Exact results on the two-dimensional Heisenberg spin-$\frac{1}{2}$ problem

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In this paper the two-dimensional Heisenberg model is considered, with a possible anisotropy in the Heisenberg interaction in the 1 direction. Helical boundary conditions are introduced and an exact mapping of the two-dimensional lattice to a one-dimensional lattice is given. This mapping allows for a determination of the form of the wave function for 1 and 2 reversed spins. For this latter nontrivial case, the quantization condition is also derived.

I. INTRODUCTION

In this paper the following Hamiltonian will be considered:

$$H=2J\sum_{i,j}\Delta\hat{s}_i^z\hat{s}_j^z+\hat{s}_i^x\hat{s}_j^x+\hat{s}_i^y s_j^y\ , \tag{1}$$

where J is the Heisenberg interaction constant, which is also called the exchange integral. The operators $\hat{s}_i^x$, $\hat{s}_i^y$, and $\hat{s}_i^z$ are the usual spin operators acting on a particle with a spin equal to $\frac{1}{2}$ at site i. The pairs i,j refer to nearest-neighbor pairs. When the value of J is positive, we are dealing with an antiferromagnetic system and when it is negative, we are dealing with a ferromagnetic system. This Hamiltonian has been introduced by Heisenberg[1] to describe ferromagnetism in metals. The constant Δ describes the z-directional anisotropy in the Hamiltonian. When Δ equals one the isotropic Heisenberg case emerges, and when $J\rightarrow 0$, but keeping $J\Delta$ constant, the Ising Hamiltonian is obtained. Therefore the just given Hamiltonian, has also been called the Heisenberg-Ising or XXZ Hamiltonian.

If the spins are arranged in such a manner that they form a chain, the one-dimensional Heisenberg model is obtained. This model has been solved, i.e., the form of its eigenfunctions and their respective energies have been determined, by Bethe[2] and Orbach.[3] These eigenfunctions are given by the so-called Bethe ansatz. This ansatz and generalizations thereof are not only the solution of the one-dimensional Heisenberg model but also have proven to be extremely important in solving other (often one-dimensional) models. Among these are the one-dimensional system containing hard-core bosons,[4] the Kondo model[5] and the six- and eight-vertex models.[6–8]

Exact results concerning a two-dimensional array of $s=\frac{1}{2}$ spins are much more scarce and mainly concern some general properties of the ground state of the two-dimensional antiferromagnetic Heisenberg model. The most important of these, with respect to the form of the ground state, are Marshall's theorem,[9] specifying the amplitudes for every spin configuration in the ground state, and the Lieb-Mattis theorem,[10] determining the total spin of the ground state. With respect to the possibility of a phase transition in the two-dimensional Heisenberg model, the Mermin-Wagner theorem[11] states that there can only be such a transition at a temperature equal to zero.

Since the advent of the new high-T_c superconductors,[12] knowledge of the two-dimensional Heisenberg model has become more and more important. These superconductors contain CuO_2 layers, which magnetic behavior can very likely be described by the antiferromagnetic Heisenberg model. If holes are introduced in this layer, an extension to this model is needed allowing for hopping of the holes through the lattice. This extended model is called the t-J model.[13] It is believed that the magnetic behavior of the Cu^{2+} ions is very important in establishing superconductivity in the high-T_c superconductors.[14,15] In trying to understand what the origin of superconductivity is, much effort has been put into determining how the magnetic background affects the conducting holes. This has been done by numerical means[16] and by analytical means.[17] Although some understanding can be obtained from these methods,[18] they always will be approximate and one cannot be sure what their real value is, with regard to the applicability of the results they supply. To overcome this problem, it is imperative to obtain exact results with respect to the two-dimensional Heisenberg model. Here we will try to give a first start in reaching such new results.

More specific, the aim of this paper is to obtain more information about the form of the eigenstates of the two-dimensional Heisenberg model using a Bethe-ansatz approach. We will concentrate on the case of two reversed spins in an otherwise ferromagnetically aligned state. In Sec. II a two-dimensional system with new helical boundaries will be introduced and its symmetry will be shortly considered. In Sec. III Bloch's method[19] will be used to derive the secular equations. In Sec. IV these equations are given for the specific case of two reversed spins. In Sec. V the exact form of the eigenfunctions will be given and its quantization condition will be derived, solving the case of two reversed spins to the same level as is done in the one-dimensional XXZ model using the Bethe ansatz. In Sec. VI these results will be discussed.

II. HAMILTONIAN AND LATTICE

Usually, for the two-dimensional problem a square lattice is used, together with periodic boundary conditions,

such that a torus emerges [Fig. 1(a)]. If the torus contains $N \times N$ particles, a typical property of this system is the fact that when one walks through the lattice along a path in one direction, one will return to the starting point after exactly N steps. Here, a system will be constructed, in which the starting point will only be reached after passing all the particles, and not just N.

Such a path can be thought of being a helix wrapped around the torus. This can be done in two, more or less perpendicular, ways, as shown in Figs. 1(b) and 1(c). If one puts particles on the crossings of these two helices, this leads to a system with N^2-1 particles, where N is the number of times a helix is wrapped around the torus. This torus can be transformed to a highly symmetric one-dimensional ring, as shown in Fig. 2.

In order to see that there are N^2-1 particles, the system will be constructed starting from a normal two-dimensional plane with N particles in both directions (i.e., with N^2 particles in total) wrapped on a torus with the usual boundary conditions. To create two helices in this system, one has to cut the torus open in two perpendicular directions, move the particles on one edge of both cuts one lattice constant, and reconnect the particles again to their nearest neighbors on the other edge. As shown in Fig. 3, this results in two overlapping particles, of which one has to be removed, hence leading to N^2-1 particles. It is interesting to note that this procedure suggests other helical systems, characterized by the number of steps the particles are moved along the cuts (to be denoted by n_1 and n_2). The total number of particles in such a system will be $N^2-n_1n_2$. Instead of moving the lattice such that particles overlap, the lattice may also be moved such that empty sites occur.[20] After adding extra particles at those empty lattice sites, one obtains systems with $N^2+n_1n_2$ particles.

Returning to the helical system defined in Fig. 2, the symmetry elements are now readily recognized. There is one C_{N^2-1} axis, going through the middle of the circle. In addition, there is a symmetry operation, which is depicted in Fig. 2. In one form, the outer circle is one of the helices on the torus and the other bonds, lying inside the circle, form the other helix. After applying the drawn operation, this last helix will then form the circle, and the bonds of the first helix, will lie inside the ring. This operation, which will be called Q, is an element of the symmetry group if the interactions along the two helices are equal. Of course, there are other symmetry operations, which also occur in the symmetry group of a normal one-dimensional ring. However, we will focus our attention a little more on the operation Q, since it does not usually occur in symmetry groups of physical systems. For the system in Fig. 2 we have

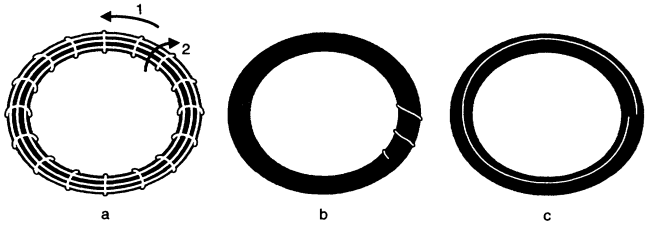

FIG. 1. (a) Shows the conventional torus chosen. Arrow 1 represents the action of the C_N axis, arrow 2 the action of the C_N circle. (b) and (c) show the two "perpendicular" helices, which can be drawn on a torus.

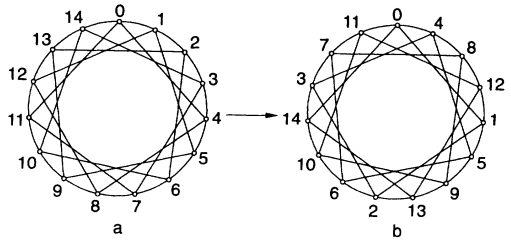

FIG. 2. (a) shows a representation of the Hamiltonian, for $N=4$, mapped onto a one-dimensional ring. This ring is one of the helices. If the lattice is drawn along the other helix, (b) is obtained. Therefore, the transformation from (a) to (b), represented by the arrow, is a symmetry operation.

$$Q \equiv (4,1)(8,2)(12,3)(9,6)(13,7)(14,11)(0)(5)(10) \tag{2}$$

or for a system of general N

$$Q \equiv \prod_{i=0}^{N^2-2}{}' (i, Ni \bmod (N^2-1)) \tag{3}$$

the following group can be constructed: E, $P, \ldots, P^i, \ldots, Q$, $QP, \ldots, QP^i, \ldots$; where P is a rotation around the C_{N_t} axis, and i ranges from 0 to N_t-1 (with $N_t \equiv N^2-1$). The prime at the product symbol indicates that only terms with $i \leq Ni \bmod (N^2-1)$ must be included. Its generators are P and Q, and one can find

$$P^{N_t}=E \ , \quad Q^2=E \tag{4}$$

and

$$QP=P^NQ \ . \tag{5}$$

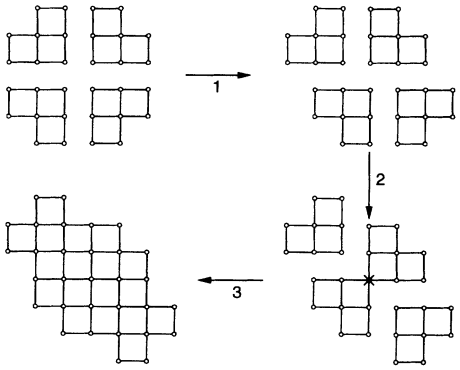

FIG. 3. To construct the helical system, the conventional torus is cut open in two directions. In the figure the part is shown where the two cuts cross. In the next step the particles along the horizontal cut are shifted one lattice spacing to the right, and after this likewise along the other cut. This leads to two overlapping particles, of which one therefore has to be removed. From this procedure then follows the last picture containing only N^2-1 particles.

A derivation is given in Appendix A.

For $N=3$, $N_t=8$, this means that the symmetry group is isomorphous with the abstract group G_{16}^{13}, as listed by Bradley and Cracknell.[21] One can take, for a general two-dimensional irreducible representation (irrep),

$$Q=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad P^n=\begin{bmatrix}\exp(kn) & 0\\ 0 & \exp(Nkn)\end{bmatrix} \tag{6}$$

as these satisfy Eqs. (4) and (5), where $k=2\pi i\lambda/N_t$, with $\lambda=0,\ldots,N_t-1$. For $\lambda=0$, $N+1$, $2(N+1)$, ... it can be derived that $N\lambda\equiv\lambda(\mathrm{mod}N_t)$, so that in these special cases a one-dimensional irrep is found (see Appendix B). This then means that for an eigenfunction transforming with a wave vector **k** under rotation, there is a degenerate (or sometimes identical) eigenfunction, transforming with a wave vector Nk, which can be obtained by operating with Q on the first eigenfunction.

The Heisenberg-Ising Hamiltonian can be written down very easily for the system drawn in Fig. 2. The Hamiltonian is

$$H=2J_1\sum_i \Delta_1 s_i^z s_{i+1}^z+s_i^x s_{i+1}^x+s_i^y s_{i+1}^y +2J_2\sum_i \Delta_2 s_i^z s_{i+N}^z+s_i^x s_{i+N}^x+s_i^y s_{i+N}^y\ , \tag{7}$$

where the summation extends from $i=0$ to N_t-1, s_i^α is the α component of the spin operator at site i, J_1 is the exchange integral for the first helix, J_2 is the exchange integral for the second helix, Δ_1 is the anisotropy parameter along helix 1, and likewise for Δ_2. The basis functions ψ will be characterized by r, the number of reversed spins from the ferromagnetic state, and the position of these reversed spins on the ring. Eigenfunctions can then be written as

$$\Psi=\sum_{n_1<n_2<\cdots<n_r} v_{n_1,\ldots,n_r}\psi_{n_1,\ldots,n_r}\ , \tag{8}$$

where the summation extends over all possible $n_1,\ldots,n_r$, with $n_i<n_j$ if $i<j$.

III. SECULAR EQUATIONS

The secular equations are found by calculating $\langle\psi_{n_1,\ldots,n_r}|H|\Psi\rangle=E\langle\psi_{n_1,\ldots,n_r}|\Psi\rangle$:

$$J_1\Delta_1/2({}^1N_{\mathrm{par}}-{}^1N_{\mathrm{antipar}})v_{n_1,\ldots,n_r}+J_2\Delta_2/2({}^2N_{\mathrm{par}}-{}^2N_{\mathrm{antipar}})v_{n_1,\ldots,n_r} +J_1\sum_1 v_{n_1',\ldots,n_r'}+J_2\sum_2 v_{n_1',\ldots,n_r'}=Ev_{n_1,\ldots,n_r}\ , \tag{9}$$

where the first line represents the result of the Ising terms, and the second line the result of the XY terms. ${}^1N_{\mathrm{par}}$ denotes the number of parallel spin pairs as seen along helix one, ${}^1N_{\mathrm{antipar}}$ the number of antiparallel spin pairs along helix 1, and likewise for ${}^2N_{\mathrm{par}}$ and ${}^2N_{\mathrm{antipar}}$. $\sum_1$ is the summation of all ${}^1N_{\mathrm{antipar}}$ spin arrangements $n_1',\ldots,n_r'$ differing from $n_1,\ldots,n_r$ by the interchange of two neighboring (as seen along helix 1) antiparallel spins, and again likewise for $\sum_2$. If $({}^1N_{\mathrm{antipar}}J_1\Delta_1+{}^2N_{\mathrm{antipar}}J_2\Delta_2)v_{n_1,\ldots,n_r}$ is added to the first two terms of Eq. (9) and is subtracted from the two summations, then one finds

$$J_1\Delta_1/2({}^1N_{\mathrm{par}}+{}^1N_{\mathrm{antipar}})v_{n_1,\ldots,n_r}+J_2\Delta_2/2({}^2N_{\mathrm{par}}+{}^2N_{\mathrm{antipar}})v_{n_1,\ldots,n_r} +J_1\sum_1(v_{n_1',\ldots,n_r'}-\Delta_1 v_{n_1,\ldots,n_r})+J_2\sum_2(v_{n_1',\ldots,n_r'}-\Delta_2 v_{n_1,\ldots,n_r})=Ev_{n_1,\ldots,n_r} \tag{10}$$

and, as ${}^1N_{\mathrm{par}}+{}^1N_{\mathrm{antipar}}={}^2N_{\mathrm{par}}+{}^2N_{\mathrm{antipar}}=N_t$,

$$J_1\sum_1(v_{n_1',\ldots,n_r'}-\Delta_1 v_{n_1,\ldots,n_r})+J_2\sum_2(v_{n_1',\ldots,n_r'}-\Delta_2 v_{n_1,\ldots,n_r})=\left[E-\frac{J_1\Delta_1+J_2\Delta_2}{2}N_t\right]v_{n_1,\ldots,n_r} \tag{11}$$

or

$$J_1'\sum_1(\Delta_1 v_{n_1,\ldots,n_r}-v_{n_1',\ldots,n_r'})+J_2'\sum_2(\Delta_2 v_{n_1,\ldots,n_r}-v_{n_1',\ldots,n_r'})=2\varepsilon v_{n_1,\ldots,n_r}\ , \tag{12}$$

where $J_1'=J_1/J$, $J_2'=J_2/J$, $J=J_1+J_2$ (hence $J_1'+J_2'=1$) and

$$-2\varepsilon=\left[E-\frac{J_1\Delta_1+J_2\Delta_2}{2}N_t\right]\Big/J\ . \tag{13}$$

For one reversed spin ($r=1$) these equations are solved trivially by $v_{n_1}=\exp(ikn_1)$ and $\varepsilon=J_1'\Delta_1+J_2'\Delta_2 -J_1'\cos(k)-J_2'\cos(Nk)$, with $k=2\pi\lambda/N_t$ and $\lambda=0,\ldots,N_t-1$. To relate this to the normal two-dimensional lattice, one should note that any number λ between 0 and N_t-1 can uniquely be written as $\lambda_1+N\lambda_2$, where λ_1 and λ_2 can have values between 0 and $N-1$, except when $\lambda_2=N-1$, then λ_1 can lie between 0 and $N-2$.

Moving the reversed spin along the J_1 helix by one step

leads to a factor in front of the wave function, with a moment containing $\lambda_1+N\lambda_2$. The momentum of the particle along the J_2 helix is associated with $N\lambda_1+\lambda_2$. If one plots all possible momenta characterized by λ in a graph, with $\lambda_1+N\lambda_2$ along the abscissa and $N\lambda_1+\lambda_2$ along the ordinate, one would obtain a slightly deformed square lattice of points (see Fig. 4). When N becomes large, the lattice becomes square, with lattice constants of 1 in both directions. The corresponding lattice consisting of the momenta would have lattice constants of $2\pi/N$ in both directions, as one would obtain in the normal two-dimensional case. Therefore when N goes to infinity the helical boundary conditions and the normal cyclic boundary conditions lead to the same eigenfunctions.

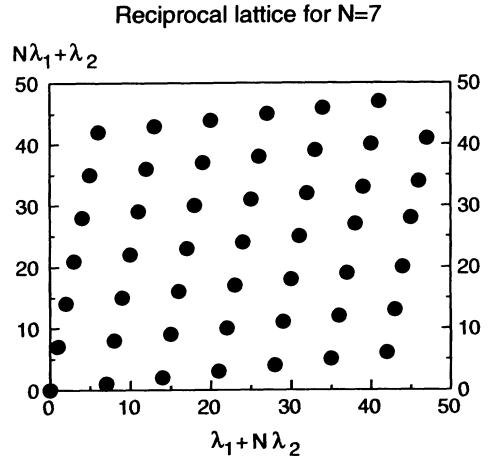

FIG. 4. The two components $\lambda_1+N\lambda_2$ and $N\lambda_1+\lambda_2$ of the momentum of one particle in a system with helical boundary conditions are depicted.

IV. SECULAR EQUATIONS FOR TWO REVERSED SPINS

By substituting the different possible spin configurations for two spins ($r=2$) into Eq. (12), the secular equations will now be written down. If one assumes that $n_2-n_1>N$ then one finds

$$2\varepsilon v_{n_1n_2}=4(J_1'\Delta_1+J_2'\Delta_2)v_{n_1n_2}-J_1'(v_{n_1-1n_2}+v_{n_1+1n_2}+v_{n_1n_2-1}+v_{n_1n_2+1})-J_2'(v_{n_1-Nn_2}+v_{n_1+Nn_2}+v_{n_1n_2-N}+v_{n_1n_2+N}) \tag{14}$$

and, if $1<n_2-n_1<N$,

$$2\varepsilon v_{n_1n_2}=4(J_1'\Delta_1+J_2'\Delta_2)v_{n_1n_2}-J_1'(v_{n_1-1n_2}+v_{n_1+1n_2}+v_{n_1n_2-1}+v_{n_1n_2+1})-J_2'(v_{n_1-Nn_2}+v_{n_2n_1+N}+v_{n_2-Nn_1}+v_{n_1n_2+N})\ . \tag{15}$$

[Take note of the fact that the seventh and eighth terms on the right-hand side of this equation are different from the ones in Eq. (14).]

The two reversed spins may also be neighbors, on both helices. One finds, for $n_2-n_1=1$,

$$2\varepsilon v_{n_1n_2}=(2J_1'\Delta_1+4J_2'\Delta_2)v_{n_1n_2}-J_1'(v_{n_1-1n_2}+v_{n_1n_2+1})-J_2'(v_{n_1-Nn_2}+v_{n_2n_1+N}+v_{n_2-Nn_1}+v_{n_1n_2+N}) \tag{16}$$

and for $n_2-n_1=N$:

$$2\varepsilon v_{n_1n_2}=(4J_1'\Delta_1+2J_2'\Delta_2)v_{n_1n_2}-J_1'(v_{n_1-1n_2}+v_{n_1+1n_2}+v_{n_1n_2-1}+v_{n_1n_2+1})-J_2'(v_{n_1-Nn_2}+v_{n_1n_2+N})\ . \tag{17}$$

If we use the following three equations to define $v_{n_1n_2}$ for $n_2\le n_1\le n_2+N-1$, Eq. (14) is valid for all $n_1<n_2$:

$$\forall n\in\{2,\ldots,N-1\}:\ v_{n_1+Nn_1+n}-v_{n_1+nn_1+N}=-v_{n_1n_1+n-N}+v_{n_1+n-Nn_1}\ , \tag{18}$$

$$J_1'(2\Delta_1v_{n_1n_1+1}-v_{n_1+1n_1+1}-v_{n_1n_1})+J_2'(v_{n_1+1n_1+N}+v_{n_1+1-Nn_1}-v_{n_1+Nn_1+1}-v_{n_1n_1+1-N})=0\ , \tag{19}$$

$$2\Delta_2v_{n_1n_1+N}-v_{n_1+Nn_1+N}-v_{n_1n_1}=0\ . \tag{20}$$

We can set both sides of the first equation equal to zero, and retain only one equation (here the equation obtained by putting the left-hand side equal to zero), since the other one follows from this equation by substituting n_1+N for n_1, which is valid because of the rotational symmetry of the system. This leads to

$$\forall n\in\{2,\ldots,N-1\}:\ v_{n_1+Nn_1+n}-v_{n_1+nn_1+N}=0\ . \tag{21}$$

Finally, the periodic boundary conditions must be satisfied:

$$v_{n_1n_2}=v_{n_2n_1+N_t}\ . \tag{22}$$

The remaining problem will now be to find a form of $v_{n_1n_2}$, which satisfies Eqs. (14), (19), (20), (21), and (22), and renders ε independent of the position of the two reversed spins.

V. FORM OF THE SOLUTION

For the one-dimensional problem Bethe proposed the following wave function:

$$v_{n_1 n_2}=e^{(ik/2)(n_1+n_2)}[ce^{a(n_2-n_1)}+c^{-1}e^{a(n_1-n_2)}] , \quad (23)$$

where k represents the cyclic symmetry and is determined from the boundary conditions. There is only one case ($n_2=n_1+1$), which is different from the equations for general (n_1,n_2), leading to an equation similar to Eq. (19). Together with the cyclic boundary condition, this equation determines c and the allowed values of a.

In our problem, there are N cases, different from the equations for general (n_1,n_2), leading to Eqs. (19), (20), and (21). To satisfy these N equations, N different c's and a's are needed, and therefore the following form of $v_{n_1 n_2}$ must be used (see Appendix C):

$$v_{n_1 n_2}=e^{(ik/2)(n_1+n_2)} \times \sum_i \alpha_i[c_i e^{a_i(n_2-n_1)}+c_i^{-1}e^{a_i(n_1-n_2)}] . \quad (24)$$

Equation (22) leads to two requirements:

$$k=\frac{2\pi\lambda}{N_t} , \quad \lambda=0,\ldots,N_t-1 , \quad (25)$$

and

$$c_i^{-2}=(-1)^{\lambda}\exp(N_t a_i) , \quad (26)$$

where α_i, c_i, and a_i can be general complex numbers.

To calculate the energy for this form of $v_{n_1 n_2}$ consider one term of the summation in Eq. (24) and substitute this into Eq. (14). This gives

$$\varepsilon=2J_1'\Delta_1+2J_2'\Delta_2-2J_1'\cos\left[\frac{k}{2}\right]\cosh(a_i) -2J_2'\cos\left[\frac{Nk}{2}\right]\cosh(Na_i) . \quad (27)$$

For all terms in Eq. (24) to lead to a correct eigenfunction all the occurring a_i's must lead to the same energy. That is, we must find all solutions for a_i of the above equation. If we let the energy be determined by one a_j (and to ensure that ε is real we could take its real part equal to zero), there are exactly $2N$ a_i's, since the right-hand side of Eq. (27) can be written as a polynomial of order $2N$ in $\exp(a_i)$. In other words, for every chosen a_j, determining ε, there are $2N$ possible a_i's (including itself), which are allowed in the summation of Eq. (24).

When a_i is a solution of the above equation then also $-a_i$ will be a solution. The $2N$ possible a_i's thus consist of pairs $(a_i,-a_i)$, which appear together in one term of $v_{n_1 n_2}$. Hence the number of different terms in $v_{n_1 n_2}$ will be exactly N, and therefore also the number of different α_i's and c_i's. Since c_i is determined by Eq. (26), we still have N constants left to be determined. The equations (19), (20), and (21) will be used for this.

When substituting $v_{n_1 n_2}$ into these equations, one finds for Eq. (19):

$$J_1'\sum_i \alpha_i\left\{c_i\left[\Delta_i e^{a_i}-\cos\left[\frac{k}{2}\right]\right] +c_i^{-1}\left[\Delta_1 e^{-a_i}-\cos\left[\frac{k}{2}\right]\right]\right\} +2J_2'\cos\left[\frac{Nk}{2}\right]\sum_i \alpha_i(c_i-c_i^{-1})\sinh[(N-1)a_i]=0 ; \quad (28)$$

for Eq. (20):

$$\sum_i \alpha_i\left\{c_i\left[\Delta_2 e^{Na_i}-\cos\left[\frac{Nk}{2}\right]\right] +c_i^{-1}\left[\Delta_2 e^{-Na_i}-\cos\left[\frac{Nk}{2}\right]\right]\right\}=0 ; \quad (29)$$

and for Eq. (21):

$$\forall n\in\{2,\ldots,N-1\}: \ \sum_i \alpha_i(c_i-c_i^{-1})\sinh[(N-n)a_i]=0 . \quad (30)$$

The first of these three equations can be rewritten as

$$J_2'\sum_i \alpha_i(c_i-c_i^{-1})\sinh[(N-1)a_i]=\frac{-J_1'}{2\cos(Nk/2)}\sum_i \alpha_i(c_i-c_i^{-1})\left[\frac{c_i[\Delta_1 e^{a_i}-\cos(k/2)]+c_i^{-1}[\Delta_1 e^{-a_i}-\cos(k/2)]}{(c_i-c_i^{-1})}\right] , \quad (31)$$

the second equation as

$$J_2'\sum_i \alpha_i(c_i-c_i^{-1})\sinh(Na_i) =J_2'\sum_i \alpha_i(c_i-c_i^{-1})\left[\frac{c_i[\Delta_2 e^{Na_i}-\cos(Nk/2)]+c_i^{-1}[\Delta_2 e^{-Na_i}-\cos(Nk/2)]}{(c_i-c_i^{-1})}+\sinh(Na_i)\right] , \quad (32)$$

and the third equation as

$$\forall n \in \{1,\ldots,N-2\}: \; J_2' \sum_i \alpha_i (c_i - c_i^{-1}) \sinh(n a_i) = 0 \; , \tag{33}$$

where $N-n$ has been replaced by n. The last two equations have been multiplied by J_2' to indicate that these two equations will not occur when $J_2'=0$.

If we use the following definitions,

$$\delta_i \equiv \alpha_i (c_i - c_i^{-1}) \; ,$$

$$P_i \equiv \frac{-1}{2\cos(Nk/2)} \left[\frac{c_i[\Delta_1 e^{a_i} - \cos(k/2)] + c_i^{-1}[\Delta_1 e^{-a_i} - \cos(k/2)]}{(c_i - c_i^{-1})} \right] , \tag{34}$$

$$Q_i \equiv \left[\frac{c_i[\Delta_2 e^{Na_i} - \cos(Nk/2)] + c_i^{-1}[\Delta_2 e^{-Na_i} - \cos(Nk/2)]}{(c_i - c_i^{-1})} \right] + \sinh(Na_i) \; ,$$

the previous three equations can again be rewritten as follows:

$$J_2' \begin{bmatrix} \sinh(a_1) & \cdots & \sinh(a_N) \\ \sinh(2a_1) & \cdots & \sinh(2a_N) \\ \vdots & \ddots & \vdots \\ \sinh[(N-1)a_1] & \cdots & \sinh[(N-1)a_N] \\ \sinh(Na_1) & \cdots & \sinh(Na_N) \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \\ \vdots \\ \delta_{N-1} \\ \delta_N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ J_1' \sum_i \delta_i P_i \\ J_2' \sum_i \delta_i Q_i \end{bmatrix} . \tag{35}$$

The matrix in this equation shows some resemblance to a Vandermonde matrix and can be diagonalized by the following method, which is similar to the one used for Vandermonde matrices.

Consider the following polynomial in $\sinh(a)$:

$$R_j(a) = \frac{\sinh(a)}{\sinh(a_j)} \prod_{\substack{k=1 \\ k \neq j}}^{N} \left[\frac{\cosh(a) - \cosh(a_k)}{\cosh(a_j) - \cosh(a_k)} \right] \equiv \sum_{k=1}^{N} A_{jk} \sinh(ka) \; . \tag{36}$$

This polynomial has the following property:

$$R_j(a_k) = \delta_{jk} \; . \tag{37}$$

This means that the matrix A, defined by the elements A_{jk} from Eq. (36), is the inverse of the matrix in Eq. (35). Multiplying Eq. (35) from the left by matrix A leads to the following equation:

$$\begin{bmatrix} -J_2' + J_1' A_{1N-1} P_1 + J_2' A_{1N} Q_1 & \cdots & J_1' A_{1N-1} P_N + J_2' A_{1N} Q_N \\ \vdots & \ddots & \vdots \\ J_1' A_{NN-1} P_1 + J_2' A_{NN} Q_1 & \cdots & -J_2' + J_1' A_{NN-1} P_N + J_2' A_{NN} Q_N \end{bmatrix} \begin{bmatrix} \delta_1 \\ \vdots \\ \delta_N \end{bmatrix} = 0 \; . \tag{38}$$

For all δ_i not to be zero, the determinant of this matrix must be zero. The determinant can be calculated as follows. First define the following quantities:

$$S \equiv (A_{1N-1} A_{2N} - A_{1N} A_{2N-1}) \; , \tag{39}$$

$$s_j^1 \equiv (A_{jN-1} A_{2N} - A_{jN} A_{2N-1})/S \; ,$$

$$s_j^2 \equiv (A_{jN} A_{1N-1} - A_{jN-1} A_{1N})/S \; ,$$

and the matrix:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ s_3^1 & s_3^2 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ s_N^1 & s_N^2 & 0 & 0 & \cdots & -1 \end{bmatrix} . \tag{40}$$

Note that the determinant of this matrix equals -1^N.

Multiplying the matrix of Eq. (38) from the left by this matrix leads to

$$\begin{bmatrix} -J_2'+J_1'A_{1N-1}P_1 & J_1'A_{1N-1}P_2 & J_1'A_{1N-1}P_3 & \cdots & J_1'A_{1N-1}P_N \\ +J_2'A_{1N}Q_1 & +J_2'A_{1N}Q_2 & +J_2'A_{1N}Q_3 & & +J_2'A_{1N}Q_N \\ J_1'A_{2N-1}P_1 & -J_2'+J_1'A_{2N-1}P_2 & J_1'A_{2N-1}P_3 & \cdots & J_1'A_{2N-1}P_N \\ +J_2'A_{2N}Q_1 & +J_2'A_{2N}Q_2 & +J_2'A_{2N}Q_3 & & +J_2'A_{2N}Q_N \\ -J_2's_3^1 & -J_2's_3^2 & J_2' & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -J_2's_N^1 & -J_2's_N^2 & 0 & \cdots & J_2' \end{bmatrix}, \tag{41}$$

and multiplying this with the same matrix from the right leads to

$$\begin{bmatrix} -J_2'+J_1'A_{1N-1}\sum_j s_j^1P_j & J_1'A_{1N-1}\sum_j s_j^2P_j & & & \\ +J_2'A_{1N}\sum_j s_j^1Q_j & +J_2'A_{1N}\sum_j s_j^2Q_j & \cdots & & \\ J_1'A_{2N-1}\sum_j s_j^1P_j & -J_2'+J_1'A_{2N-1}\sum_j s_j^2P_j & & & \\ +J_2'A_{2N}\sum_j s_j^1Q_j & +J_2'A_{2N}\sum_j s_j^2Q_j & \cdots & & \\ 0 & 0 & -J_2' & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -J_2' \end{bmatrix}. \tag{42}$$

Because $\det(AB)=\det(A)\det(B)$ and the determinant of the matrix in Eq. (40) is not equal to zero, the determinant of this matrix should be zero. Hence

$$\begin{vmatrix} -J_2'+J_1'A_{1N-1}\sum_j s_j^1P_j+J_2'A_{1N}\sum_j s_j^1Q_j & J_1'A_{1N-1}\sum_j s_j^2P_j+J_2'A_{1N}\sum_j s_j^2Q_j \\ J_1'A_{2N-1}\sum_j s_j^1P_j+J_2'A_{2N}\sum_j s_j^1Q_j & -J_2'+J_1'A_{2N-1}\sum_j s_j^2P_j+J_2'A_{2N}\sum_j s_j^2Q_j \end{vmatrix}=0. \tag{43}$$

Calculating this determinant, and realizing that

$$\begin{aligned} &A_{1N-1}s_j^1+A_{2N-1}s_j^2=A_{jN-1}, \\ &A_{1N}s_j^1+A_{2N}s_j^2=A_{jN}, \\ &s_j^1s_{j'}^2-s_{j'}^1s_j^2=(A_{jN-1}A_{j'N}-A_{jN}A_{j'N-1})/S, \end{aligned} \tag{44}$$

one finds that

$$\begin{vmatrix} -J_2'+J_1'\sum_j A_{jN-1}P_j & J_1'\sum_j A_{jN}P_j \\ J_2'\sum_j A_{jN-1}Q_j & -J_2'+J_2'\sum_j A_{jN}Q_j \end{vmatrix}=0. \tag{45}$$

This is the quantization condition. Equation (27) determines the allowed a_j's for a given energy, and Eq. (45) determines which energies are allowed. In principle, one can subsequently, with Eq. (35) and a normalization condition for the wave function, determine the form of the α_i's, but since they do not affect the energy of the wave function, we will not deal with this task here.

VI. DISCUSSION

In order to elucidate the previous result a little more, it will be investigated where the solutions of the quantization condition can be found. To start with, I would like to remark that the given method is exact, under the provisions made in Appendix C, and therefore should supply all the necessary solutions. On the basis of group theory and the given total number of spin configurations for $r=2$, the total number of solutions should be as follows:

$$\left.\begin{aligned} &\forall\lambda \text{ even}: \frac{N_t}{2} \\ &\forall\lambda \text{ odd}: \frac{N_t}{2}-1 \end{aligned}\right\} \text{ in total}: \frac{N_t}{2}\frac{N_t}{2}+\frac{N_t}{2}\left[\frac{N_t}{2}-1\right] = \left[\frac{N_t}{2}\right] \tag{46}$$

where N_t has been taken to be even. Although all these solutions should be contained in Eq. (45), it is not yet clear what the actual values of the momenta a_i for these solutions will be. To gain some insight in this problem, the structure of the quantization condition will be examined by first considering some special cases and then the general case. Before doing so, it will be useful to rewrite

P_i and Q_i as follows:

$$P_i=\frac{-1}{2\cos(Nk/2)}\{\coth(\varphi_i/2)[\Delta_1\cosh(a_i)-\cos(k/2)] +\Delta_1\sinh(a_i)\}\ , \tag{47}$$

$$Q_i=\coth(\varphi_i/2)[\Delta_2\cosh(Na_i)-\cos(Nk/2)] +(1+\Delta_2)\sinh(Na_i)\ ,$$

where $c_i=\exp(\varphi_i/2)$ has been substituted.

Also, it is important to see that when one a_i is chosen all other parameters, as the other a_i's and all φ_i's are then determined (for given k and J_1',J_2'). The other way around, for determining the solutions of Eq. (45), there is only one parameter a_i, which can be varied. Whenever this parameter is referred to it will be called a_j, instead of a_i. In general, a_j may be a complex number; however, confining a_j to the area

$$\{\mathrm{Re}(a_j)=0\cap 0\le \mathrm{Im}(a_j)\le\pi\}\ , \quad \cup\{0\le\mathrm{Re}(a_j)<\infty\cap\mathrm{Im}(a_j)=0\}\ , \quad \cup\{0\le\mathrm{Re}(a_j)<\infty\cap\mathrm{Im}(a_j)=\pi\} \tag{48}$$

ensures that ε is real but still can obtain all values between $+\infty$ and $-\infty$.

A. Special case $J_2'=0$

When J_2' equals zero, the normal one-dimensional chain is obtained, and hence a similar quantization condition to (45) should emerge. As noted in Appendix C, here it is not possible to obtain N different a_i's, and hence only in this case our derivation of Eq. (45) cannot be used.

However, if one considers Eq. (35), one finds

$$J_1'\sum_i \delta_i P_i=0\ . \tag{49}$$

Since in fact $N-1$ of the P_i's do not exist, one may take their accompanying α_i's equal to zero, and retain only one P_j belonging to a_j, leading to

$$\coth\left[\frac{\varphi_j}{2}\right]=\frac{-\Delta_1\sinh(a_j)}{\Delta_1\cosh(a_j)-\cos(k/2)} \tag{50}$$

which is essentially the same condition as derived by Orbach.[3] To get some idea of the structure of this equation, let us consider its solutions in the area of a_j, where $\mathrm{Re}(a_j)=0$. According to Eq. (26):

$$\varphi_j=-N_t a_j+i\pi\lambda' \tag{51}$$

where λ' is 0 when λ is even and λ' is 1 when λ is odd. Hence, the left-hand side of (50) goes from $-\infty$ to $+\infty$, when $\mathrm{Re}(a_j)=0$ and $\mathrm{Im}(a_j)$ goes from $2\pi(\gamma+\lambda'/2)/N_t$ to $2\pi(\gamma+\lambda'/2+1)/N_t$, with γ an integer. This means that $\coth(\varphi_j/2)$ crosses the right-hand side (rhs) of (50) for every γ once and leads to a solution, unless the rhs diverges. Therefore, for λ even there are $N_t/2-1$ different γ's for a given λ leading to a solution. For λ odd, one additional γ must be excluded because $a_j=0$ is a solution of (50), but leads to $\varphi_j=\pi$, and hence to $v_{n_1n_2}=0$. This means that when λ is odd, there are $N_t/2-2$ solutions for a given λ, with $\mathrm{Re}(a_j)=0$. The other solutions are to be found in the other regions of (48) and lead to bound states. A detailed analysis is given by Orbach and Bethe. The important fact to remember is that the majority of solutions is in the area where $\mathrm{Re}(a_j)=0$, because then $\coth(\varphi_j/2)$ shows it divergences, leading to the solutions.

B. Special case $J_1'=0$

When J_1' equals zero, again, a one-dimensional chain remains, however, with its particles numbered in an unusual fashion, leading to a quantization condition, somewhat different from the Orbach form. When J_1' equals zero, Eq. (45) leads to

$$\sum_i A_{iN}Q_i=1 \tag{52}$$

or, in a more explicit form,

$$\sum_i A_{iN}\left\{\coth\left[\frac{\varphi_i}{2}\right]\left[\Delta_2\cosh(Na_i)-\cos\left[\frac{Nk}{2}\right]\right] +(1+\Delta_2)\sinh(Na_i)\right\}=1\ . \tag{53}$$

From Eq. (36) follows

$$A_{iN}=\frac{1}{\sinh(a_i)\prod_{\substack{k=1\\k\neq i}}^{N}2[\cosh(a_i)-\cosh(a_k)]}\ . \tag{54}$$

Again, it will be indicated that most of the solutions are to be found in the area where $\mathrm{Re}(a_j)=0$ (hence, when a_j is discussed we mean $\mathrm{Im}(a_j)$, unless explicitly stated). First it will be argued that all $A_{iN}\coth(\varphi_i/2)$ are all increasing or decreasing functions, for every i, of a_j. The a_i's are the solutions to $\cosh(Na_i)=\cosh(Na_j)$ (i.e., all a_i including a_j lead to the same energy). If the a_i's (including a_j) are ordered according to increasing a_i, it is easy to see that if a_j is increasing, its neighbors a_{j-1} and a_{j+1} are decreasing, and vice versa. It is also clear from (54) that the sign of A_{jN} is opposite to the sign of its neighbors A_{j-1N} and A_{j+1N}. Therefore, the $A_{1N}\coth(\varphi_i/2)$ are all decreasing or increasing at the same time. Furthermore, the factors $[\Delta_2\cosh(Na_i)-\cos(Nk/2)]$ do all have the same value for all a_i for a given a_j.

Next it will be shown that a_j cannot be allowed to vary from 0 to π, since this would lead to overcounting the number of solutions. This is very simple to see because, when a_j traverses some area, in fact the other a_i's traverse $N-1$ other areas. If a solution is found in a_j's area, the same solution will be found when a_j traverses one of the other a_i's areas. To avoid this overcounting the domain of a_j must be restricted. The following restriction is proposed:

$$\text{if } \left[\frac{d\varepsilon}{da_j}\right]_{a_j=(2\pi/N)\left[\gamma+\lambda'/2\right]}<0\,,$$

$$\text{then } \frac{2\pi}{N}\left[\gamma+\frac{\lambda'}{2}\right]\le a_j<\frac{2\pi}{N}\left[\gamma+\frac{\lambda'}{2}+\frac{1}{N}\right], \tag{55}$$

$$\text{if } \left[\frac{d\varepsilon}{da_j}\right]_{a_j=(2\pi/N)\left[\gamma+\lambda'/2\right]}>0\,,$$

$$\text{then } \frac{2\pi}{N}\left[\gamma+\frac{\lambda'}{2}\right]\ge a_j>\frac{2\pi}{N}\left[\gamma+\frac{\lambda'}{2}-\frac{1}{N}\right],$$

$$\text{with } \gamma\in\{0,\ldots,N_t/2\}$$

where any subarea, with a γ leading to an a_j smaller than zero or larger than π, or with a γ such that the derivative of the energy is zero, will be excluded. These subareas have been chosen, as to satisfy the following conditions.

(1) The sum in Eq. (50) does only diverge at the beginning and the end of each subarea because $a_i=a_j+2\pi v_i/N$ and $a_{i'}=\pi-a_j-2\pi v_{i'}/N$, where the ν_i's must be chosen in such a way that the a_i's are also between 0 and π.

(2) If a_j goes from $2\pi(\gamma+\lambda'/2)/N_t$ to its other boundary, the energy ε decreases.

These conditions, in fact, ensure that every subarea is traversed only by a_j and not by any other a_i, which prevents the solutions from being overcounted. This can be seen as follows: the divergence at $2\pi(\gamma+\lambda'/2)/N_t$ is caused by $\coth(\varphi_j/2)$ and a_j starts at this value moving in the lower-energy direction until it strikes some divergence [caused by another $\coth(\varphi_i/2)$] from the higher-energy direction. Because of the fact that if one $\coth(\varphi_i/2)$ diverges, only this $\coth(\varphi_i/2)$ diverges and, because of the fact that if a_j moves in the lower-energy direction all a_i move in the lower-energy direction, indeed every subarea is only covered by a_j.

It is now clear that if neither A_{Jn} nor $[\Delta_2\cosh(Na_j)-\cos(Nk/2)]$ change sign in a subarea, the sum in Eq. (53) goes from $-\infty$ to $+\infty$, if a_j traverses this subarea. A_{Jn} will change sign if some $2\pi v_i/N$ or $\pi-2\pi v_{i'}/N$ is included in the subarea. This, however, will happen only for one γ for a given k, and only for λ odd. $[\Delta_2\cosh(Na_j)-\cos(Nk/2)]$ will also change sign for only one γ for a given k. Therefore, the same number of solutions are found as in the previous one-dimensional case in the area where $\mathrm{Re}(a_j)=0$.

C. General J_1', J_2'

For general J_1', J_2', the case is not as simple as above. Again, it is necessary to restrict the allowable values of $a_{j'}$ to avoid overcounting of solutions.

Because the four terms in the determinant of Eq. (45) have divergences for the $a_{j'}$ this is, in fact, possible. This is illustrated in Fig. 5. In this picture the abscissa represents a_j [$\mathrm{Re}(a_j)$ still being zero], and the ordinate is

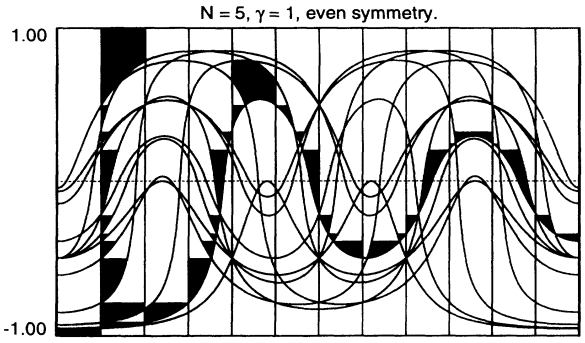

FIG. 5. Depicted are the lines of divergence for the quantization condition for λ even. The abscissa represents a_j, ranging from 0 to π. The ordinate represents $J_1'\cos(k/2)$, ranging from -1 to 1. A detailed explanation is given in the text.

the value of $J_1'\cos(k/2)$. $J_2'\cos(Nk/2)$ has been chosen to be $1-|J_1'\cos(k/2)|$. The black straight and curved lines are the points where any of the four terms in the determinant diverge. The straight lines are the divergences of $\coth(\varphi_j/2)$ (i.e., whenever a_j equals some $2\pi(\gamma+\lambda'/2)/N_t$), and the curved lines are the divergences of a $\coth(\varphi_i/2)$, which occurs when an a_i, defined by a_j by having the same energy, assumes the value of $2\pi(\gamma+\lambda'/2)/N_t$.

One can also say that for every allowable $2\pi(\gamma+\lambda'/2)/N_t$ there is one straight line in the figure (representing the fact that a_j assumes this value), and there is one additional curved line [representing the fact that when a_j is on this line, one of the a_i assumes the value $2\pi(\gamma+\lambda'/2)/N_t$]. This means that there are pairs of lines, one straight and one curved, such that every pair belongs to one γ.

The domain of a_j can now be restricted in a way similar to the case with $J_1'=0$, using the following method (where one should bear in mind that we are looking for solutions for a given J_1', J_2' and k).

> Start with a_j at a $2\pi(\gamma+\lambda'/2)/N_t$ and determine its accompanying a_i's. Let a_j move in a direction such that their energy decreases. Stop with a_j moving, whenever a_j or any of its a_i's encounter another "divergence" line. If a_j encounters a minimum in ε as a function of a_j, let any of the a_i, which still can move, move in such a way that the energy lowers [which could mean that $\mathrm{Re}(a_j)$ no longer equals zero, although ε remains real] until it encounters a divergence line or the edges of the total domain, 0 or π. The values, which a_j has now traversed, including its starting point and excluding its end point, constitute one of the subareas, which again is a part of the restricted domain of a_j.

As an example this method has been used to construct the black area in Fig. 5. It is clear that none of these subareas is covered more than once, since one starts from one $2\pi(\gamma+\lambda'/2)/N_t$ moving downwards, until one of the a_i encounters another $2\pi(\gamma'+\lambda'/2)/N_t$ from above.

The case that one of the a_i's strikes 0 or π and no

divergence happens only when λ is odd because for λ even, also at 0 and π there are divergences and only for one γ, since only one divergence line (straight or curved) is closest to 0 or π. This one area must probably be excluded (as had to be done with the previous one-dimensional case when A_{jN} changed sign), since the determinant will not cover all values from $-\infty$ to $+\infty$, and hence might not lead to a solution. For certain values of J_1', J_2' and k, divergence lines may cross, which might lead to a complication in constructing the subareas. This, however, can be overcome by constructing the subareas for $J_1'+\delta$, with δ small and positive, and taking the limit for $\delta \downarrow 0$. This makes the construction of the subareas unambiguous, although some areas may have a length approaching zero.

The main problem now is, that it is not clear how the value of the determinant will behave on any of these subareas. It is clear that it will diverge at the beginning and at the end of every subarea. Unfortunately, it does not necessarily do so from $-\infty$ to $+\infty$. One may just hope for some kind of conservation of solutions in the subareas, meaning that if, by varying J_1', a solution disappears from one subarea (e.g., because the value of the determinant diverges to $-\infty$ at both sides of the subarea, instead of diverging from $-\infty$ to $+\infty$), an additional solution may appear in a neighboring area (where, for example, the determinant now diverges to $+\infty$ at both sides, however, including 0, thereby satisfying the quantization condition, and leading to two solutions).

Despite these problems, one should bear in mind that the quantization condition is exact and will supply all solutions. It is just not clear what the exact momenta of these solutions will be. Future work on this problem should of course consider this. However, probably the most important question to answer is how to extend the above results to a general number of reversed spins. The solution of the $r=2$ case is a first step in this direction but not, by far, the only step to be made.

We would like to note that this result could only have been obtained through the use of the helical boundary conditions. These conditions allow for a one-dimensional numbering of the particles and, hence, of the reversed spins, conserving a high symmetry (at least C_{N^2-1}) of the system. If we had used the usual two-dimensional numbering, the secular equations would have been difference equations in at least two variables. For such an equation, it is not possible to write its general solution in terms of a finite sum of exponentials, and the quantization condition cannot be derived. As this is possible using the helical boundary conditions, it is certainly advisable to use them.

To extend the described results, one may look for some ansatz or employ related vertex models. We are currently pursuing our research in this last field.

VII. CONCLUSIONS

In this paper the form of the eigenfunctions up to $r=2$ of the two-dimensional Heisenberg Hamiltonian with helical boundary conditions have been derived. The $r=2$ result is nontrivial. In this case the eigenfunction consists of a sum of exponential terms, containing the position of the reversed spins and an associated moment. The different moments for the exponential terms are uniquely defined by the energy of the eigenfunction. Also the quantization condition is given, which determines which momenta are allowed (and of course which energies are allowed).

APPENDIX A: DERIVATION OF EQ. (5)

Equation (5) can be proven as follows. As noted before any symmetry operation is in fact a permutation of the particles. A symmetry operation R can, hence, be written as

$$R=\prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ f(j)\end{pmatrix}, \tag{A1}$$

where $f(j)$ is some function of j. For the terms occurring in the product the particle, which is at position j after application of the permutation, was at position $f(j)$ before the permutation. Since one particle cannot be on two different positions after a permutation, $f(j)$ must cover the whole collection of numbers $\{0,\ldots,N_t-1\}$ when j goes from 0 to N_t-1. This means that the product of two permutations can be written as

$$\begin{aligned} RR' &= \prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ f(j)\end{pmatrix}\prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ g(j)\end{pmatrix} \\ &= \prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ f(j)\end{pmatrix}\prod_{j=0}^{N_t-1}\begin{pmatrix} f(j) \\ g(f(j))\end{pmatrix} \\ &= \prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ g(f(j))\end{pmatrix}. \end{aligned} \tag{A2}$$

Now, P and Q are as follows:

$$P=\prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ j+1 \bmod N_t\end{pmatrix}, \quad Q=\prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ Nj \bmod N_t\end{pmatrix}. \tag{A3}$$

The left-hand side of (5) reads

$$\begin{aligned} QP &= \prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ Nj \bmod N_t\end{pmatrix}\prod_{j=0}^{N_t-1}\begin{pmatrix} Nj \bmod N_t \\ Nj+1 \bmod N_t\end{pmatrix} \\ &= \prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ Nj+1 \bmod N_t\end{pmatrix}, \end{aligned} \tag{A4}$$

and, since $(N^2 \bmod N_t)=1$, the right-hand side gives

$$\begin{aligned} P^N Q &= \prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ j+N \bmod N_t\end{pmatrix}\prod_{j=0}^{N_t-1}\begin{pmatrix} j+N \bmod N_t \\ Nj+N^2 \bmod N_t\end{pmatrix} \\ &= \prod_{j=0}^{N_t-1}\begin{pmatrix} j \\ Nj+1 \bmod N_t\end{pmatrix}. \end{aligned} \tag{A5}$$

Q.E.D.

APPENDIX B: DERIVATION OF EQ. (6)

The irreps of the group defined by Eqs. (4) and (5) will be derived, using these equations and the great orthogonality theorem (GOT). Define the vectors $\mathbf{r}_{ij}^{l}$ in the h-dimensional space (with h the order of the group) as follows: take from an irrep $D^{l}(R)$ (which is a matrix) its component $D_{ij}^{l}(R)$, where R is a symmetry operation, and l numbers the irreps. The components of $\mathbf{r}_{ij}^{l}$ are the values of $D_{ij}^{l}(R)$ for all different symmetry operations. That is

$$\mathbf{r}_{ij}^{l}=(D_{ij}^{l}(R_1),D_{ij}^{l}(R_2),\ldots,D_{ij}^{l}(R_h)) . \tag{B1}$$

In our case $h=2N_t$, with the ordering of the symmetry elements as follows: E, P, $P^2,\ldots,P^{N_t-1}$, Q, QP, $QP^2,\ldots,QP^{N_t-1}$. The GOT now states that all possible $\mathbf{r}_{ij}^{l}$ (which are $2N_t$ in total) must be orthogonal to each other and are normalized to $(h/d_l)^{1/2}$, where d_l is the dimension of its irrep.

Also bear in mind that

$$\sum_{j=0}^{N_t-1} e^{i(k-k')j}=0 \text{ for } k\neq k' , \quad k=\frac{2\pi\lambda}{N_t} , \quad k'=\frac{2\pi\lambda'}{N_t} , \quad \lambda \text{ and } \lambda' \text{ integer} ,$$
$$=N_t \text{ for } k=k' . \tag{B2}$$

First the one-dimensional irreps will be derived.

Since $Q^2=E$, for a one-dimensional irrep Q can be ±1. $P^{N_t}=E$, so

$$P=e^{ik} , \quad k=2\pi\lambda/N_t , \quad \lambda \text{ integer} . \tag{B3}$$

But, since $QP=P^NQ$, one finds

$$P=P^N \Longrightarrow \lambda=\gamma(N+1) , \quad \gamma=0,\ldots,N-2 . \tag{B4}$$

Therefore, the one-dimensional irreps are

$$Q=\pm1 , \quad P=e^{ik} , \quad k=2\pi\lambda/N_t , \quad \lambda=\gamma(N+1) , \quad \gamma=0,\ldots,N-2 . \tag{B5}$$

Now consider the two-dimensional irreps. First the basis functions will be chosen in such a way, that P is always diagonal. Next, with $Q^2=E$, one finds

$$Q\equiv\begin{bmatrix} a & b \\ c & d \end{bmatrix} , \quad Q^2=\begin{bmatrix} a^2+bc & b(a+d) \\ c(a+d) & bc+d^2 \end{bmatrix}=\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \Longrightarrow \begin{matrix} a^2+bc=1 , & b(a+d)=0 , \\ bc+d^2=1 , & c(a+d)=0 . \end{matrix} \tag{B6}$$

If $a\neq-d$, this would mean that $b=c=0$ and, hence, that Q is diagonal. If this were the case, all matrices in the irrep would be diagonal and then the irrep would not be irreducible, and therefore not even an irrep. Hence, $a=-d$, and the following Q will be used:

$$Q=\begin{bmatrix} a & b \\ c & -a \end{bmatrix} , \quad bc=1-a^2 . \tag{B7}$$

Since $P^{N_t}=E$, P can be written as

$$P=\begin{bmatrix} e^{ik} & 0 \\ 0 & e^{ik'} \end{bmatrix} \text{ with } k=2\pi\lambda/N_t , \quad k'=2\pi\lambda'/N_t , \quad \lambda \text{ and } \lambda' \text{ integer} . \tag{B8}$$

It is now clear that b and c may not be equal to zero, since, if this were the case, an $\mathbf{r}_{ij}^{l}$ can be constructed (e.g., when $b=0$, then $i=1$, $j=2$) with all of its components equal to zero, violating the GOT. One now has to satisfy Eq. (5):

$$QP=\begin{bmatrix} ae^{ik} & be^{ik'} \\ ce^{ik} & -ae^{ik'} \end{bmatrix} , \quad P^NQ=\begin{bmatrix} ae^{iNk} & be^{iNk} \\ ce^{iNk'} & -ae^{iNk'} \end{bmatrix} \Longrightarrow ae^{iNk}=ae^{ik} , \quad be^{iNk}=be^{ik'} , \quad ce^{iNk'}=ce^{ik} , \quad ae^{iNk'}=ae^{ik'} . \tag{B9}$$

If $a\neq0$, this leads to $k=k'$ and $\lambda=\gamma(N+1)$. Note that these λ values also occur in the one-dimensional irreps. With $bc=1-a^2$, and $b\neq0$ and $c\neq0$ it is clear that $a\neq\pm1$. This means that an $\mathbf{r}_{11}^{l}$ from a two-dimensional irrep with a $\lambda=\gamma(N+1)$ can never be orthogonal to the one-dimensional irrep with the same λ, and therefore $a=0$.

This means that

$$Q=\begin{bmatrix} 0 & b \\ 1/b & 0 \end{bmatrix} \text{ and } k'=Nk , \tag{B10}$$

where λ may have all integer values between 0 and N_t-1, except for the values occurring in the one-

dimensional irreps. Furthermore, every λ may occur only once, either as λ, either as $N\lambda \bmod N_t$.

Finally, b has to be determined by the normalization condition, leading to $|b|^2=1$ or $b=\exp(i\phi)$. Any value of ϕ may be chosen. However, if one has been chosen, no other ϕ is allowed, since this would lead to violation of the GOT. $\phi=0$ will be chosen. Therefore, we find for the two-dimensional irreps:

$$Q=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad P=\begin{bmatrix}e^{ik} & 0\\ 0 & e^{iNk}\end{bmatrix}, \quad k=\frac{2\pi\lambda}{N_t} \tag{B11}$$

with λ restricted as indicated above.

Finally, all vectors $\mathbf{r}_{ij}^l$ occurring in these irreps are orthogonal to the one-dimensional irreps, and hence these irreps are indeed irreducible. Every λ generates two $\mathbf{r}_{ij}^l$ (two per λ in the one-dimensional case because $Q=\pm 1$, and two per λ in the two-dimensional case, since a two-dimensional irrep generates four $\mathbf{r}_{ij}^l$ and uses two λ's) and therefore $2N_t$ $\mathbf{r}_{ij}^l$'s have been generated. Since the order of the group is also $2N_t$, there are no irreps of dimensionality higher than two.

APPENDIX C: DERIVATION OF EQ. (24)

Equation (24) will be derived, using some calculus of finite differences. Equation (14) is the central equation to be solved, the other equations should be considered as boundary conditions. Equation (14) appears to be a homogeneous linear difference equation with constant coefficients in two variables, namely, n_1 and n_2. However, using the C_{N_t} symmetry of the system, group theory justifies the following substitution:

$$v_{n_1 n_2}=e^{(k/2)(n_1+n_2)}v'_{n_2-n_1}, \tag{C1}$$

where k is the same as in Eq. (25).

Substituted into Eq. (14), this leads to

$$\begin{aligned}\varepsilon v'_{n_2-n_1}=&2(J'_1\Delta_1+J'_2\Delta_2)v'_{n_2-n_1}\\ &-J'_1\cos\left[\frac{k}{2}\right](v'_{n_2-n_1-1}+v'_{n_2-n_1+1})\\ &-J'_2\cos\left[\frac{Nk}{2}\right](v'_{n_2-n_1-N}+v'_{n_2-n_1+N})\end{aligned} \tag{C2}$$

resulting into a finite difference equation in one variable (n_2-n_1) of order $2N$. According to the theory of finite differences, it can be solved by determining the $2N$ roots r_i of its characteristic equation:

$$\begin{aligned}&J'_2\cos\left[\frac{Nk}{2}\right]r^{2N}+J'_1\cos\left[\frac{k}{2}\right]r^{N+1}\\ &+(\varepsilon-2J'_1\Delta_1-2J'_2\Delta_2)r^N\\ &+J'_1\cos\left[\frac{k}{2}\right]r^{N-1}+J'_2\cos\left[\frac{Nk}{2}\right]=0 .\end{aligned} \tag{C3}$$

Since r may not be zero, if one substitutes $\exp(a_i)$ for r, this equation is the same as Eq. (27). It can now be shown that the general solution for $v'_{n_2-n_1}$ is

$$v'_{n_2-n_1}=\sum_i c'_i r_i^{n_2-n_1}, \tag{C4}$$

which leads to Eq. (24). We have assumed here that none of the possible roots are multiple, which might, however, occur for some energies [at maximum N different energies, all the other variables being constant in the energy expression (27)]. This means, that for some k values possibly some solutions have been discarded (at maximum N per k value, whereas approximately $N_t/2$ are to be found, *vide infra).*

Finally it is important to note that $J'_2\cos(Nk/2)$ may not be equal to zero, since then it is no longer possible to determine $2N$ different roots and to satisfy the boundary conditions. This does not pose us with any real problems because when J'_2 is zero the normal one-dimensional chain remains and the Bethe ansatz may be used, and $\cos(Nk/2)$ is only equal to zero when $N=3$ and $\lambda=4$, which will therefore not be considered.

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FIG. 1. (a) Shows the conventional torus chosen. Arrow 1 represents the action of the C_N axis, arrow 2 the action of the C_N circle. (b) and (c) show the two "perpendicular" helices, which can be drawn on a torus.