Analytical approach to the Heisenberg antiferromagnet with nearest- and next-nearest-neighbor exchange

Holger Köhler and Klaus W. Becker
Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany
(Received 13 November 1996)

We investigate the ground-state energy of a two-dimensional Heisenberg antiferromagnet with competing nearest- and next-nearest-neighbor exchange interactions J_1 and J_2. On the basis of a recently introduced cumulant technique we describe the transition from the usual antiferromagnetic phase to a so-called layered antiferromagnetic phase as a function of the ratio J_2/J_1. Whereas in the former phase the spins are approximately aligned antiparallel along the up and down sublattice, in the layered phase each of the two sublattices forms an antiferromagnetic lattice by itself. The result for the ground-state energy and for respective order parameters agree well with findings obtained from numerical methods. [S0163-1829(97)00937-5]

I. INTRODUCTION

Since the discovery of high-temperature superconductivity the investigation of ground-state properties of two-dimensional Heisenberg antiferromagnets has again become of central theoretical interest. In this paper, we study the ground-state energy of a two-dimensional Heisenberg antiferromagnet on a quadratic lattice with competing nearest- and next-nearest-Heisenberg interactions

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \, \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \, \mathbf{S}_j \, . \tag{1}$$

The brackets $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ denote summations over nearest and next-nearest-neighbors, respectively. As is easily seen, the model has the following asymptotic behavior: For $J_1 \gg J_2$ the usual antiferromagnetic ground state for nearest-neighbor interactions is found, whereas for $J_1 \ll J_2$ a so-called layered antiferromagnetic ground state is expected. In the latter phase, next-nearest-neighbor spins are approximately aligned antiparallel on two interpenetrating sublattices, as shown in Fig. 1. The transition between the two limits was extensively studied in the literature, mainly by numerical methods.[2–8] For classical spins ($S \to \infty$) the transition takes place exactly at $J_2 = J_1/2$. This was shown by Einarson *et al.*[1] by transforming the Hamiltonian (1) to the nonlinear σ model. The same value for J_2/J_1 was also found for quantum spins $S = 1/2$ if one neglects spin fluctuations, i.e., if one reduces the model to that of pure Ising interactions. Dagotto *et al.*[7] were the first who suggested the appearance of an additional phase in the intermediate range between the two competing antiferromagnetic phases. They believed this phase to be a spin liquid. Especially since Anderson's suggestion of a resonating valence bond (RVB) state for high-temperature superconductors the properties of spin liquids have attracted large interest. Recently, a possible chiral order was also concluded from numerical investigations of different spiral order parameters.[6]

In this paper, we study the ground state of the Hamiltonian (1) in the framework of a new analytical method which is based on the introduction of cumulants.[9,10] This approach automatically guarantees size consistency. Another advantage is that this method is easy applicable also to strongly correlated electrons and spins systems. The diagrammatic methods fail or are not appropriate, because generalized Feynman rules are too complex for practical, i.e., analytical purposes. It was applied before to the Heisenberg antiferromagnet with nearest-neighbor interaction J_1 (Ref. 11) as well as to a number of other systems. The method starts from an unperturbed ground state to which successive fluctuations are added by applying the perturbation. For the Heisenberg antiferromagnet, the Néel state is taken as an unperturbed ground state. By application of the transverse part of H, pairs of spin defects are generated. They give rise to the true ground state for the Heisenberg model. For the $J_1 - J_2$ model (1) we also start from the Néel state being the approximate ground state for $J_1 \gg J_2$. Application of spin fluctuation proportional to J_1 along either rows or columns generates new states, denoted as strings These new states also tend to minimize the next-nearest-neighbor exchange $\sim J_2$ (compare Fig. 2). The transition to the layered antiferromagnet can be described by taking into account longer and longer strings since their weight increases with increasing J_2/J_1.

The paper is organized as follows. In the next section (Sec. II) the cumulant method will be briefly reviewed as well as the above mentioned previous application to the

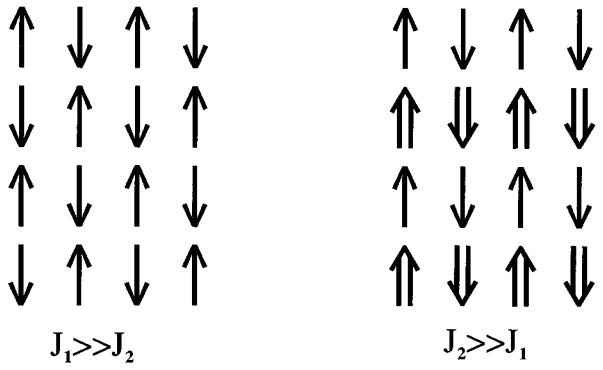

FIG. 1. Néel state for $J_1 \gg J_2$ (left) and layered Néel state for $J_2 \gg J_1$ (right).

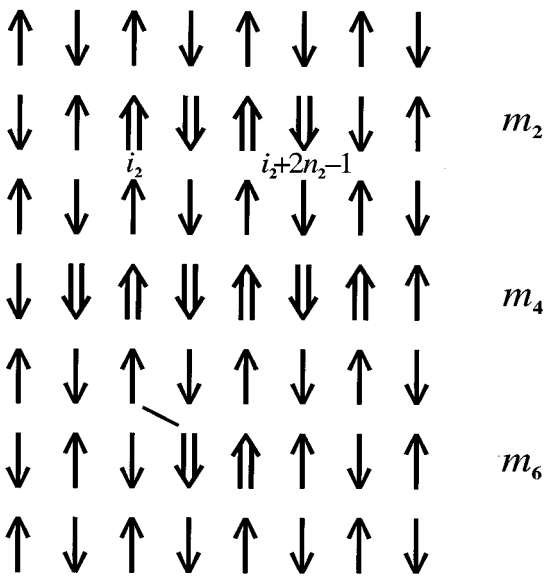

FIG. 2. This figure shows three strings of various lengths which are created by $H_1^{\perp}$ in each second row. The site i_2 is the starting position for a string in row m_2 and n_2 denotes the length of this string [compare Eq. (31)]. The diagonal line shows a pair of next-nearest-neighbor spins which can be flipped by application of $H_2^{\perp}$.

Heisenberg model with nearest-neighbor exchange $\sim J_1$ only. Section III represents the main part of the paper. Here, the cumulant approach is applied to the J_1-J_2 model by introducing generalized string operators. At the end of this section the layered antiferromagnet for $J_2/J_1 \gg 1$ will be discussed. Its ground state can be considered as the new layered Néel state to which spin fluctuations are induced by applying the transverse part of the J_2 exchange. This is in complete analogy to the case of the nearest-neighbor exchange model.

II. CUMULANT APPROACH

In this section, we briefly review the basic ideas of the cumulant approach:[9,10] Note that the spin operators $\vec{S}_i$ in Eq. (1) do not obey simple commutation or anticommutation relations. Therefore the usual diagrammatic techniques which are based on the validity of Wick's theorem are not easily applied. This situation is quite similar to that of strongly correlated electrons where so-called Hubbard operators are introduced which describe the creation or annihilation of electrons. Due to the strong local Coulomb repulsion, the Hubbard operators are only defined in a subspace of the Hilbert space which does not contain doubly occupied sites. Therefore, the Hubbard operators do not obey simple anticommutation relations. This is why, for systems like Eq. (1) it is not possible to apply the well-established Feynman technique and to relate perturbation processes of any order to Feynman diagrams. This is the deeper reason for the difficulties existing in strongly correlated systems or Hamiltonians like Eq. (1). For each of these systems one would have to introduce generalized diagrams as has been done for spins. However, the underlying new correspondence between graphs and analytical expressions are usually far from being simple and cannot easily be applied. In all these cases the cumulant method, as used in this paper, provides an alternative theoretical approach. The advantage of the method is that only cumulant expressions enter in any physical quantities. Cumulants can be considered as a generalization of connected diagram techniques and guarantee that all physical quantities turn out to be size consistent, i.e., that they scale properly with the size of the system. The occurrence of cumulants corresponds to the famous linked-cluster theorem.

The method starts from the definition of a function $f(\lambda)$

$$f(\lambda)=\ln\langle\phi_0|\exp[-\lambda(H_0+H_1)]\exp(\lambda H_0)|\phi_0\rangle \tag{2}$$

from which an expression for the ground state in terms of cumulants can be derived. We start from a separation of the total Hamiltonian H into an unperturbed part H_0 and into a perturbation H_1. In Eq. (2) the state $|\phi_0\rangle$ is the ground state of H_0 with eigenvalue ϵ_0, i.e., $H_0|\phi_0\rangle=\epsilon_0|\phi_0\rangle$. Introducing the Liouville operator L_0, which is defined by $L_0A=[H_0,A]$ for any operator A of the unitary space, Eq. (2) can be transformed into[9,10]

$$f(\lambda)=\ln\langle\phi_0|\exp[-\lambda(H_1+L_0)]|\phi_0\rangle. \tag{3}$$

For the Laplace transform $\tilde{f}(x)$,

$$\tilde{f}(x)=-\int_0^{\infty} f(\lambda)\exp(\lambda x)\,d\lambda, \quad \mathrm{Re}\,\{x\}<0, \tag{4}$$

one can show that the shift of the ground-state energy δE_g with respect to the unperturbed energy ϵ_0 is given by

$$\delta E_g=E_g-\epsilon_0=\lim_{x\to 0}x^2\tilde{f}(x). \tag{5}$$

On the other hand, Eq. (3) suggests the introduction of cumulants.[12] One is led to the following cumulant expression for the ground-state energy:

$$\delta E_g=\lim_{x\to 0}\left\langle\phi_0\left|H_1\left(1+\frac{1}{x-(H_1+L_0)}\,H_1\right)\right|\phi_0\right\rangle^c. \tag{6}$$

Here and in the following, the index c denotes cumulant expectation values formed with the unperturbed ground state of H_0. As is well known, cumulants can be considered as a generalization of connected diagrams known from usual diagram techniques. They can be defined in terms of usual expectation values according to

$$\langle\phi_0|A_1^{n_1}\cdots A_m^{n_m}|\phi_0\rangle^c=\frac{\partial^{n_1}}{\partial\lambda_1^{n_1}}\cdots\frac{\partial^{n_m}}{\partial\lambda_m^{n_m}}\ln\left\langle\phi_0\left|\prod_{i=1}^{m}\exp(\lambda_iA_i)\right|\phi_0\right\rangle\Bigg|_{\lambda_1=\cdots=\lambda_m=0}. \tag{7}$$

In Eq. (6) both quantities H_1 and L_0 are subject to the cumulant ordering procedure according to (7). For the following, it is also convenient to introduce a bilinear form of operators A and B by

$$\langle \phi_0|A^\dagger B|\phi_0\rangle^c=(A|B). \tag{8}$$

Note, the last equation does not define a mathematical scalar product since the bilinear form (8) is not positive definite. The expression for δE_g is rewritten as

$$\delta E_g=(H_1|\Omega), \tag{9}$$

$$|\Omega)=\lim_{x\to 0}\left|1+\frac{1}{x-(H_1+L_0)}H_1\right\rangle, \tag{10}$$

where we have introduced a new quantity Ω, called the wave operator or Moeller operator, which is known from scattering theory. Obviously, the physical meaning of Ω is to transform the unperturbed ground state $|\phi_0\rangle$ into the full ground state $|\Psi_0\rangle$ of H. In the past, Eqs. (9) and (10) have been used to evaluate ground-state properties for a number of different physical systems.[11,13,14] One possibility to further evaluate Eqs. (9) and (10) is based on a projection technique. Recently, a different evaluation scheme was proposed in, Ref. 17 which we shall use in the following. This starts from an exponential ansatz for the wave operator

$$|\Omega)=\left|\exp\left(\sum_\mu \alpha_\mu S_\mu\right)\right\rangle=:|e^S). \tag{11}$$

Here, a set of the so-called relevant operators S_μ have been introduced which has to be chosen in such a way that the S_μ can generate, but not annihilate, fluctuations in the unperturbed ground state. As is easily seen, this guarantees that the power series of the exponential usually stops after a few steps. The unknown parameters α_μ in Eq. (11) have to be evaluated from the following additional set of equations

$$(S_\nu|H\Omega)=0 \quad \text{for all } S_\nu \text{ from the set } \{S_\nu\}. \tag{12}$$

Note the close analogy of Eq. (11) to the usual exponential ansatz for the ground-state wave function within the so-called coupled-cluster method. For a closer review of this method see the review article.[16] Equations (9), (11), and (12) allow the evaluation of the ground-state energy. Due to the introduction of cumulants the result will always be size consistent.

In the next section, we shall use these equations to evaluate the ground-state energy for the J_1-J_2 model. Note that the cumulants can be eliminated again. Assuming

$$\langle \phi_0|(S_\mu)^n|\phi_0\rangle=0 \quad \text{for all integer } n>0, \tag{13}$$

it was shown in Ref. 18 that Eqs. (9), (11), and (12) can be rewritten as

$$E_g=(H|\Omega)=\langle \phi_0|He^S|\phi_0\rangle, \tag{14}$$

$$0=(S_\nu|H\Omega)=\langle \phi_0|S_\nu^\dagger He^S|\phi_0\rangle-\langle \phi_0|S_\nu^\dagger e^S|\phi_0\rangle \times\langle \phi_0|He^S|\phi_0\rangle, \tag{15}$$

or by combining both equations

$$\left\langle \phi_0\left|S_\nu^\dagger H\exp\left(\sum_\mu \alpha_\mu S_\mu\right)\right|\phi_0\right\rangle =E_g\left\langle \phi_0\left|S_\nu^\dagger\exp\left(\sum_\mu \alpha_\mu S_\mu\right)\right|\phi_0\right\rangle. \tag{16}$$

At first sight, the set of equations (16) looks similar to a variational problem with a variational wave function $\exp(\Sigma_\mu\alpha_\mu S_\mu)|\phi_0\rangle$. However, a comparison to an eigenvalue equation is more adequate since Eq. (16) can be used to determine both the parameters α_μ and the ground-state energy E_g. However, note that Eq. (16) is always size consistent, in contrast to equations obtained for instance by a configuration interaction (CI) approach.[15]

As a simple example let us discuss the Heisenberg antiferromagnet with nearest-neighbor exchange in two dimensions. According to the above procedure, we start by dividing the Hamiltonian into the Ising and the transverse part, denoted by H_0 and H_1

$$H_0=J_1\sum_{\langle i,j\rangle} S_i^z S_j^z$$

$$H_1=\frac{J_1}{2}\sum_{\langle i,j\rangle}(S_i^+S_j^-+\text{H.c.}). \tag{17}$$

For the wave operator Ω, we choose

$$|\Omega)=|\exp(\lambda A)) \quad \text{with } A=\sum_{\langle i,j\rangle} S_i^+\ S_j^- \ , \quad i\in\downarrow,\ j\in\uparrow. \tag{18}$$

By applying Ω on the Néel state, i.e., the unperturbed ground state of H_0, pairs of spin fluctuations are generated. Note, in the fluctuation operator A the sites i and j are taken from the down spin and up spin sublattices, respectively. This is important for the power series of Ω to stop after a few terms. Note, this would not be the case if also the adjoint spin-flip operators would be present in A. An improved ansatz for Ω was used in Refs. 17 and 16 which allows the parameter λ_{ij} also to depend on the distance between i and j. In this case not only accurate values for the ground-state energy but also for the sublattice magnetization result.[18,16] Following the outlined procedure, Eqs. (17) and (18) lead to

$$E_g=\epsilon_0+\lambda\ \ (H_1|A), \tag{19}$$

where ϵ_0 is the Néel energy. Note that the power series of Ω has stopped after the first order in A since higher spin fluctuations, induced by higher powers in A, cannot be remedied again by H. The equation for the parameter λ is given by

$$(A|(H_0+H_1)(1+\lambda A+\tfrac{1}{2}\lambda^2A^2))=0. \tag{20}$$

The first-order term in λ creates pairs of spin fluctuations on nearest-neighbor sites in the Néel state which are healed again by application of $A^\dagger$. This term measures the difference in Ising energy between the Néel state with one additional pair of spin fluctuations and the pure Néel state. The contribution from λ^2 describes processes with two pairs of spin fluctuations which are healed by H_1 and $A^\dagger$ on the left. Since in the cumulant formation size consistency is maintained only pairs of spin fluctuations close to each other can contribute. For later reference let us rewrite Eq. (20) explicitly by eliminating the cumulant expressions

$$\frac{1}{2}\lambda^2(\langle\phi_0|A^\dagger H_1 AA|\phi_0\rangle - 2\langle\phi_0|A^\dagger A|\phi_0\rangle\langle\phi_0|H_1 A|\phi_0\rangle) + \lambda(\langle\phi_0|A^\dagger H_0 A|\phi_0\rangle$$
$$-\langle\phi_0|H_0|\phi_0\rangle\langle\phi_0|A^\dagger A|\phi_0\rangle) + \langle\phi_0|A^\dagger H_1|\phi_0\rangle = 0. \quad (21)$$

From Eq. (21) it is easy to evaluate the parameter λ. One finds $\lambda = -0.1771$. This is close to $-1/6$, a value one would obtain by neglecting the term $\sim\lambda^2$ altogether. For the ground-state energy E_g already a very good value results from this simple approach.[11,18] As was mentioned before for the staggered magnetization, one would have to extend the ansatz for Ω by allowing the parameter λ to depend on the distance $R_i - R_j$,

$$|\Omega) = \left|\exp\left(\sum_{i,j} \lambda_{ij} S_i^+ S_j^-\right)\right). \quad (22)$$

S_i^+ and S_j^- are now spin fluctuations on sites i and j on the down and up sublattices, respectively, which can be located arbitrarily away from each other.[16,18]

III. INTRODUCTION OF GENERALIZED STRING STATES

We are now in the position to evaluate the ground-state energy of the $J_1 - J_2$ model. As unperturbed Hamiltonian H_0 we choose the Ising part of Eq. (1), i.e.,

$$H_0 = J_1 \sum_{\langle i,j\rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j\rangle\rangle} S_i^z S_j^z =: H^{||}. \quad (23)$$

In two dimensions, this Hamiltonian was discussed by Baxter.[19] For small $J_2 \ll J_1$, the ground state is approximately the usual Néel state. For increasing J_2 a layered antiferromagnetic Néel state will develop (compare Fig. 2). Contrary to the usual Néel state which is twofold degenerate, the layered ground state is fourfold degenerate. Parallel strings either in the horizontal or in the vertical direction are possible. Therefore, with the time reversed states altogether four layered states result. Note, in the limit $J_2 \to \infty$ also noncollinear antiferromagnetic states are possible. They are again formed by two antiferromagnetic sublattices on next-nearest-neighbor sites. The two sublattices, however, may have an arbitrary angle with each other. In what follows, J_1/J_2 will always be finite so that noncollinear states do not occur.

Our aim is to describe the ground state of Eq. (1) in both limits $J_1 \gg J_2$ and $J_2 \ll J_1$ by a proper choice of the wave operator Ω. Our starting point is the usual Néel state. The intermediate regime $J_1 \approx J_2$ is described by an extrapolation between the two antiferromagnetic states. The layered Néel state will be built up by local string operators applied on the usual Néel state. These new states contain strings of flipped spins in every second row (or column), as shown in Fig. 2. The physical picture is as follows: For increasing J_2, longer strings become more and more important since they are leading to a gain in energy. The layered antiferromagnet Néel state is formed when all strings in parallel rows (or columns) have infinite length. Additional spin fluctuations around the layered Néel state lead to a further gain in energy, similar to spin fluctuations for the case of the usual antiferromagnet.

Let us now introduce generalized string operators in order to construct the wave operator. For simplicity, let us disregard at first the transverse part of the exchange J_2, i.e., we replace H_1 by

$$H_1 \Rightarrow \frac{J_1}{2} \sum_{\langle i,j\rangle} (S_i^+ S_j^- + \text{H.c.}) =: H_1^\perp. \quad (24)$$

Moreover, we only consider strings along one row in order to clarify the construction scheme of string operators. A string A_n of length $2n$ is defined by

$$\tilde{A}_n = \frac{1}{\sqrt{L/2}} \sum_{i\in\downarrow} (S_i^+ S_{i+1}^- S_{i+2}^+ S_{i+3}^- \cdots S_{i+2n-2}^+ S_{i+2n-1}^-),$$
$$n = 1,2,\ldots,\frac{L}{2}, \quad (25)$$

where the summation over i runs over all sites of the down sublattice within one row only. Application of $\tilde{A}_n$ to the original Néel state shows that strings of $2n$ spin defects (or n pairs of overturned neighboring spin pairs) are generated in one row starting from site i. The summation over i in Eq. (25) means that strings may start from any site of the down sublattice in the considered row. Obviously, by applying operators $\tilde{A}_n$ on every second row a layered antiferromagnetic state can be constructed. This is exactly the scheme we are going to follow. For the present (one-dimensional) case the wave operator, for the moment denoted by Ω_1, is given by

$$|\Omega_1) = \left|\exp\left(\sum_{n=1}^{L/2} \alpha_n \tilde{A}_n\right)\right). \quad (26)$$

Using Eqs. (14) and (15) the equations for the ground-state energy and the coefficients α_n read

$$E_g = (H^{||} + H_1^\perp|\Omega_1), \quad (27)$$

$$0 = (\tilde{A}_n|(H^{||} + H_1^\perp)\Omega_1). \quad (28)$$

As discussed before, due to the introduction of cumulants only connected diagrams contribute to physical quantities. This property can be used to simplify Eqs. (27) and (28). Expanding the exponential of Ω_1 also, states will be generated which consist of more than one string starting at different positions within the considered row. However, in Eq. (27) only string operators $\tilde{A}_1$ of length one with one pair of flipped spins can contribute. The reason is that $H^\perp$ in the ''bra'' of Eq. (27) can at most annihilate one pair of spin defects. However, due to the appearance of the string $\tilde{A}_n^\dagger$ in

the bra also longer strings (of length $2n-2$ and $2n+2$) may contribute to Eq. (28). Moreover, states from the expansion of Ω_1 with two strings of total length $2n-2$ could contribute, in case that they can be connected by the explicit $H_1^\perp$ in Eq. (28). For simplicity, we shall neglect this possibility. Having this simplification in mind, the exponential form (26) is equivalent to a linear ansatz

$$\left|\exp\left(\sum_n \alpha_n \widetilde{A}_n\right)\right) = \left|1+\sum_{n=1} \gamma_n \widetilde{A}_n\right), \tag{29}$$

where new coefficients γ_n have been introduced. Like the α_n also the new coefficients γ_n are determined by the set of equations (28). This leads to a system of linear equations for the γ_n.

Next, let us generalize the concept of string operators to the full two-dimensional case, i.e., to all rows (or columns). In the following we discuss the case of string operators along rows. As noted before, strings can be generated in every second row. The $L/2$ rows are denoted by $m_2, m_4, \ldots, m_L$. Again L is the linear length of the lattice. Moreover, we introduce an index vector $\underline{n}$ with $L/2$ components $n_2, n_4, \ldots, n_L$. The components n_i indicate the string length within the rows m_i and are integer numbers. The complete string operator is defined by $\widetilde{A}_{\underline{n}}$

$$\begin{aligned}\widetilde{A}_{\underline{n}} = \frac{1}{\sqrt{\left(\frac{2}{L}\right)^{L/2}}} \sum_{i_2 i_4 \cdots i_L} & S^+_{i_2}(m_2) S^-_{i_2+1}(m_2) \cdots S^+_{i_2+2n_2-2}(m_2) S^-_{i_2+2n_2-1}(m_2) \\ & \times S^+_{i_4}(m_4) S^-_{i_4+1}(m_4) \cdots S^+_{i_4+2n_4-2}(m_4) S^-_{i_4+2n_4-1}(m_4) \\ & \times S^+_{i_L}(m_L) S^-_{i_L+1}(m_L) \cdots S^+_{i_L+2n_L-2}(m_L) S^-_{i_L+2n_L-1}(m_L)\end{aligned} \tag{30}$$

The summation indices i_2, i_4 to i_L denote the starting points of the strings in the corresponding row thus generalizing the notation of Eq. (25) (Fig. 2). The lengths of the strings are given by the n_i's. Obviously, the string operator A_n, as defined by Eq. (30), generates strings in $L/2$ rows, where also strings of length zero are allowed. Therefore, situations as, for instance, shown in Fig. 2 are described. Note that the starting site of any string within a row is not important. Due to the summation over all lattice sites a string of a given length may start from any lattice sites.

The new exponential ansatz for the wave operator corresponds to that of Eq. (26):

$$|\Omega_1) = \left|\exp\left(\sum_{\underline{n}} \alpha_{\underline{n}} \widetilde{A}_{\underline{n}}\right)\right). \tag{31}$$

As in Eq. (29) we assume the strings to form a complete basis, so that Ω_1 is equivalent to

$$|\Omega_1) = \left|1+\sum_{\underline{n}} \gamma_{\underline{n}} \widetilde{A}_{\underline{n}}\right). \tag{32}$$

The new coefficients $\gamma_{\underline{n}}$ depend on the index vector $\underline{n}$. As before they can be determined from a linear set of equations (28). Equation (33) together with Eqs. (27) and (28) modified for the present case give a complete evaluation scheme for the ground-state energy. Up to now we have neglected the transverse part $H_2^\perp$ of the next-nearest-neighbor exchange

$$H_2^\perp = \frac{J_2}{2} \sum_{\langle\langle i,j\rangle\rangle} (S_i^+ S_j^- + \text{H.c.}). \tag{33}$$

Now we are able also to consider the full Hamiltonian (1)

$$H = H_0 + H_1,$$

where

$$H_1 = H_1^\perp + H_2^\perp, \tag{34}$$

where H_0 is again given by Eq. (23). In analogy to the treatment of the nearest-neighbor exchange from Sec. II, the wave operator will be generalized to include also spin fluctuations due to $H_2^\perp$

$$|\Omega) = \left|\exp\left(\mu A_\mu + \sum_{\underline{n}'} \alpha_{\underline{n}'} \widetilde{A}_{\underline{n}'}\right)\right) \tag{35}$$

$$A_\mu = {\sum_{\langle\langle i,j\rangle\rangle}}' S_i^+ S_j^-. \tag{36}$$

Note, the summation over i,j in the fluctuation operator A_μ only runs over next-nearest-neighbor sites, where the prime Σ' indicates that A_μ can only generate pairs of spin fluctuations on next-nearest-neighbor sites in the layered Néel order. Obviously, A_μ like $H_2^\perp$ applied on the original Néel state gives zero. Therefore, before A_μ can be applied, the new layered Néel state has to be generated. Note that the spin fluctuation operator A_μ and the string operators $\widetilde{A}_{\underline{n}}$ do not commute with each other so that the wave operator does not factorize into a product of a spin fluctuation and a string part. However, to simplify the further calculations we shall henceforth use such a product form,

$$|\Omega) = \left| e^{-\mu A_\mu} \left(1+\sum_{\underline{n}'} \gamma_{\underline{n}'} \widetilde{A}_{\underline{n}'}\right) \right). \tag{37}$$

Here, already the approximation from Eq. (31) to Eq. (32) has been used. A more formal justification for Eq. (37) is given in Appendix A. There, by a slight generalization of the

string operators $\tilde{A}_{\underline{n}}$, it can be shown that the form (35) can indeed be reduced to Eq. (37).

Next, the cumulant equations for evaluating the ground-state energy can be given. In analogy to the introductory example from the preceding section they read

$$E_g=(H|\Omega), \tag{38}$$

$$0=(\tilde{A}_{\underline{n}}|H\Omega), \tag{39}$$

$$0=(A_\mu\tilde{A}_{\underline{n}}|H\Omega). \tag{40}$$

The first equation gives the ground-state energy as before, whereas the unknown parameter α_n and μ are determined by the second and third equations. As mentioned above in Eq. (40), first a local layered Néel state has to be formed. In the ''bra'' vector $\tilde{A}_{\underline{n}}$ acts on the original Néel state. Only then the spin fluctuation operator A_μ can be applied. Replacing the cumulant averages by the usual expectation values in analogy to Sec. II one finds

$$\langle\phi_0|\tilde{A}^\dagger_{\underline{n}}H\Omega|\phi_0\rangle-\langle\phi_0|\tilde{A}^\dagger_{\underline{n}}\Omega|\phi_0\rangle E_g=0, \tag{41}$$

$$\langle\phi_0|\tilde{A}^\dagger_{\underline{n}}A^\dagger_\mu H\Omega|\phi_0\rangle-\langle\phi_0|\tilde{A}^\dagger_{\underline{n}}A^\dagger_\mu\Omega|\phi_0\rangle E_g=0, \tag{42}$$

with Ω given by Eq. (37). The ground-state energy is again

$$E_g=\langle\phi_0|H\Omega|\phi_0\rangle. \tag{43}$$

The only condition used to derive Eqs. (41) and (42) is $\langle\phi_0|S^\nu|\phi_0\rangle=0$ for all powers $\nu>0$ and $A_\mu|\phi_0\rangle=0$. Let us discuss in some detail the first equation, (41). Expanding Ω in terms of string operators one finds

$$\left\langle\phi_0\left|\tilde{A}^\dagger_{\underline{n}}(H^{\|}+H_1^\perp+H_2^\perp)\exp(\mu A_\mu)\left(1+\sum_{\underline{n}'}\gamma_{\underline{n}'}\tilde{A}_{\underline{n}'}\right)\right|\phi_0\right\rangle-\left\langle\phi_0\left|\tilde{A}^\dagger_{\underline{n}}\exp(\mu A_\mu)\left(1+\sum_{\underline{n}'}\gamma_{\underline{n}'}\tilde{A}_{\underline{n}'}\right)\right|\phi_0\right\rangle E_g=0. \tag{44}$$

Here, the part $H^{\|}$ from the Hamiltonian $H=H^{\|}+H_1^\perp+H_2^\perp$ measures the Ising contributions of the strings. The part $H_1^\perp$ either enlarges or cuts the strings by one pair of flipped spins. The contribution from $H_2^\perp$ are virtual spin flips, as shown in Fig. 2. Finally, the prefactor of the energy term represents the expectation value of strings with the Néel state. Equation (44) can formally also be written as

$$\sum_{\underline{n}'}\gamma_{\underline{n}'}\left([E^{\|}(\underline{n})+\mu E_2^\perp(\underline{n})-E_g]\prod_{i=1,3,\ldots}^{L}\delta_{n_i\,n_i'}+E_1^\perp(\underline{n}')\sum_{i=1,3,\ldots}^{L}(\delta_{n_i\,n_i'+1}+\delta_{n_i\,n_i'-1})\prod_{j=1,3,\ldots(\neq i)}^{L}\delta_{n_j\,n_j'}\right)=0 \tag{45}$$

with obvious definitions for $E^{\|},E_2^\perp$, and $E_1^\perp$. As discussed before, there are altogether $L/2$ rows, where strings can be created. The different terms still depend on the length of the strings as indicated by the index vectors n and n'. Obviously, there are no fluctuations which connect different rows. Therefore, we can restrict the calculations to contributions from one row only. Defining ϵ_g as the ground-state energy contribution from one row, i.e., $E_g=(L/2)\ \epsilon_g$, Eq. (45) leads to

$$\begin{pmatrix}\epsilon(0)-\epsilon_g & J_1/2 & 0 & 0 & \cdots\\ J_1/2 & \epsilon(1)-\epsilon_g & J_1/2 & 0 & \cdots\\ 0 & J_1/2 & \epsilon(2)-\epsilon_g & J_1/2 & \cdots\\ \cdot & \cdot & \cdot & \cdot & \cdots\\ \cdot & \cdot & \cdot & \cdot & \cdots\\ \cdot & \cdot & \cdot & \cdot & \cdots\end{pmatrix}\begin{pmatrix}\tilde{\gamma}_0\\ \tilde{\gamma}_1\\ \tilde{\gamma}_2\\ \cdot\\ \cdot\\ \cdot\end{pmatrix}=\begin{pmatrix}0\\ 0\\ 0\\ \cdot\\ \cdot\\ \cdot\end{pmatrix}. \tag{46}$$

Here we have used the following definitions:

$$\epsilon(n)=\epsilon^{\|}(n)+\mu\epsilon_2^\perp(n),$$

where

$$\epsilon_2^\perp(n)=4J_2n \tag{47}$$

and

$$\epsilon^{\|}(n)=\begin{cases}-(J_1-J_2)\ L, & n=0,\\ -(J_1-J_2)\ L+\dfrac{1}{2}J_1+2\ (J_1-2J_2)n, & 0<n<\dfrac{L}{2},\\ -J_2L, \quad n=\dfrac{L}{2}.\end{cases} \tag{48}$$

The new coefficients $\tilde{\gamma}_n$, introduced in Eq. (46), are related to the former coefficients γ_n by

$$\gamma_n = \frac{\tilde{\gamma}_n}{\tilde{\gamma}_0}, \quad n = 1,2,3,\ldots L/2 \quad \text{with} \sum_{n=0}^{L/2} \tilde{\gamma}_n^2 = 1. \tag{49}$$

Note that the set of equations (46) defines an eigenvalue problem from which $L/2$ eigenvalues ϵ_λ and eigenvectors $\tilde{\gamma}_n^\lambda$ can be determined. The number of possible eigenvalues and eigenvectors are given by the number of independent string states within one row. Being L the length of a string there is altogether $L/2$ independent string states. Therefore the dimension of the eigenvalue problem is $L/2$ as well. Its lowest energy gives the ground-state energy ϵ_g we are looking for. The ground-state wave function is found from the corresponding eigenvector $\tilde{\gamma}_n^g$. In the next section the solution of Eq. (46) will be discussed in more detail.

Next, let us proceed with the discussion of Eq. (42) which is much simpler to evaluate than Eq. (41). From this equation the spin fluctuation parameter μ can be found. Inserting expression (37) for Ω one is led to

$$\langle \phi_0 | \tilde{A}_n^\dagger A_\mu^\dagger H_2^\perp \tilde{A}_n | \phi_0 \rangle + \mu \langle \phi_0 | \tilde{A}_n^\dagger A_\mu^\dagger H^{||} A_\mu \tilde{A}_n | \phi_0 \rangle + \frac{\mu^2}{2} \langle \phi_0 | \tilde{A}_n^\dagger A_\mu^\dagger H_2^\perp A_\mu^2 \tilde{A}_n | \phi_0 \rangle - E_g \mu \langle \phi_0 | \tilde{A}_n^\dagger A_\mu^\dagger A_\mu \tilde{A}_n | \phi_0 \rangle = 0. \tag{50}$$

Note, none of the spin fluctuations changes the length of the strings. We extract the value for μ from the case of maximum string length L, i.e., $n = L/2$ frustrated bonds, when the string extends over the whole lattice. In Eq. (50) we have already eliminated all cumulants in favor of usual expectation values formed with the original Néel state. Therefore, formally also nonconnected contributions enter Eq. (50). One finds

$$\mu^2 (8L^4 J_2 + 4L^2 J_2) + \mu(-4L^4 J_2 + 12 J_2 L^2 - 8L^2 E_g) + 2L^2 J_2 = 0. \tag{51}$$

The contributions to the first bracket are caused by application of twice the fluctuation operator A_μ. The contributions proportional to L^4 are due to nonconnected spin fluctuations whereas terms in L^2 are caused by neighboring fluctuations, i.e., by connected contributions. Similarly, in the next bracket there is one term from the Ising energy arising from the whole lattice, which is also proportional to L^4. The second one can be interpreted as the difference in Ising energy between the layered Néel state and the same state in which one pair of spins is flipped. Finally, the last term in Eq. (51) represents one pair of spin fluctuations in the layered Néel state. Note that all terms of order L^4 exactly cancel, if the large J_2 result for the ground-state energy (Appendix B) is used

$$E_g = -\frac{J_2 L^2}{2} + \mu J_2 L^2. \tag{52}$$

The remaining terms form an equation for μ which exactly coincides with the equation for the spin fluctuation parameter we already know from the discussion of the usual antiferromagnet from Sec. II. This is the justification that for $J_2/J_1 \gg 1$ the layered Néel state is reached. To make this more explicit we may also insert expression (43) for E_g into the original equation (42) for μ. Taking into account only contributions from the maximal string length L we find

$$\langle \tilde{A}_{L/2}\phi_0 | A_\mu^\dagger H_2^\perp | \tilde{A}_{L/2}\phi_0 \rangle + \mu \langle \tilde{A}_{L/2}\phi_0 | A_\mu^\dagger H^{||} A_\mu | \tilde{A}_{L/2}\phi_0 \rangle + \frac{\mu^2}{2} \langle \tilde{A}_{L/2}\phi_0 | A_\mu^\dagger H_2^\perp A_\mu^2 | \tilde{A}_{L/2}\phi_0 \rangle - \mu (\langle \tilde{A}_{L/2}\phi_0 | H^{||} | \tilde{A}_{L/2}\phi_0 \rangle$$
$$+ \mu \langle \tilde{A}_{L/2}\phi_0 | H^\perp A | \tilde{A}_{L/2}\phi_0 \rangle) \langle \tilde{A}_{L/2}\phi_0 | A_\mu^\dagger A_\mu | \tilde{A}_{L/2}\phi_0 \rangle = 0. \tag{53}$$

The action of $\tilde{A}_{L/2}$ applied on the original Néel state generates the layered Néel state $|\phi_0\rangle$. Note that Eq. (53) is completely equivalent to Eq. (21) for the nearest-neighbor Heisenberg antiferromagnet from Sec. II. One also finds that μ varies between $\mu = 0$ (for $J_2 = 0$) and approximately 1/6 (for $J_2/J_1 \gg 1$). In the next section we shall discuss the solutions for the ground-state energy of the full Hamiltonian, as given by Eqs. (46) and (50).

IV. RESULTS

For a better understanding of the results let us start with the pure Ising system and neglect at first all contributions from $H_1^\perp$ and $H_2^\perp$. For the Ising system $H^{||} = \Sigma_{\langle i,j \rangle} S_i^z S_j^z + \Sigma_{\langle\langle i,j \rangle\rangle} S_i^z S_j^z$, the energies are not degenerate except for $J_2 = J_1/2$. As is usually done in literature, we vary J_2 only between 0 and J_1. For $J_2 \ll J_1$ the lowest state is always the usual Néel state, whereas in the opposite limit the layered Néel state has the lowest energy. The eigenvectors of Eq. (46) coincide in this case with the string states $A_n^\dagger |\phi_0\rangle$ The eigenvalues are given by the Ising energies $(J_1 - 2J_2)n$. Thus the energy spectrum as function of J_2 is symmetric with respect to $J_2 = J_1/2$. Going through this point, the ground state and the state with highest energy change their role. The ground-state energy has its maximum value here and therefore also frustration has its maximum value.

Next, let us include spin fluctuations from the nearest-neighbor exchange $H_1^\perp$. The exchange $H_2^\perp$ is still kept zero, so that the parameter μ remains $\mu = 0$. Also in this case the energy spectrum as function of J_2 is symmetric with respect to $J_2 = J_1/2$. This property can be understood from the form of Eq. (46) if μ is set to 0. From this symmetry follows that

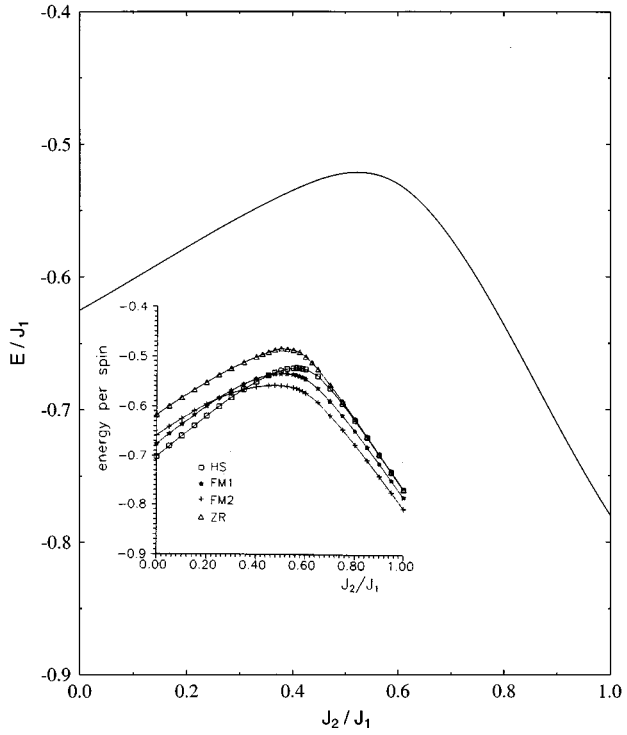

FIG. 3. Ground-state energy per spin in units of J_1 vs J_2/J_1. The small figure contains the numerical results of Richter (Ref. 6). For details compare this reference.

within the present approximation the model with $J_2=0$, i.e., with nearest neighbor exchange only, has the same ground-state energy as the J_1–J_2 model at $J_1=J_2$. For the two corresponding ground states the Ising contribution to the energy is the same. In addition the same contributions from spin fluctuations are added. As is easily seen, for the model with $J_2=0$ spin fluctuations $\sim H_1$ enlarge the length of the strings, whereas for $J_2=J_1$ spin fluctuations always shorten the string length.

Finally, we also include spin fluctuations from the next-nearest-neighbor exchange $H_2^{\perp}$. The respective spin fluctuation parameter μ changes from 0 (for $J_2=0$) to $\approx 1/6$ (for $J_2=J_1$). The ground-state energy as function of J_2 is shown in Fig. 3. For comparison the figure also contains the numerical results obtained from exact diagonalization of small clusters.[6] Note that the ground-state energy is no longer symmetric with respect to $J_2=J_1/2$. Instead it has its maximum value close to $J_2\approx 0.54J_1$ in almost perfect agreement with the numerical result. At this point again frustration has its maximum value.

It may also be worthwhile to discuss the other solution of the eigenvalue problem (46). We assume that its eigenvectors can also be considered as approximate excited states of the J_1–J_2 model. This is concluded from Eq. (44) which tells us that the linear combinations of strings $\exp(\mu A_\mu)(1+\Sigma_n \gamma_n \tilde{A}_n)$ applied on the Néel state $|\phi_0\rangle$ are eigenstates of H in the subspace formed by the strings. Table I shows the energy differences between the first excited state and the ground state. Note that approaching to the maximum value of the ground-state energy at $J_2\approx J_1/2$ the first excitation approaches the ground state. This behavior was already

TABLE I. Ground-state energy (E_g) and first excited-state energy (E_1) per spin as function of J_2 of the present work. For comparison the respective values (E_g^D) and (E_1^D) of Dagotto *et al.* (Ref. 7) are also shown.

J_2	E_g	E_1	E_g^D	E_1^D
0.475	−0.523845	−0.4984	−0.532989	−0.5080
0.55	−0.522227	−0.5135	−0.523595	−0.5127
0.575	−0.525096	−0.5190	−0.523592	−0.5154
0.6	−0.530000	−0.5277	−0.525896	−0.5190
0.6625	−0.552126	−0.5428	−0.544653	−0.5402
0.7	−0.571055	−0.5610	−0.563858	−0.5585
0.75	−0.601411	−0.5889	−0.594282	−0.5846
0.8	−0.635938	−0.6125	−0.627335	−0.6117
0.875	−0.691635	−0.6715	−0.679219	−0.6536

observed by Dagotto[7] and was taken as evidence for the possible existence of a new phase in the region between the Néel phase and the layered Néel phase. It is also interesting to consider the weight of the strings with different length which contribute to the ground-state wave function. Starting again from $J_2=0$ and increasing the value of J_2, longer and longer strings contribute. In the transition region, i.e., at $J_2\approx 0.54J_1$, strings of all lengths are equally important and contribute to the ground-state wave function. This may be an indication for the tendency of the ground state to show disorder. Finally, for still larger J_2 the longest string has also the largest weight. As discussed before it extends over the whole lattice and forms the layered Néel state (see Fig. 4). In Fig. 5 the staggered magnetizations M_N and M_L are shown. These quantities are the respective order parameters for the

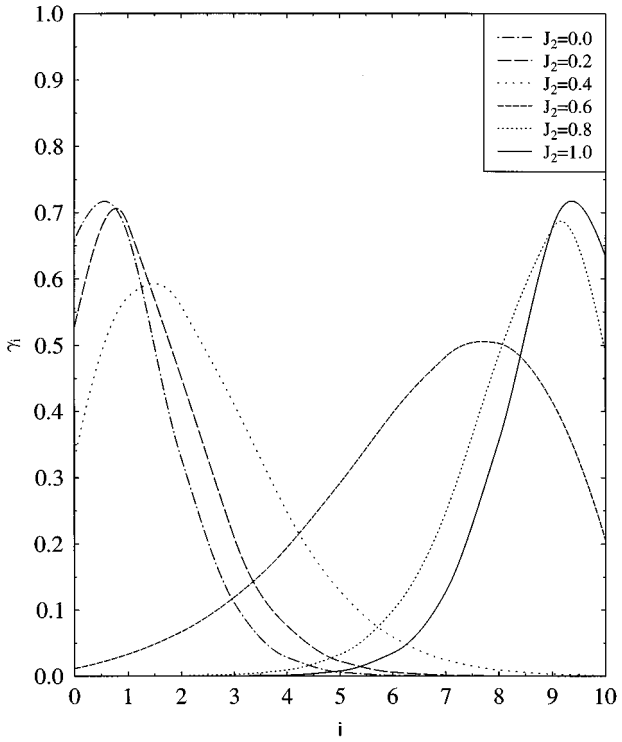

FIG. 4. Eigenvectors γ_i of Eq. (50) for various numbers of exchange constants J_2/J_1 $(J_1=1)$.

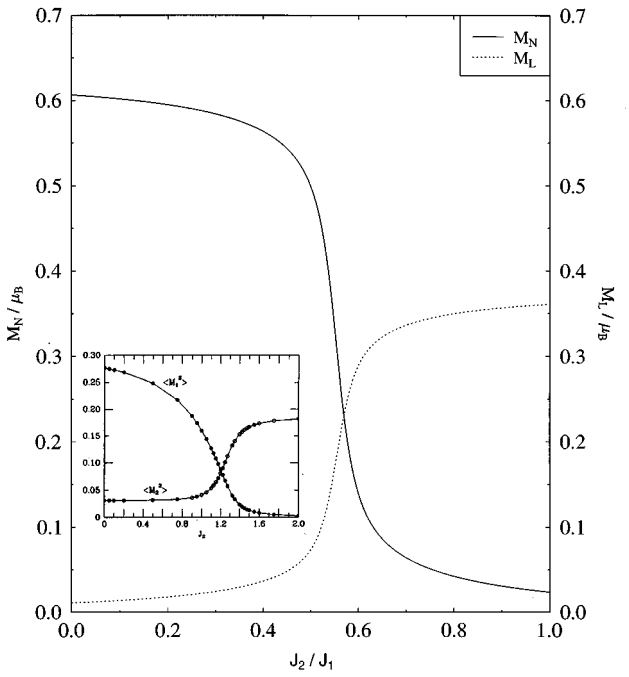

FIG. 5. Staggered magnetizations M_N (Néel state) and M_L (layered Néel state) in units of Bohr magnetons. The small figure shows the results of Dagotto *et al.* (Ref. 7) for the expectation values of the square of the respective staggered magnetizations as function of $J_2/2J_1$. Note that M_1 of Dagotto *et al.* (Ref. 7) corresponds to M_N and M_2 to M_L.

nearest-neighbor and next-nearest-neighbor antiferromagnet. The results are found from a ground-state calculation by adding to the Hamiltonian the respective staggered magnetic fields for the two antiferromagnetic phases. Again, note the remarkable agreement of our analytical results with those from numerical evaluation. As before for the energy, the asymmetry for the two order parameters as function of J_2/J_1 is caused by the spin fluctuations $\sim\mu$ induced by $H_2^{\perp}$. Especially, the maximum value of $\tilde{M}_L$ at $J_2\approx J_1$ is strongly reduced by both $H_1^{\perp}$ and $H_2^{\perp}$ as compared to the value of M_N at $J_2\approx 0$. The value for M_N at $J_2=0$ is close to results obtained from spin-wave theory and also from numerical methods.[7] Note, however, that our approach is completely different from linear spin-wave theory.

ACKNOWLEDGMENT

The authors are grateful to J. Richter (Magdeburg) for a number of stimulating discussions.

APPENDIX A: DEFINITIONS OF GENERALIZED STRING OPERATORS

As was mentioned below, Eq. (33) the definition (26) of string operators can be generalized so that the transformation to the linearized form (33) of the wave operator becomes exact. To show this, we again consider strings which are embedded in an antiferromagnetic surrounding (Fig. 5). For simplicity, we consider the one-dimensional case with strings defined in one row. Note that next to both sides of a given string there is always a pair of parallel spins directed either in up or in down direction. This property is used to define a projector $\mathcal{Q}$

$$\mathcal{Q}=1-\mathcal{P} \quad \text{with} \quad \mathcal{P}=\prod_i \frac{1}{2}(1-\sigma_{i-1}^z\sigma_i^z), \tag{A1}$$

by which one can decide whether a string is present in a given state or not. Here σ_i^z is the Pauli spin operator and the index i runs over all sites of the considered row. If there is a pair of two neighboring spins the corresponding factor in the projector $\mathcal{P}$ gives zero. Thus it follows that $\mathcal{P}$ applied on any string state gives 0 whereas $\mathcal{Q}$ gives 1. Vice versa, if $\mathcal{P}$ and $\mathcal{Q}$ is applied on the original Néel state one obtains 1 and 0. To be able also to enlarge a given string it should be possible to identify the beginning or end of a string. We therefore introduce a local projector $\mathcal{E}_i$

$$\mathcal{E}_i=\frac{1}{4}(\hat{1}-\sigma_{i-1}^z)(\hat{1}-\sigma_i^z). \tag{A2}$$

$\mathcal{E}_i$ gives 1 if it is applied on that side of the string which is formed by two neighboring down spins, located at positions $i-1$ and i. With this definition we define a generalized string creation operator by

$$\tilde{A}_n=\frac{1}{\sqrt{L/2}}\sum_i (S_i^+S_{i+1}^-\cdots S_{i+2n-2}^+S_{i+2n-1}^-)(\mathcal{P}+\mathcal{E}_i\mathcal{Q}). \tag{A3}$$

Note that Eq. (A3) can only generate connected strings. The first term creates a string of length $2n$ in the Néel state whereas the second term enlarges an already present string by adding $2n$ overturned spins. Obviously the definition (A3) leads to the desired linearization (37) of the wave operator Ω.

APPENDIX B: RIGOROUS BOUNDS OF EIGENVALUES

From the tridiagonal form of the eigenvalue problem (46) it follows that three adjacent coefficients $\tilde{\gamma}_{n-1},\tilde{\gamma}_n,\tilde{\gamma}_{n+1}$ are always connected with each other:

$$\frac{J_1}{2}\tilde{\gamma}_{n-1}+a_{n+1,n+1}\tilde{\gamma}_n+\frac{J_1}{2}\tilde{\gamma}_{n+1}=0, \quad n=1,2,3,\ldots. \tag{B1}$$

Here we have abbreviated the diagonal elements of Eq. (46) by a_{nn}, i.e., $a_{nn}=\epsilon_n-\epsilon$. Relation (B1) is also valid for $n=0$ if $\tilde{\gamma}_{-1}$ is set identical to zero. Starting with $n=0$ and inserting successively the preceding equation in the next equation one can always eliminate the lowest coefficient. In this way one is led to the following sequence of equations:

$$P_1\tilde{\gamma}_0+\frac{J_1}{2}P_0\tilde{\gamma}_1=0,$$

$$P_2\tilde{\gamma}_1+\frac{J_1}{2}P_1\tilde{\gamma}_2=0,\ldots \tag{B2}$$

or in general

$$P_n\tilde{\gamma}_{n-1}+\frac{J_1}{2}P_{n-1}\tilde{\gamma}_n=0. \tag{B3}$$

The quantities P_n obey the following recursion relation:

$$P_n=a_{nn}P_{n-1}-\left(\frac{J_1}{2}\right)^2 P_{n-2}, \quad n=1,2,3,\ldots, \tag{B4}$$

where we have defined $P_0=1$ and $P_{-1}=0$. The first three equations of Eq. (B4) read explicitly

$$P_1=a_{11},$$

$$P_2=a_{22}a_{11}-\left(\frac{J_1}{2}\right)^2, \tag{B5}$$

$$P_3=a_{33}\left(a_{22}a_{11}-\frac{J_1}{2}\right)-\left(\frac{J_1}{2}\right)^2 a_{11},\ldots.$$

Remember, the coefficients a_{nn} are functions of energy ϵ. Therefore, the P_n's are polynomials of order n in the energy. Note that $P_{L/2}$ is the highest polynome possible. Its zeros correspond exactly to the $L/2$ eigenvalues ϵ_λ of the $L/2$-dimensional eigenvalue problem (46). The sequence of polynomes (B5) is called a ''Sturm chain.'' In the literature, there are given some exact theorems[20] for Sturm chains from which one can conclude exact properties for the eigenvalues: All eigenvalues of Eq. (46) are nondegenerate. Moreover, they are located in intervals, given by

$$|\epsilon_\lambda-\epsilon(n)|\leqslant J_1 \tag{B6}$$

with $\epsilon(n)=\epsilon^{||}(n)+\mu\epsilon_2^{\perp}(n)$ given by Eqs. (46) and (47). Note that for lattice size $L^2\to\infty$ the relative differences between two excited states goes to zero whereas the absolute difference does not. For the lowest eigenvalue $E_g=(L/2)\epsilon_g$ one finds from Eq. (B6)

$$J_1\geqslant\left|E_g+\frac{J_2L^2}{2}-\mu J_2L^2\right|. \tag{B7}$$

Since J_1 on the LHS can be neglected for large L this inequality turns into the former Eq. (52).

[1] T. Einarsson and H. Johannesson, Phys. Rev. B **43**, 5867 (1991).
[2] M. P. Gelfand, R. R. P. Singh, and D. A. Huse, Phys. Rev. B **40**, 10 801 (1989).
[3] N. Read and S. Sachdev, Phys. Rev. Lett. **62**, 1694 (1989).
[4] P. Chandra, P. Coleman, and A. J. Larkin, J. Phys.: Condens. Matter **2**, 7933 (1990).
[5] R. P. Rajiv Singh and R. Naranyana, Phys. Rev. Lett. **65**, 1072 (1990).
[6] J. Richter, Phys. Rev. B **47**, 5794 (1993).
[7] E. Dagotto and A. Moreo, Phys. Rev. B **39**, 4744 (1989).
[8] C. Bruder and F. Mila, Europhys. Lett. **17**, 463 (1992).
[9] K. W. Becker and P. Fulde, Z. Phys. B **72**, 423 (1988).
[10] K. W. Becker and W. Brenig, Z. Phys. B **79**, 195 (1990).
[11] K. W. Becker, H. Won, and P. Fulde, Z. Phys. B **75**, 335 (1988).
[12] R. Kubo, J. Phys. Soc. Jpn. **17**, 1100 (1962).
[13] K. W. Becker and U. Muschelknautz, Phys. Rev. B **48**, 13 826 (1993).
[14] K. W. Becker, R. Eder, and H. Won, Phys. Rev. B **45**, 4864 (1992).
[15] R. K. Nesbet, Rev. Mod. Phys. **33**, 28 (1961).
[16] R. F. Bishop, Theor. Chim. Acta **80**, 95 (1991).
[17] T. Schork and P. Fulde, Int. J. of Chem. **51**, 113 (1994).
[18] M. Vojta and K. W. Becker, Ann. Phys. (Leipzig) **5**, 456 (1996).
[19] R. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, New York 1992).
[20] J. Stoer and R. Burlisch, *Introduction to Numerical Analysis* (Springer-Verlag, New York, 1980).