}{3!}+O\left(\frac{1}{N^4}\right)\right]dx+\frac{1}{N}\left|\cos\left(\frac{2\pi\ell}{N}\right)-\cos\left(\frac{2\pi\ell}{N}+\frac{\pi}{N}\right)\right| \tag{88}$$

for $N\to\infty$, where $f_\ell(x)=|\cos(2\pi\ell/N)-\cos x|$. From the symmetries of f_ℓ and its derivatives, it follows that Eq. (88) becomes

$$E_{\rm vac}^{\rm diff}(g_\ell)\sim\frac{1}{N}\sqrt{\left[\cos\left(\frac{2\pi\ell}{N}\right)-\cos\left(\frac{2\pi\ell}{N}+\frac{\pi}{N}\right)\right]^2}\sim\frac{2J\pi^2\ell}{N^3},\quad N\to\infty \tag{89}$$

(see Fig. 13). Therefore, in the thermodynamic limit, the forerunners of the quantum phase transition in the isotropic *XX* model approach the ground state faster than the ones of the *XY* model (with $\gamma\neq0$). Compare Figs. 10 and 13.

As shown in Fig. 12, the intersection points of the two vacua [which coincide with the level crossing points $g_c(n)$ discussed in Sec. III] are characterized by a discontinuity of the first derivative for finite-size chains. By deriving the energy difference (73), one can show that the discontinuity of the first derivative at the points of level crossing scales like

$1/N$. Therefore in the thermodynamic limit, the divergence of the second derivative vanishes, as for the *XY* Hamiltonian with $\gamma \neq 0$.

Let us finally consider the points $g = \pm 1$. On one hand, they are level crossing points ($g = \pm\sqrt{1-\gamma^2}, \gamma = 0$). On the other hand, following the same criterion introduced for the *XY* model, they can be considered as forerunners of quantum phase transitions. What happens in this particular case is that these points belong to the ground state already for finite N. Another crucial difference between the anisotropic case and the *XX* model is that, since all Bogoliubov fermions are single, there are $N+1$ points forerunning the quantum phase transition. Thus in the $N \to \infty$ limit, they densely fill the interval $[-1,1]$ of g and yield, as one expects [4], a continuous quantum phase transition in this interval.

V. CONCLUSIONS

In this paper, we analyzed the *XY* model on a circle with periodic boundary conditions. Being interested in finite-size systems, we did not neglect the boundary term which derives from the Jordan-Wigner transformation. The Hamiltonian can be diagonalized by deforming the discrete Fourier transform with a local gauge coefficient depending on the parity of spins down (see, for example, [4,26]). We accomplished it by following a approach based on the solution of a modular equation that derives from the invariance of the Hamiltonian under translations. We then showed that in the Fourier space, there are two classes of fermions: single and coupled ones. This distinction is crucial in order to determine the Bogoliubov transformation. The main point that, quite surprisingly, has been neglected in the large literature on finite-size spin models is that the Bogoliubov transformation has a gauge freedom. By its very definition, a gauge freedom does not change the physical results. However, it paves the way to a deeper comprehension of physical phenomena. We have shown that, rather than being just a trick for doing numerical calculations, the gauge freedom is deeply rooted in the mathematical structure of the model and allows for many equivalent descriptions of the spin system. A particularly simple description, well adapted to the thermodynamic limit, is the mechanism that gives rise to vacua competition. The very fact that such a description has been used in previous numerical analysis strengthens our results and makes them of interest for numerical applications.

Moreover, we revealed an unexpected link with the quantum phase transition. In fact, the combination of the Bogoliubov gauge with the conservation of parity sectors uniquely determines in the finite-size model the points where quantum phase transition will occur when the size of the system becomes infinite. They are associated to single Bogoliubov fermions. Indeed, while the gauge of Bogoliubov pairs does not affect parity, the gauge of single fermions does change it and couples physical states with unphysical ones (with wrong parity). It is just at the level crossings of these states that quantum phase transitions will occur.

There is considerable interest in the study of entanglement for quantum spin chains, both in view of applications and because of their fundamental interest (see, for example, the results concerning the *XX* chain [16,33,32]). Our approach can be used in the study of the properties of multipartite entanglement of the ground state in terms of the distribution of bipartite entanglement [34,35] and in the investigation of the possible connections with quantum phase transitions in the thermodynamic limit.

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