

Antiferromagnetic Heisenberg-Ising ring in the presence of a magnetic flux: Relevance of domain-wall dynamics

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We consider a system of charged spinless fermions in a ring governed by the antiferromagnetic Heisenberg-Ising Hamiltonian and in the presence of a magnetic flux. We find that the two broken-symmetry ground states evolve adiabatically with increasing flux with a period corresponding to two flux quanta, while the period of the total spectrum is one flux quantum. This behavior, already observed for this system in the gapless regime [B. Sutherland and B. S. Shastry, *Phys. Rev. Lett.* **65**, 1833 (1990)], is shown to be a natural consequence of the relevant degrees of freedom involved in the low-energy physics of this system: antiferromagnetic domain walls or solitons, with half the charge of the original particles. A space-time approach is introduced to describe the dynamics of these objects, affording a complete topological classification of space-time histories of the system. This allows a physically complete understanding of the ground-state-subspace evolution with increasing flux in the antiferromagnetic broken-symmetry regime. In this case, the flux period doubling can be explained in terms of the Berry's phase gained by the two degenerate broken-symmetry ground states upon adiabatic switching of the flux.

I. INTRODUCTION

The one-dimensional spin- $\frac{1}{2}$ XXZ (Heisenberg-Ising) Hamiltonian occupies an important role in many-body physics as one of the nontrivial, highly correlated systems for which a solution can be constructed. In spite of its being solvable, the solution is neither technically nor physically simple. This difficulty explains the long history between Bethe's work,¹ paving the way for solution and obtaining information for physically relevant properties such as long-range static correlations. In fact, our knowledge of properties such as dynamical correlations is still incomplete.² In spite of these difficulties, the low-energy physics of this problem can be considered to be well known,³⁻⁷ and the results are physically very interesting. There is, for instance, a gapless fermion phase with no Fermi-liquid behavior (Luttinger liquid^{8,9}), while, in the antiferromagnetic insulator regime, unusual kink-like excitations^{10,11} replace the otherwise expected traditional spin waves. From an experimental point of view, this Hamiltonian is relevant for describing magnetic excitations of quasi-one-dimensional magnetic insulator¹²⁻¹⁵ where very faithful representations of this model in different regimes can be found.

In a recent paper, Sutherland and Shastry¹⁶ (hereafter referred to as SS) have studied this system in the presence of a magnetic flux. They have shown that, in the gapless regime, the continuous evolution with increasing flux of low-lying states shows a flux periodicity which doubles the spectrum periodicity. As mentioned by SS, this suggests that the underlying dynamics corresponds to objects with half the charge of the particles coupled to the flux in the normal representation.

The purpose of this work is to provide an explanation for the above-mentioned period doubling by identifying the fractionally charged objects as domain walls (DW's), or solitons, between opposite antiferromagnetic (AF)

domains. Based on a previously developed mapping of the problem in terms of DW's,¹¹ we analyze the effect of the flux on the DW dynamics by means of a space-time description. This scheme allows a topological classification of space-time histories of the system in terms of closed DW loops. We show that the period doubling is a rather general property of DW dynamics, valid not only in the gapless regime but also in the broken-symmetry AF regime. In this latter case, the analysis can be pursued further to obtain the wave function with flux from the wave function with no flux, relating the physically relevant (gauge-invariant) effect of the flux to a class of space-time paths. Finally, in the AF regime, the period doubling admits a simple explanation as the different Berry's phase¹⁷ acquired by both degenerate broken-symmetry ground states (GS's) upon piercing the flux slowly in time.

The paper is organized as follows. In Sec. II, different representations of the Hamiltonian in the presence of magnetic flux are described, and the mapping in terms of DW's is reviewed, introducing the space-time picture for their dynamics. Section III analyzes the effect of a magnetic flux on the DW picture and studies the flux evolution of the ground-state manifold in the AF broken-symmetry regime. Section IV shows the period doubling as a general feature of DW dynamics, and demonstrates how the space-time picture can be used in the AF regime to obtain the GS wave function with flux from that in the absence of flux. Section V interprets the period doubling in the AF regime as a manifestation of Berry's phase under adiabatic time evolution. The work is summarized in Sec. VI.

II. FORMALISM

A. Hamiltonian in the presence of magnetic flux

The spin- $\frac{1}{2}$ XXZ Hamiltonian has the following form:

$$\begin{aligned}\mathcal{H} &= \sum_{i=1}^N h_{i,i+1} \\ &= \sum_{i=1}^N \left[\frac{1}{2}(s_i^+ s_{i+1}^- + \text{H.c.}) + \Delta s_i^z s_{i+1}^z \right],\end{aligned}\quad (1)$$

where s^α are the operators corresponding to the spin- $\frac{1}{2}$ algebra and the sum runs over N sites in a closed ring. We restrict ourselves to an equal number of up and down spins ($N/2$) and, as usual, each up-spin site can be considered as a particle (hard-core boson or Wigner-Jordan fermion⁶) in a background (vacuum) of down-spin sites. In this particle representation, the first term in \mathcal{H} models the hopping of particles between nearest-neighbor sites, while the last term represents, apart from a trivial additive constant, the interaction between nearest-neighbor particles.

If we pierce a flux Φ through the ring, each particle (unit charge) picks up a phase Φ upon completing a loop around the lattice. The effect of this flux can be accounted for by either appropriate boundary conditions or by suitable modification of the hopping term. Adopting the latter procedure, the presence of the flux modifies the original Hamiltonian in the following way:

$$\mathcal{H}_1(\Phi) = \sum_{i=1}^{N-1} h_{i,i+1} + \frac{1}{2}(e^{i\Phi} s_N^+ s_1^- + \text{H.c.}) + \Delta s_N^z s_1^z, \quad (2)$$

where the ring geometry amounts to imposing periodic boundary conditions. The Bethe-ansatz solution of $\mathcal{H}_1(\Phi)$ can be shown to be completely equivalent to the treatment of SS.

There are, in fact, infinitely many gauge-equivalent Hamiltonians for a fixed flux Φ , reflecting the fact that what matters is the total flux picked up in a closed loop around the lattice, irrespective of the particular amount gained in every elementary hopping event. In \mathcal{H}_1 all the flux is gained in the bond between sites N and 1 . We call this \mathcal{H}_1 the gauge-1 representation. If, for instance, we distribute the flux homogeneously through the lattice, we arrive at the following gauge-equivalent, translational-invariant version of the problem (the gauge-2 representation):

$$\mathcal{H}_2(\Phi) = \frac{1}{2} \sum_{i=1}^N (e^{i\Phi/N} s_i^+ s_{i+1}^- + \text{H.c.}) + \Delta \sum_{i=1}^N s_i^z s_{i+1}^z. \quad (3)$$

Another useful gauge representation (gauge 3) is the following:

$$\begin{aligned}\mathcal{H}_3(\Phi) &= \sum_{i=1}^{N-2} h_{i,i+1} + \frac{1}{2}(e^{i\Phi/2} s_{N-1}^+ s_N^- + \text{H.c.}) \\ &\quad + \Delta s_{N-1}^z s_N^z + \frac{1}{2}(e^{i\Phi/2} s_N^+ s_1^- + \text{H.c.}) \\ &\quad + \Delta s_N^z s_1^z,\end{aligned}\quad (4)$$

where the total flux has been evenly distributed between two adjacent bonds. Gauge transformations relating equivalent Hamiltonians can be thought of as local rotations around the z axis in Eq. (1), such that the total rotation moving along the ring equals the flux. The 2π periodicity of the spectrum with flux, as is evident from

\mathcal{H}_1 , corresponds to the particular values of flux that can be accommodated without discontinuities in this process of local rotations.

B. Antiferromagnetic domain walls or solitons

Following previous suggestions, it has been shown that the relevant degrees of freedom controlling the low-energy physics of this problem are DW's between opposite AF domains. This was done by performing an exact mapping¹¹ of the original \mathcal{H} in terms of these DW's and showing that an approximate solution of the resulting Hamiltonian reproduces the basic features of the known exact solution, providing a clear physical image of the physics involved.

The mapping of \mathcal{H} [Eq. (1)] in terms of DW's can be summarized as follows (for details see Ref. 11). There are two degrees of freedom per site and, correspondingly, two degrees of freedom per nearest-neighbor bond. These two bond degrees of freedom correspond to either antiferromagnetic ($\uparrow\downarrow$ or $\downarrow\uparrow$) or ferromagnetic ($\uparrow\uparrow$ or $\downarrow\downarrow$) alignment of the sites defining the bond. If we associate a spin- $\frac{1}{2}$ algebra (σ^α) to each bond, with the up degree of freedom corresponding to ferromagnetic-bond status and the down degree of freedom to antiferromagnetic-bond status, each ferromagnetic bond can be viewed as a DW or soliton between opposite AF domains. The Hamiltonian in this representation is

$$\mathcal{H}_{\text{DW}} = \mathcal{H}_{\text{even}} + \mathcal{H}_{\text{odd}} + \mathcal{H}_{\text{constraint}}, \quad (5)$$

where

$$\mathcal{H}_{\text{even}} = \frac{1}{2} \sum_{i \text{ even}} (\sigma_i^+ \sigma_{i+2}^- + \sigma_i^- \sigma_{i+2}^+ + \text{H.c.}) + \frac{\Delta}{2} \sum_{i \text{ even}} \sigma_i^z, \quad (6)$$

$$\mathcal{H}_{\text{odd}} = \frac{1}{2} \sum_{i \text{ odd}} (\sigma_i^+ \sigma_{i+2}^- + \sigma_i^- \sigma_{i+2}^+ + \text{H.c.}) + \frac{\Delta}{2} \sum_{i \text{ odd}} \sigma_i^z, \quad (7)$$

and

$$\begin{aligned}\mathcal{H}_{\text{constraint}} &= -\frac{1}{2} \sum_i (\sigma_i^z + \frac{1}{2}) \\ &\quad \times (\sigma_{i-1}^+ \sigma_{i+1}^- + \sigma_{i-1}^- \sigma_{i+1}^+ + \text{H.c.}).\end{aligned}\quad (8)$$

Notice that the index i runs over bonds (not sites), and only alternate bonds are coupled in $\mathcal{H}_{\text{even,odd}}$. This means that the bonds are divided into even and odd sublattices, the action of the Hamiltonian being the same within each sublattice. \mathcal{H}_{DW} represents a system of solitons (ferromagnetic bonds) being created and annihilated (in pairs) and hopping within each sublattice in a background of AF bonds (vacuum), plus a static contribution measuring the energy associated with the number of solitons. $\mathcal{H}_{\text{even,odd}}$ are, in fact, the well-known, exactly solvable and physically interesting Ising + transverse-field model,^{18,19} the one-dimensional (1D) quantum version of the classical 2D Ising model at finite temperature.

The many-body nature of this problem manifests itself in the contribution $\mathcal{H}_{\text{constraint}}$, which couples DW's in different sublattices. This term can be interpreted as a geometrical constraint which forbids world lines (in the space-time image to follow) of solitons in different sublattices to cross each other.¹¹

A useful picture of DW dynamics can be obtained in a space-time diagram which, in our ring geometry, becomes a space-time cylinder. A DW moving in the vacuum, classical Néel (CN) state, is represented by a world-line on the surface of the space-time cylinder. This world line separates domains with opposite AF order. There are only two types of topologically different closed soliton-antisoliton loops in space time, described as path 1 and path 2 in Fig. 1. Path 1 represents a particular space-time history of the system, interpolating between the two vacua of this problem: the two opposite classical Néel states, $|\text{CNS1}\rangle$ and $|\text{CNS2}\rangle$,

$$|\text{CNS1}\rangle = \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\cdots, \quad (9)$$

$$|\text{CNS2}\rangle = \downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\cdots. \quad (10)$$

Path 2 represents a local quantum fluctuation of one of the two vacua. There is no continuous deformation between both classes of paths, whereof their being called topologically inequivalent. Within each class, a further distinction can be made according to whether the path runs within the even or odd bond sublattices.

The physical image of the low-energy physics of \mathcal{H} in the AF regime ($\Delta > 1$) afforded by the previous mapping is very clear. There are two degenerate, broken-symmetry ground states [quantum Néel (QN) states $|\text{QNS1}\rangle$, $|\text{QNS2}\rangle$], which can be thought of as the quantum renormalized version of the corresponding classical Néel states:

$$|\text{QNS1}\rangle = |\text{CNS1}\rangle + \text{quantum fluctuations}, \quad (11)$$

$$|\text{QNS2}\rangle = |\text{CNS2}\rangle + \text{quantum fluctuations}. \quad (12)$$

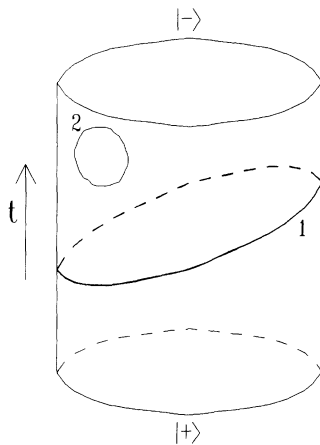


FIG. 1. Topological classification of closed space-time soliton loops. Each line represents a soliton world line moving in the background of a classical Néel state. The shown history interpolates between the two classical Néel states. The discrete nature of the lattice is not explicit.

These quantum fluctuations can be interpreted as the dressing of the CN states with virtual (bound) soliton-antisoliton pairs (path 2 in Fig. 1). This dressing does not destroy long-range order but renormalizes the CN states providing a finite correlation length (ξ) for the fluctuations of the order parameter. This correlation length can be viewed as the characteristic spatial size of the quantum fluctuation created by the soliton-antisoliton type-2 closed loop.

There is a gap between the GS's and excitations. These are (massive) free domain walls (though dressed with soliton-antisoliton pairs) running through the lattice. The number of these excitations is always even due to periodic boundary conditions, but they behave as independent entities (no binding).

The existence of two degenerate GS's ($|\text{QNS1}\rangle$ and $|\text{QNS2}\rangle$) is valid in the limit of an infinite ring or, for a finite ring, in the presence of the appropriate staggered fields. For a large, but finite, ring without staggered field, the true GS is known to be nondegenerate. This means that the two broken-symmetry QN states are coupled, whereof their splitting in energy. This coupling can be visualized as the probability amplitude for these QN states reaching each other upon application of the Hamiltonian. In our space-time picture, this coupling is identified as the probability of having an odd number of closed soliton loops of type 1 in the space-time cylinder between the two QN states. This coupling can be thought of as a quantum fluctuation in which a soliton-antisoliton pair delocalizes and runs through the lattice to merge again upon completing a cycle. It is immediately obvious that the existence of a gap for the creation of free (massive) solitons implies that such an event has a probability decreasing exponentially with size in the form $\exp(-N/\xi)$, where ξ is the correlation length for fluctuations in the GS. It is also clear that, for large lattices, the events picturing this probability amplitude are those with a single closed loop of type 1 (contributions from paths with 3,5,7, . . . loops are exponentially small corrections to the probability amplitude of one loop).

Therefore, the effective Hamiltonian describing the coupling between the states $|\text{QNS1}\rangle$ and $|\text{QNS2}\rangle$ is given a 2×2 matrix of the form

$$\mathcal{H} = \begin{pmatrix} E_0 & V \\ V & E_0 \end{pmatrix}, \quad (13)$$

where E_0 represents the energy of the two QN states and V their coupling. This V is exponentially small [$\exp(-N/\xi)$], and corresponds to paths between QN states with a single type-1 loop. Taking into account the two-sublattice nature of the domain-wall Hamiltonian, this V can be further decomposed according to whether the path follows the even or odd sublattice:

$$V = V_{\text{even}} + V_{\text{odd}}, \quad (14)$$

where, on symmetry grounds, $V_{\text{even}} = V_{\text{odd}}$.

In analogy with the electron-phonon problem, one can consider the 2×2 matrix describing the ground-state manifold as the effective Hamiltonian controlling the slow degrees of freedom (interplay between the two QN

states) once the fast degrees of freedom (dressing of CN states with quantum fluctuations) have been integrated out. In our case, the existence of long-range AF order guarantees that such a decoupling between slow and fast degrees of freedom becomes asymptotically exact in the limit of large lattices.

III. DOMAIN WALLS IN THE PRESENCE OF FLUX

The presence of a flux through the ring modifies trivially the DW Hamiltonian in those terms involving soliton dynamics. Assuming, for instance the gauge-2 representation, creation of a pair of solitons ($\sigma_i^+ \sigma_{i+2}^+$) adds a phase ($e^{i\Phi/N}$). Motion to the right of the right soliton and to the left of the left soliton adds the same phase. Motion in the reverse sense changes the sign of the phase ($e^{-i\Phi/N}$). Finally, annihilation ($\sigma_i^-, \sigma_{i+2}^-$) of a pair of solitons (restoring the original vacuum) changes the sign of the creation phase. This is true for action in a given sublattice. The corresponding actions in the other sublattice have opposite signs in the phase. The rule for motion of solitons defined with respect to the opposite vacuum and for other gauge representations can be inferred straightforwardly. In general, to get the phase of an elementary event involving DW's, it suffices to remember that, in the spin picture of \mathcal{H} , any event is always the interchange of two nearest-neighbor up and down spins, from where the phase to be picked up is obvious.

The effect of the flux on the closed paths of Fig. 1 is very simple. Assuming the gauge-2 representation for simplicity, the total phase picked in a type-1 loop is $e^{\pm i\Phi/2}$, corresponding to half the total flux (the sign depending on the path sublattice). This reflects the fact that, for each sublattice, only $N/2$ elementary events are required to complete a cycle. In this sense, we can think of a DW or soliton as a particle with half the charge of an up spin in the original representation. This phase is not gauge invariant, but any gauge transformation amounts to merely adding a constant phase to all type-1 paths, irrespective of sublattice.

The phase associated with a type-2 closed loop is zero, irrespective of the sublattice involved and gauge invariant. Therefore, the probability amplitude of this class of paths is the same whether the flux is present or not.

We can now analyze the evolution with flux of the two quasidegenerate ground states, $|\text{QNS1}\rangle$ and $|\text{QNS2}\rangle$, of the AF regime ($\Delta > 1$). It suffices to realize that a single type-1 loop gets opposite phase in different sublattices (gauge 2) and the effective coupling now becomes $V \cos(\Phi/2)$. Therefore, the matrix describing the ground-state manifold in the gauge-2 representation is

$$\mathcal{H}_2(\Phi) = \begin{pmatrix} E_0 & V \cos(\Phi/2) \\ V \cos(\Phi/2) & E_0 \end{pmatrix}. \quad (15)$$

Changing the gauge representation modifies this matrix in a trivial way. Thus, for instance,

$$\mathcal{H}_1(\Phi) = \begin{pmatrix} E_0 & V(1+e^{i\Phi})/2 \\ V(1+e^{-i\Phi})/2 & E_0 \end{pmatrix} \quad (16)$$

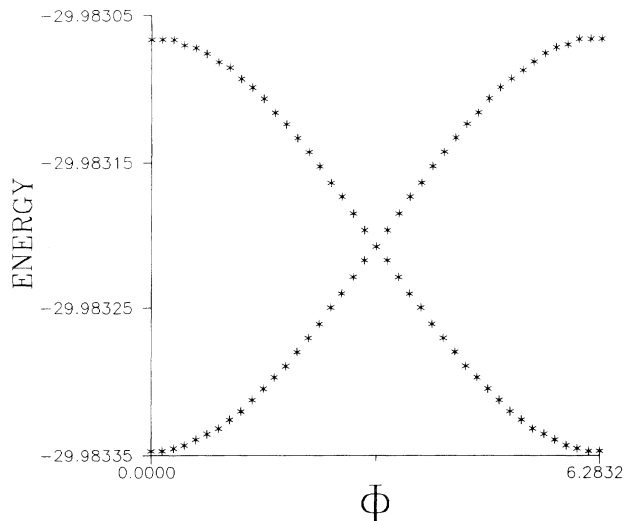


FIG. 2. Energy of the two quasidegenerate ground states vs total flux from the exact solution of Bethe-ansatz equations for $\Delta = 1.5$ and $N = 202$ sites.

and

$$\mathcal{H}_3(\Phi) = \mathcal{H}_2(\Phi). \quad (17)$$

These equivalent matrices imply that the splitting between both quasidegenerate GS's has a cosinelike form with increasing flux, with a periodicity corresponding to 4π (two flux quanta). This periodicity is exactly that found by SS in their analysis of this problem in the gapless regime ($\Delta \leq 1$). We show here that it is also valid in the AF regime, and that it is driven by the nature of the dynamical objects: DW's.

To substantiate the validity of all these arguments, we have solved the exact Bethe-ansatz equations for this Hamiltonian in the presence of a total flux using a gauge-2 representation.²⁰ The results for the energy of the quasidegenerate GS's versus flux are shown in Fig. 2, where the behavior corresponding to the diagonalization of the previous equivalent 2×2 matrices is evident.

It is important to stress that the reasoning leading to this result is completely rigorous and valid for large enough lattices in the phase with AF long-range order. All that is required is a large enough lattice to ensure that the dominant contribution to the coupling between quasidegenerate QN states can be represented by a single type-1 closed loop whose size, therefore, scales with the ring size, implying an exponentially small coupling. The size for which the cosinelike form of the splitting sets in depends (exponentially) on the lattice size, measured in units of the correlation length ξ . This can be seen by comparing Figs. 2 and 3. Notice that the value of Δ , the same in both figures, is close to the transition point ($\Delta = 1$) where the correlation length diverges. Therefore, very large sizes are required to change the splitting curve from a distorted parabolic form to the correct cosinelike asymptotic result. It is interesting to observe that, though the curve changes from a perfect cosinelike form upon decreasing the lattice size, the periodicity of the continuously evolved GS's does not change. This indi-

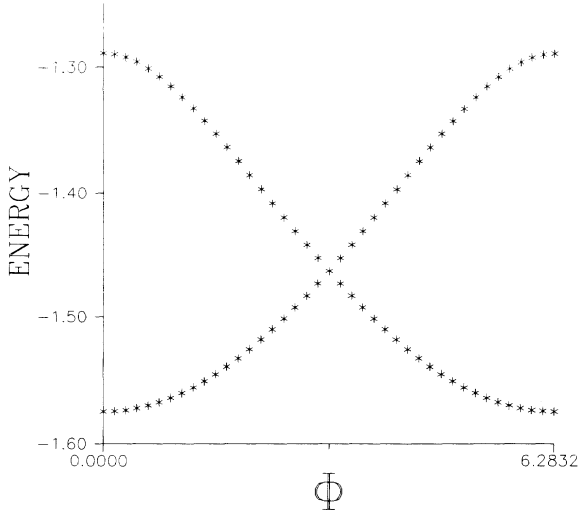


FIG. 3. Same as in Fig. 2 for $N = 14$ sites.

cates that the existence of long-range order is not related to the appearance of this periodicity, as is evident from the results of SS obtained in the critical regime. Indeed, we will show that this doubling of the spectrum periodicity is a natural feature of events involving DW's or solitons.

IV. FLUX PERIODICITY OF TIME EVOLUTION: WAVE-FUNCTION RIGIDITY

In this section we will consider the flux dependence of the probability amplitude for the time evolution between a classical Néel state ($|\text{CNS1}\rangle$, for instance) and an arbitrary state $|\Psi\rangle$ specified by its particular arrangement of DW's. For any time t , this probability is $\langle\Psi|e^{-it\mathcal{H}}|\text{CNS1}\rangle$. Upon Trotter-Suzuki cutting to the desired degree of accuracy, this probability can be interpreted as the weighted sum of space-time histories of the system between both states. Given a particular history, the weight of such a path with flux is the weight without flux but multiplied by $e^{i\theta}$, where θ is a path-dependent phase. We can classify all paths connecting both states according to this phase in the following manner.

Each path can be considered as part of a path which begins at $|\text{CNS1}\rangle$ and ends at $|\text{CNS2}\rangle$ passing through $|\Psi\rangle$. If we fix the trajectory between $|\Psi\rangle$ and $|\text{CNS2}\rangle$ (the same for all paths going between them), it is clear that the global phase between both CN states is that corresponding to an odd number of type-1 closed loops. Assuming gauge-2 representation for simplicity, this means that

$$\theta = \theta_{\text{ref}} + m\Phi/2, \quad (18)$$

where $m = \pm 1, \pm 3, \dots$ and θ_{ref} is a reference phase picked up in the fixed path between $|\Psi\rangle$ and $|\text{CNS2}\rangle$. This classification is topological: once the closing reference path has been fixed, paths belonging to classes with different m 's cannot be continuously deformed into each other. Changing m implies modification of the number of closed type-1 loops. The periodicity of this classification is that of the closed type-1 loops: the representative path

of the class with given m changes its phase by 2π when the total flux changes by 4π .

One can get rid of possible gauge-dependent effects in the periodicity choosing, for instance, the gauge-3 representation where only the physical flux appears explicitly in the phase corresponding to any path between $|\text{CNS1}\rangle$ and $|\Psi\rangle$. Then, the previous construction guarantees that θ_{ref} is an integer number of times $\Phi/2$. Therefore, the physical periodicity of the phase (gauge independent) is that of the classification of paths: two flux quanta. This means that the probability amplitude for the time evolution between a classical Néel state and an arbitrary state will repeat itself every two flux quanta. Adding states with appropriate coefficients, things can be arranged such that cancellations manifest as a larger period (this is the case for the adiabatic evolution of the ground state of the XY model), but the key point is that the periodicity of the spectrum is not the periodicity of the time evolution as a consequence of DW dynamics.

It is important to stress that the difference between the spectrum periodicity and the time evolution periodicity with flux is a real property, not related to a particular gauge representation. In other words, there is no gauge transformation that could render the time evolution flux periodicity and the spectrum flux periodicity to the same value 2π . To see this, it suffices to realize that, for a change of flux corresponding to the spectrum periodicity 2π , the relative sign of the phase corresponding to paths reaching a state from both classical Néel states reverses. This means that such a change is not reducible to a global phase and, therefore, cannot be gauged away.

The previous construction makes natural the appearance of the 4π periodicity observed in the adiabatic evolution of the ground state, but does not tell us how to construct the wave function with flux in terms of that with no flux. In the remaining part of this section, we will show that we can accomplish this task in the AF ordered region ($\Delta > 1$) by means of our space-time image.

According to the previous discussion, the GS's are (in gauge-2 representation) the even and odd combination of both QN states [see Eq. (15)]. While we have analyzed the flux dependence of the coupling between these QN states in terms of single space-time type-1 loops, nothing has been said about changes of the wave function of each QN state with increasing flux. This wave function can be obtained as follows. We can imagine that we generate the QN state evolving the corresponding CN state in imaginary time τ :

$$|\text{QNS1}\rangle \propto e^{-\tau\mathcal{H}}|\text{CNS1}\rangle. \quad (19)$$

The above procedure is known to produce the true GS (equally weighted combination of both QN states). If we want to make sure that only one QN state is developed, we simply ignore paths that connect both CN states. This can be done in the following way. We select all paths implied by Eq. (19) for which we can draw a straight line along the (imaginary) time axis in the space-time cylinder such that each soliton world line crosses this line an even number of times. This guarantees that no closed type-1 loop is in the intermediate region between the corresponding CN state and the final state.

This construction is equivalent to selecting those paths with a fixed m in the classification of Eq. (18). It is important to emphasize that the apparent constraint in selecting paths is harmless to the final result. What we are doing is constructing from the corresponding CN states the QN states in the diagonal entries of the 2×2 matrix of Eq. (15), or, in other words, integrating the fast degrees of freedom of one of the two broken-symmetry ground states independent of the opposite ground state. The paths describing the interplay between both GS's are taken care of by the off-diagonal entries of matrix (15) already considered.

The important point of this construction is that the effect of the flux is now very easy: all the paths so constructed connecting a CN state with a given state acquire the same (gauge-dependent) phase in the presence of a flux. Therefore, the coefficient of a given state in a QN wave function with flux is that obtained in the absence of flux, but multiplied by a unit complex number whose phase only depends on this state. Therefore, the recipe to construct explicitly both GS's in gauge-2 representation is the following:

$$|\text{GS}\rangle = |\text{QNS1}(\Phi)\rangle \pm |\text{QNS2}(\Phi)\rangle, \quad (20)$$

where the QN states are modified with flux in a trivial way: just attach to the coefficient of a given configuration the well-defined phase shared by all paths connecting it to the corresponding CN state. We name this path-independent phase the *canonical* phase, and call this property of the wave-function *rigidity*.

This rigidity of the GS wave functions in the AF regime can be readily verified from the exact solution of the Bethe-ansatz equations for a gauge-2 representation. If

we calculate the ratio of the coefficients with which a particular state appears in the Bethe-ansatz solution for the GS wave function with and without flux, in the limit of large lattice sizes, this ratio should be a unit complex number whose phase is the canonical phase of the state under consideration. (The global phase of the wave function is always fixed such that the coefficient of the reference CN state is 1). If, for instance, one takes the state obtained from a classical Néel state by just one elementary event (interchange of two adjacent opposite spins), the canonical phase is, obviously, $e^{\pm i\Phi/N}$. In Fig. 4 we show as a function of lattice size,²¹ the (normalized by N) difference between the (Bethe ansatz) calculated phase of the above-mentioned ratio of coefficients and the canonical phase for the state described above, for a total flux $\Phi = 2\pi$. We see that this value approaches zero exponentially with size, as is expected from our previous analysis. The same exponential approach to unity can be obtained for the modulus of this ratio. This rigidity of the wave function appears immediately if one does perturbation theory around the CN states. It should be emphasized, however, that this property is exact in all the range of parameters for which there is AF long-range order and not a feature of perturbation theory. Indeed, the absolute value of the coefficient of the described state is very different from the lowest-order perturbation result around the corresponding CN state for the value of Δ of Fig. 4, yet the phase is the same irrespective of the value of Δ , depending only on the total flux through the ring (in the gauge-2 representation). Of course, the lattice size necessary to observe the canonical phase depends on the correlation length of the GS, as can be seen by comparing Figs. 4. and 5 for different values of Δ . In Fig. 5, a smaller value of Δ implies a larger correlation length, and, therefore, a slower convergence towards the canonical phase with increasing lattice sizes.

This rigidity of the wave function of a QN state is nothing but a gauge transformation. This means that,

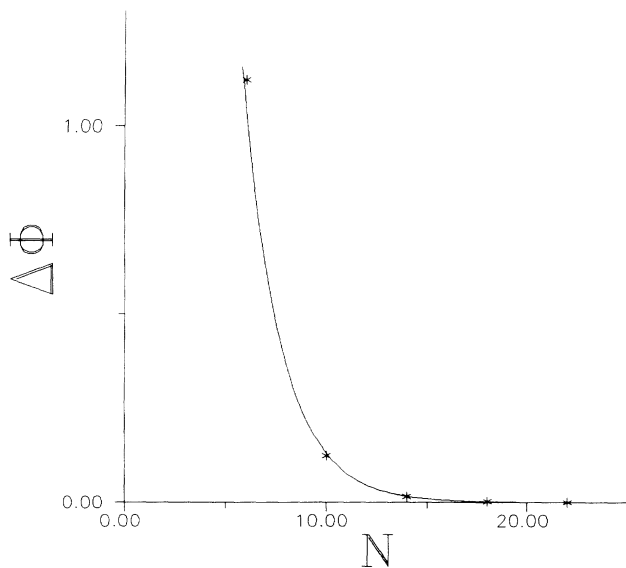


FIG. 4. Exponential approach to the canonical phase (see text) of the coefficient of the state with a soliton-antisoliton pair (at minimum distance) in the background of a perfect Néel state vs lattice size. Asterisks: Bethe-ansatz exact solution (gauge 2) for $\Delta=5$. Solid line: exponential fit. The total flux through the lattice is 2π .

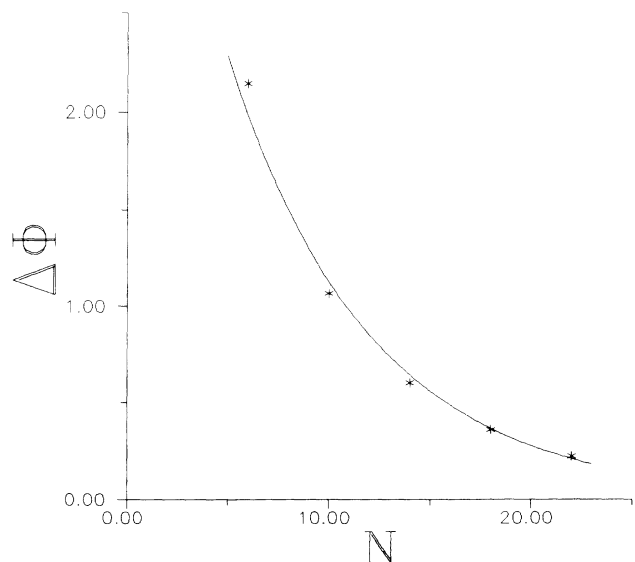


FIG. 5. Same as in Fig. 4 for $\Delta=2$.

within each QN state, the effect of the flux can be gauged away so that physical (gauge-invariant) properties do not change with flux. This explains, for instance, why the only change in energy upon increasing the flux depends on the off-diagonal coupling between QN states. In principle, we could have expected the diagonal term to depend on Φ (as does the QN wave function). Now we understand why it does not: within each QN state, the effect of the flux can be gauged away and the energy (gauged-independent property) remains the same as in the absence of flux. Therefore, the only change in energy is due to the coupling between QN states, described pictorially by type-1 closed loops. This coupling, though gauge dependent, is not gauge removable. Of course, the energy splitting this coupling gives rise to is gauge independent.

The situation previously described admits a simple pictorial interpretation. The typical fluctuation of the CN state is a type-2 closed loop whose phase is zero, therefore, flux independent. Only the interplay between both QN states will be affected by the flux in the manner dictated upon identifying this coupling with type-1 closed loops. In other words, to see the effect of the flux, one has to make sure that the dynamical objects complete a cycle around the lattice.

V. BERRY'S PHASE

In this section we show how the period doubling can be interpreted in terms of Berry's phase of adiabatic evolution.¹⁷ So far, we have used the word adiabatic as synonym of continuous in the flux-dependent properties of the GS's. Now we give a truly dynamical meaning to it. We imagine that a flux is slowly pierced through the ring and see the system evolve in time. In the AF ordered regime, if we start with the true GS and pass a flux $\Phi=2\pi$ slowly in time, we end up in the other quasidegenerate GS with an additional exponentially small increase in energy (the crossing taking place at $\Phi=\pi$ does not affect the adiabatic theorem because there is a conserved quantity, crystalline momentum in the gauge-2 representation, which guarantees continuity). This is the dynamical content of the adiabatic theorem.

We can state this adiabatic theorem in terms of QN states. If we start with a QN state, the time scale for the Rabi oscillations [see Eq. (15)] between QN states is given by $e^{N/\xi}$. This means that we can always choose a large enough lattice size such that, to the desired accuracy, starting with a QN state, its wave function evolves with time such that, at each time, this wave function is the QN state wave function corresponding to the instantaneous flux passed through the ring. In other words, the existence of a gap implies that a QN state is robust versus adiabatic changes of flux provided we do not wait long enough so as to see the effect of the slow degrees of freedom (Rabi oscillations between both QN states). But this result leads to an apparent puzzle if one uses a gauge-1 representation. In that case, the effective coupling between QN states has the form of the matrix (16), and this means that the true ground state changes upon adiabatic fluxing from being the even combination of QN states at $\Phi=0$ to the odd one at $\Phi=2\pi$. Yet, in terms of QN

states, and in this gauge representation, the wave function of each QN state has a flux period of 2π . Therefore, while the true GS has a flux period of 4π for adiabatic time evolution, the wave functions for each QN state making the true GS show a flux period of 2π for the same time adiabatic evolution. How does this come about?

The answer is the following. If we let the QN states evolve in time between $\Phi=0$ and $\Phi=2\pi$, within the specified conditions for adiabaticity and using the effective Hamiltonian $\mathcal{H}_1(\Phi)$, we get the following results:

$$|QNS1(t)\rangle = e^{i\phi_{\text{Berry}}^1} e^{i\phi_{\text{dynamical}}} |QNS1(0)\rangle + \text{exponentially small corrections}, \quad (21)$$

$$|QNS2(t)\rangle = e^{i\phi_{\text{Berry}}^2} e^{i\phi_{\text{dynamical}}} |QNS2(0)\rangle + \text{exponentially small corrections}, \quad (22)$$

where t is the time corresponding to $\Phi=2\pi$. We see that, after completing a cycle in parameter space (flux from zero to $\Phi=2\pi$), each QN state returns to the original state with a global phase, in agreement with the adiabatic theorem. This phase has a rapidly varying dynamical part, $\phi_{\text{dynamical}}$, the same for both states, and a geometrical (time-independent) contribution, different for each QN state, and such that, upon increasing the flux by 2π , then

$$\phi_{\text{Berry}}^1 - \phi_{\text{Berry}}^2 = \pi. \quad (23)$$

This geometrical phase is nothing but Berry's phase¹⁷ and, in this case, it is responsible for reconciling the flux periodicity of 4π of the true GS's with a flux periodicity of 2π for the QN states under real slow time evolution. In our case, we can even associate a space-time picture to the origin of this phase: closed type-1 soliton-antisoliton paths. If we artificially remove the contribution of these paths, the flux periodicity of the wave function (for gauge-1 representation) for real slow time evolution coincides with that of the spectrum (2π).

VI. SUMMARY

We have studied the spin- $\frac{1}{2}$ XXZ Hamiltonian in a ring with a magnetic flux through it. We have found that, in the AF regime, the two GS's evolve continuously upon increasing the flux with a periodicity twice the spectrum periodicity. This result already shown by SS in the gapless regime, suggests that the underlying dynamics corresponds to objects with half the charge of the particles of the original representation. These objects have been identified as kinks or domain walls between opposite AF domains. Using a mapping previously introduced to describe this Hamiltonian in terms of these objects, the effect of the flux has been incorporated and given a simple geometrical interpretation with a path-integral space-time diagram. This approach allows a complete classification of space-time paths in terms of the number of soliton-antisoliton closed loops around the ring. This classification explains the observed doubling of the flux

spectrum periodicity as a general property of the dynamics of this problem, in the sense that it is the natural flux periodicity for the matrix element of the time evolution operator between any two states. In the AF long-range-ordered regime, this scheme shows that, for sufficiently large rings, the physical effect of the flux manifests itself only in the relative coupling of the two degenerate broken-symmetry QN states. Within each QN state, the wave function is rigid in the presence of flux: its effect of flux amounts to a gauge transformation and it can be removed by a suitable choice of gauge, leaving physical (gauge-invariant) properties unchanged within each QN

state. Finally, in the AF region, the doubling of the flux periodicity has been given a dynamical meaning. It arises as a consequence of the different Berry's phase developed by both QN states as the total flux through the ring increases slowly with time. Again, the space-time paths responsible for this Berry's phase have been identified as closed soliton-antisoliton loops around the lattice.

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²⁰We use the simplest iterative scheme dictated by the structure of the Bethe-ansatz equations for gauge-2 representation. The convergence is fast and numerically stable. Unlike the procedure reported in Ref. 1, no need for different iterative schemes depending on flux is found.

²¹Unlike the energy, obtaining the coefficient of a particular state from the Bethe-ansatz expression for the eigenstates is a time consuming task. This is related to the necessity of generating all the permutations of N objects. Accordingly, the lattice sizes of Figs. 4 and 5 are much smaller than those used for the energy.