Anisotropic Heisenberg antiferromagnet in the presence of a magnetic field for arbitrary dimension and spin

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In this work we study the Heisenberg *XXZ* antiferromagnetic model for spin S and dimension d in the presence of an external longitudinal magnetic field. First, we essay a variational approach which uses as trial function a version of the analytic expression for the ground state given by the paired nonmagnetic excitation (PNME) theory [M. Lagos and G. G. Cabrera, Solid State Commun. **67**, 221 (1988); Phys. Rev. B **38**, 659 (1988)], generalized in order to incorporate the external field. The ground-state energy, sublattice magnetization, and magnetic susceptibility are obtained. Subsequently, we solve the problem numerically for a chain of 12 spins ($S=1$ and $S=\frac{3}{2}$) using the Lanczös method [E. Dagotto and A. Moreo, Phys. Rev. D **31**, 865 (1985)]. The two approaches give excellent concordance over a wide range of the parameters of the model. We show that our analytic trial function represents accurately the ground state of the system for anisotropies ranging from the Ising limit to the almost isotropic Heisenberg model for all values of the field. Moreover, it accounts for the several antiferromagnetic and ferromagnetic phases occurring for different values of the magnetic field with the same precision. The critical fields of the transitions are predicted correctly. Also, results for various spin values S in two and three dimensions are presented.

I. INTRODUCTION

In one dimension, for $S=\frac{1}{2}$, the antiferromagnetic *XXZ* Heisenberg Hamiltonian was completely solved by the Bethe ansatz,[1-3] but for larger spin or higher dimension no exact analytical solution is known. Numerical solutions become more difficult as well, as the dimension or the spin size increase. The study of the spin dynamics in real lattices thus resorts to approximate approaches. Among them, spin-wave theory has shown to describe accurately the magnetic excitations of a number of antiferromagnetic crystals. The minimum error for the ground-state energy of spin-wave theory is obtained for the isotropic case which corresponds to an anisotropy parameter $\alpha=1$ (3 and 2% error in one and two dimensions, respectively), and the error rapidly increases as α departs from unity.

In order to focus our discussion we study a magnetic system that can be divided into two sublattices, one associated with vectors $\mathbf{R}$ and the other with vectors $(\mathbf{R}+\delta)$, where δ connects nearest neighbors of different sublattices. Thus we have the following Hamiltonian:

$$\mathcal{H}=J\frac{\alpha}{2}\sum_{\mathbf{R},\delta}[S^{+}(\mathbf{R})S^{-}(\mathbf{R}+\delta)+S^{+}(\mathbf{R}+\delta)S^{-}(\mathbf{R})]$$
$$+J\sum_{\mathbf{R},\delta}S^{z}(\mathbf{R})S^{z}(\mathbf{R}+\delta)$$
$$-\mu_b gH\sum_{\mathbf{R}}[S^{z}(\mathbf{R})+S^{z}(\mathbf{R}+\delta_0)]\ , \qquad (1.1)$$

where $\mathbf{S}(\mathbf{R})$ is the spin at the site $\mathbf{R}$, J is the exchange coefficient, and H is the magnetic field.

Recently, an approximate solution for the Hamiltonian was proposed for the $S=\frac{1}{2}; d=1$ case. This solution was based in a variational version of the "paired nonmagnetic excitation theory" (hereafter PNME).[4-12] This denomination deserves a comment: actually the PNME excitation operators are not "nonmagnetic," because although they conserve the z component of total spin, they do not commute with the other components of the total spin.

The PNME method applies in the quasi-Ising limit ($\alpha<0.5$) and renders excellent agreement (much better than spin-wave theory) when compared with numerical calculations for the ground-state energy and correlation functions. The ground state proposed by the PNME method is a coherent state even for very high anisotropy and the apparent structure is disordered similar to the Anderson[13] solution but on the average the antiferromagnetic order is preserved. Then, it is not surprising that the theory fails when a sufficiently high magnetic field is applied; in this case a ferromagnetic phase is expected which is well beyond the capability of the simple version of the PNME theory.

In this work we address the Heisenberg antiferromagnetic model for spin S and the anisotropic exchange in the presence of an external longitudinal magnetic field. First, we essay a variational approach which uses as trial function a version of the analytic expression for the ground state given by the PNME theory, generalized in order to incorporate the external field. The calculations are done for arbitrary dimension. The matrix elements are calculated as a power series in the anisotropic parameter α up to fourth order. The ground-state energy, sub-

lattice magnetization, and magnetic susceptibility are obtained. Subsequently we approach the problem numerically and solve it for a chain of 12 spins ($S=1$ and $S=\frac{3}{2}$) using the Lanczös method.

The two approaches give excellent concordance over a wide range of the parameters of the model. We show that our analytic trial function represents accurately the ground state of the system for anisotropies ranging from the Ising limit to the almost isotropic Heisenberg model for all values of the field. Moreover, it accounts for the several antiferromagnetic and ferromagnetic phases occurring for different values of the magnetic field with the same precision. The critical fields of the transitions are also predicted correctly.

II. THE MODEL

We consider the trial variational state

$$|g(\theta_1,\theta_2,\alpha')\rangle = R_y(\theta_1,\theta_2)|g(\alpha')\rangle \ , \tag{2.1}$$

where the unitary operator

$$R_y(\theta_1,\theta_2) = \prod_{\mathbf{R}} \exp\left[\frac{i}{2}[\theta_1 S_y(\mathbf{R}+\delta_1)+\theta_2 S_y(\mathbf{R})]\right] , \tag{2.2}$$

is simply a rotation in θ_1 (sublattice $\mathbf{R}$) and θ_2 (sublattice $\mathbf{R}+\delta$) around the y axis (the angles are measured from the antiferromagnetic state along the z direction). Finally

$$|g(\alpha')\rangle = \exp\left[-\frac{\alpha'}{(2zS-1)}\sum_{\mathbf{R},\delta}[S^+(\mathbf{R}+\delta)S^-(\mathbf{R})-S^+(\mathbf{R})S^-(\mathbf{R}+\delta)]\right]|\mathcal{N}\rangle \tag{2.3}$$

corresponds to the PNME ground-state solution, $|\mathcal{N}\rangle$ the Néel state (spin up in the $\mathbf{R}$ sublattice and down in the $\mathbf{R}+\delta$ sublattice), α' is a variational parameter which measures the degree of disorder from the ordered Néel state, and z is the number of nearest neighbors.

In our calculations only two variational angles are considered, each one corresponding to a sublattice mean spin direction. This poses a limit to the possible magnetic structures which can be obtained; for example, an helical phase with arbitrary pitch is disregarded. Nevertheless, antiferromagnetic, ferromagnetic, or spin flop phases are obtained as a minimum of the energy functional. α' is a variational parameter which controls the magnitude of the sublattice magnetic moment; then in principle, a paramagnetic phase is also an accessible solution.

The energy functional is

$$F(\theta_1,\theta_2,\alpha') = \langle g(\alpha')|R_y^\dagger(\theta_1,\theta_2)\mathcal{H}R_y(\theta_1,\theta_2)|g(\alpha')\rangle \ . \tag{2.4}$$

Taking advantage of the unitary character of the operators $R(\theta)$ one can view Eq. (2.4) as the expectation value of the transformed operator $R^\dagger\mathcal{H}R$ with respect to the state $|g(\alpha')\rangle$. To accomplish the transformation just substitute in Eq. (1.1)

$$S^x \to \cos\theta S^x - \sin\theta S^z \ , \tag{2.5}$$

$$S^y \to S^y \ , \tag{2.6}$$

$$S^z \to \sin\theta S^x + \cos\theta S^z \ . \tag{2.7}$$

Then replace the resulting expression in place of $R^\dagger\mathcal{H}R$ in Eq. (2.4). Recalling that $S^x=(S^+ + S^-)/2$ and $S^y=(S^+ - S^-)/(2i)$ one readily arrives at

$$\frac{F(\theta_1,\theta_2,\alpha')}{N} = \frac{Jz}{2}\{H_I(\cos\theta_1\cos\theta_2+\alpha\sin\theta_1\sin\theta_2)+\tfrac{1}{2}H_{XY}(\sin\theta_1\sin\theta_2+\alpha\cos\theta_1\cos\theta_2+\alpha)\} - \frac{hSM_z}{2}(\cos\theta_1-\cos\theta_2) \ , \tag{2.8}$$

where $h=g\mu_b\hbar H$ is the reduced longitudinal magnetic field. The coefficients

$$H_I = \langle g(\alpha')|S^z(\mathbf{R}+\delta)S^z(\mathbf{R})|g(\alpha')\rangle \ , \tag{2.9}$$

$$H_{xy} = \langle g(\alpha')|S^x(\mathbf{R}+\delta)S^x(\mathbf{R}) + S^y(\mathbf{R}+\delta)S^y(\mathbf{R})|g(\alpha')\rangle \ , \tag{2.10}$$

$$M_z = \frac{1}{S}\langle g(\alpha')|S^z(\mathbf{R})|g(\alpha')\rangle \tag{2.11}$$

do not depend on the angles θ_i, but only on α'. The mean values presented in Eqs. (2.9)–(2.11) are known exactly in one dimension[5,6] for $S=\frac{1}{2}$:

$$H_I = -\tfrac{1}{4}[J_0^2(2\alpha')+J_1^2(2\alpha')] \ , \tag{2.12}$$

$$H_{xy} = -\tfrac{1}{2}J_1(2\alpha') \ , \tag{2.13}$$

$$M_z = J_0(2\alpha') \ , \tag{2.14}$$

where $J_n(x)$ are the Bessel functions of integer order.

For arbitrary dimension d and spin values S the matrix elements are not known in a closed analytical expression. In the Appendix we show a method to obtain them as a

power series in the anisotropy parameter α. The results are

$$H_I=-\frac{zS^2}{2}\left[1-\frac{\alpha'^2}{2Sz-1}+\frac{\alpha'^4}{3(2Sz-1)^4}\times\left\{(Sz-2)\left[4Sz-1-\frac{2S^2\Gamma}{z}\right]+3S^2z^2\right\}\right], \tag{2.15}$$

$$H_{xy}=-\frac{2zS^2\alpha'}{2zS-1}\left[1-\frac{\alpha'^3}{3(2Sz-1)^2}\left\{4zS-1-\frac{2S^2\Gamma}{z}\right\}\right], \tag{2.16}$$

$$M_z=1-\frac{Sz\alpha'^2}{(2Sz-1)^2}+\frac{Sz\alpha'^4}{6(2Sz-1)^4}\left[4Sz-1-\frac{2S^2\Gamma}{z}\right], \tag{2.17}$$

where

$$\Gamma=\sum_{\delta_a,\delta_b,\delta_c,\delta_d}\delta(\delta_a+\delta_b+\delta_c+\delta_d),$$

is the number of closed loops which can be constructed with four steps between nearest neighbors. Our problem then is reduced to minimizing with respect to θ_i, and α'. The extremum equations are

$$[-4B\sin\xi+P\sin\eta]\cos\xi=0, \tag{2.18}$$

$$[-4A\sin\eta+P\sin\xi]\cos\eta=0, \tag{2.19}$$

$$\frac{\partial}{\partial\alpha'}F(\theta_1,\theta_2,\alpha')=0, \tag{2.20}$$

where we have defined the quantities

$$A=\frac{Jz}{4}(1-\alpha)[H_I-\tfrac{1}{2}H_{XY}], \tag{2.21}$$

$$B=\frac{Jz}{4}(1+\alpha)[H_I+\tfrac{1}{2}H_{XY}], \tag{2.22}$$

$$P=hM_zS \tag{2.23}$$

and the new variables η and ξ as

$$\eta=\tfrac{1}{2}[\theta_1+\theta_2], \tag{2.24}$$

$$\xi=\tfrac{1}{2}[\theta_1-\theta_2]. \tag{2.25}$$

III. THE RESULTS

The set of minimization equations has four types of solution:

$$\text{(i)}\quad\begin{cases}\cos\eta=0,\\ \cos\xi=0.\end{cases} \tag{3.1}$$

This solution represents two configurations:

(a) The sublattice magnetizations point along the same direction against the magnetic field and obviously represent a maximum of energy. In fact the rotation angles are $\theta_1=\pi$, $\theta_2=0$.

(b) The two sublattice magnetizations point against the direction of the field and represent a minimum of energy. The rotation angles are $\theta_1=0$, $\theta_2=\pi$.

$$\text{(ii)}\quad\begin{cases}\eta=\dfrac{\pi}{2},\\ \sin\xi=\dfrac{\mu g\hbar SHM_z}{Jz(1+\alpha)(1/2H_{xy}+H_I)}.\end{cases} \tag{3.2}$$

This solution represents a spin-flop configuration in which the sublattice magnetizations point along directions symmetric with respect to the z axis. Here the rotation angles are given by

$$\theta_1=\frac{\pi}{2}+a\arcsin\left[\frac{\mu g\hbar SHM_z}{Jz(1+\alpha)(1/2H_{xy}+H_i)}\right], \tag{3.3}$$

$$\theta_2=\frac{\pi}{2}-a\arcsin\left[\frac{\mu g\hbar SHM_z}{Jz(1+\alpha)(1/2H_{xy}+H_I)}\right]. \tag{3.4}$$

For a small magnetic field the two sins are oriented antiferromagnetically in the x direction.

$$\text{(iii)}\quad\begin{cases}\sin\eta=\dfrac{\mu g\hbar SHM_z}{Jz(1-\alpha)(-1/2H_{xy}+H_I)},\\ \xi=\dfrac{\pi}{2}.\end{cases} \tag{3.5}$$

In this solution the sublattice magnetizations point along the same direction ; the rotation angles are

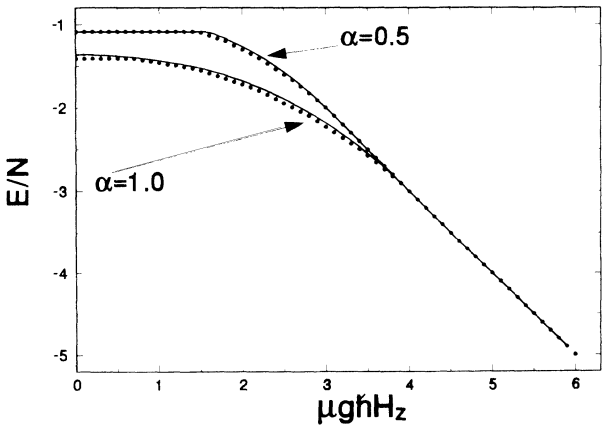

FIG. 1. Energy curves in one dimension, associated with values of the anisotropy $\alpha=0.5,1.0$ for spin $S=1$. The solid line represents results from the Lanczös method, and the variational approach is given by the scattered line.

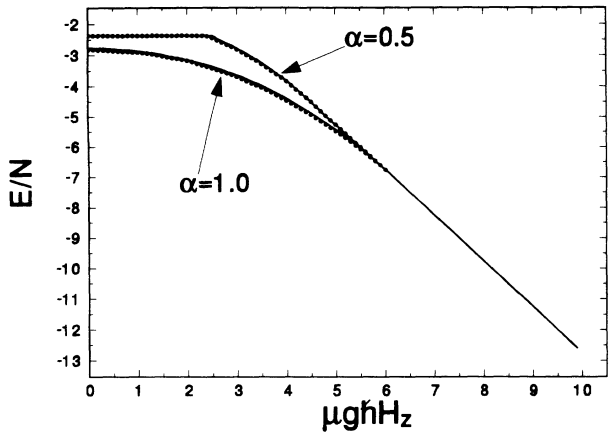

FIG. 2. Energy curves in one dimension, associated with the values of the anisotropy $\alpha=0.5,1.0$ for spins $S=\frac{3}{2}$. The solid line represents results from the Lanczös method, and the variational approach is given by the scattered line.

$$\theta_1=\frac{\pi}{2}+a\arcsin\left[\frac{\mu g\hbar SHM_z}{Jz(1-\alpha)(-1/2H_{xy}+H_I)}\right], \quad (3.6)$$

$$\theta_2=-\frac{\pi}{2}+a\arcsin\left[\frac{\mu g\hbar SHM_z}{Jz(1-\alpha)(-1/2H_{xy}+H_I)}\right], \quad (3.7)$$

and obviously represent a maximum. For a small magnetic field the two spins are oriented ferromagnetically in the x direction.

Finally

$$\text{(iv)}\ \xi=\eta=0\ . \quad (3.8)$$

In this case the spins remain oriented antiferromagnetically along the z axis and the energy is minimum. In this case the ground-state energy, sublattice magnetization, and correlation functions are the same as the case in which there is no magnetic field and the susceptibility is zero.

The minimization equation for α' has a known closed form only for the special case of $d=1$, $S=\frac{1}{2}$. For general spin S and dimension d, as a consequence of the length of the calculations, the mean values of the quantities involved are known as a series expansion in α' only to fourth order, and is necessary to solve numerically the resultant polynomial equation. It is also expected that as α' goes from zero to unity, the series expansion becomes less exact.

We solved Eqs. (2.20) numerically for different values of the reduced magnetic field h, and spin S. Also we have developed numerical solutions for spin $S=1$ and $S=\frac{3}{2}$ in chains of 12 and 10 spins, respectively, using the modified Lanczös algorithm.[14] The energy and the rotation angles were then evaluated for each case.

Figures 1 and 2 show energy curves in one dimension, associated with different values of the anisotropy α for spin 1 and $\frac{3}{2}$ (see Ref. 7 for an $S=\frac{1}{2}$ chain). The agreement is excellent especially near the Ising limit.

Figure 3 shows the field-dependent magnetization as given by our variational approach (continuous lines) and by the computer simulation (black circles), for two values

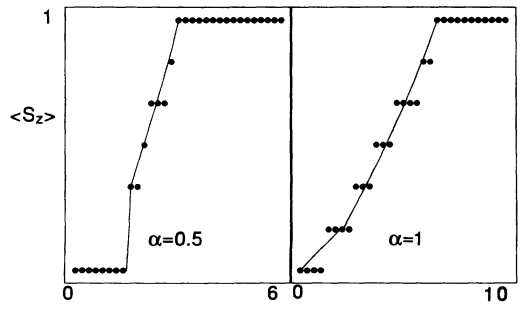

FIG. 3. Magnetization curves in one dimension, associated with values of the anisotropy $\alpha=0.5,1.0$ for spin $S=1$. The solid circles represent the numerical simulation with a 12-site chain. The variational approach is given by the solid line.

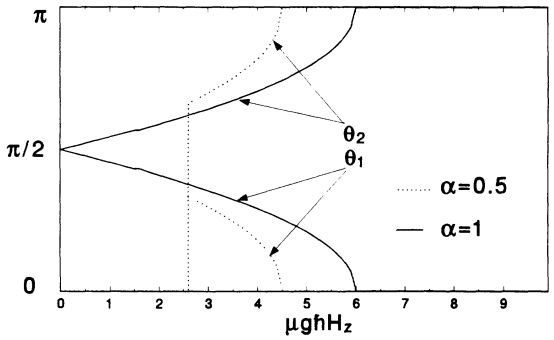

FIG. 4. Variational angles θ_1 and θ_2 as functions of the strength of the magnetic field for $S=\frac{3}{2}$ in a linear chain.

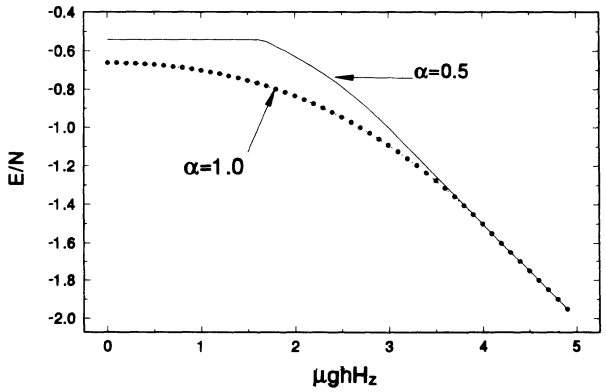

FIG. 5. Energy per bond as a function of the strength of the magnetic field, for the $S=\frac{1}{2}$, $d=2$ case, for $\alpha=0.5,1.0$.

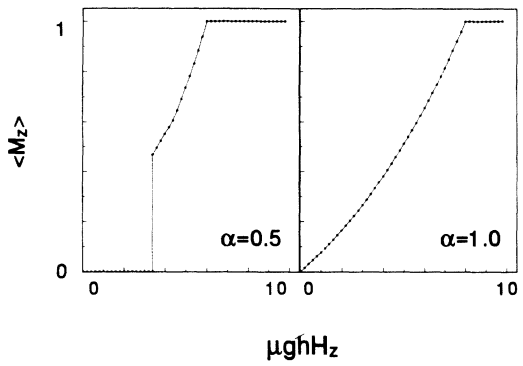

FIG. 6. Magnetization in the direction of the z axis as a function of the strength of the magnetic field for the $S=\frac{1}{2}$, $d=2$ case, for $\alpha=0.5, 1.0$.

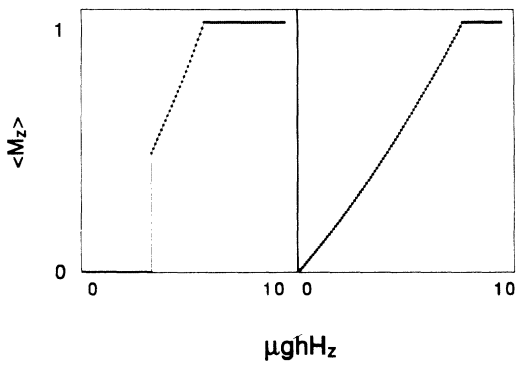

FIG. 8. Magnetization in the direction of the z axis as a function of the strength of the magnetic field for the $S=1$, $d=2$ case, for $\alpha=0.5, 1.0$.

of the anisotropy parameter α. The computer calculation assumes a chain of 12 sites, which explains the stepped shape of the numeric results. But for this technical aspect both approaches exhibit very good agreement.

The character of the several phases that the model goes through at $T=0$ as the strength of the external field is varied, can be visualized from the values assumed by θ_1 and θ_2. These are the mean angles subtended by the spins in the two sublattices with respect to a perfect antiferromagnetic configuration oriented along the z axis. This way, for example, $\theta_1=\theta_2$ and $\theta_1=-\theta_2=\pi/2$ correspond to an antiferromagnetic and a ferromagnetic situation, respectively.

Figure 4 plots θ_1 and θ_2 as functions of the strength of the magnetic field for $S=\frac{3}{2}$ in a linear chain (for an $S=\frac{1}{2}$ linear chain, see Ref. 7). The behavior for anisotropies toward the Ising ($\alpha=0.5$) and isotropic ($\alpha=1.0$) limits exhibit interesting differences. For example, in the case $S=\frac{3}{2}$, $\alpha=0.5$, the system has three phases and two transitions. For low parallel fields the spins persist in an antiferromagnetic configuration oriented along the z axis. When the reduced magnetic field increases up to about $h_z=2.6$ the spins jump abruptly to a new configuration,

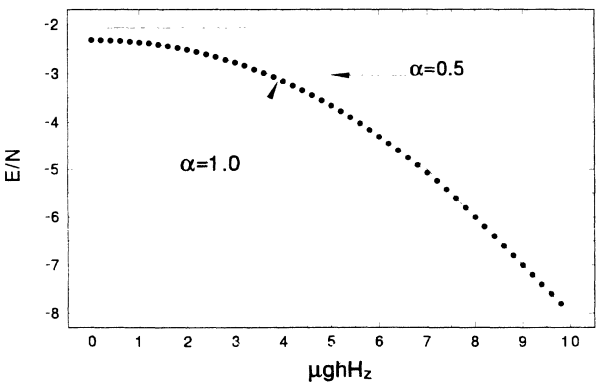

FIG. 7. Energy per bond as a function of the strength of the magnetic field, for the $S=1$, $d=2$ case, for $\alpha=0.5, 1.0$.

which may be thought of as an antiferromagnetic alignment of the spin components in the x-y plane together with ferromagnetic order of the z components. The magnetization along the z axis increases with h_z and the system keeps in this regime until the reduced parallel field reaches the point $h_z=4.5$, where the x-y antiferromagnetic component disappears and the system goes through a ferromagnetic phase oriented in the z direction. While the first transition is abrupt the second is continuous. For $\alpha=1.0$, that is, for an isotropic system, the system behaves quite differently. In agreement with previous results,[12] at $h_z=0$ the system has antiferromagnetic order in the x-y plane. As h_z increases, the field increases the ferromagnetic magnetization along the z axis. Close to $h_z=6.0$ the system enters a new phase, in which the spins fluctuate around a perfect ferromagnetic configuration.

In the two-dimensional isotropic case at zero field and $S=\frac{1}{2}$, a Monte Carlo treatment by Barnes, Kotchan, and Swanson[15] gives, for ϵ_0 the value -0.669, agrees with our result of -0.667 within a difference of 0.3%. For the two- and three-dimensional cases our results are essentially new, and we do not have reliable results with a nonzero magnetic field for comparison. Figure 5 displays the energy for the $S=\frac{1}{2}$, $d=2$ case, for $\alpha=0.5$ and for the isotopic case $\alpha=1.0$. Figure 6 shows the magnetization in the direction of the magnetic field in the same cases.

Figure 7 displays the energy for the $S=1$, $d=2$ case, for two representative values of α. Figure 8 shows the magnetization in the direction of the magnetic field in the same case. The value of the energy for zero field and $\alpha=1$ estimated by a real-space renormalization-group treatment by Mattis and Pan[16] is -1.907, and our result gives the value -2.32, lower than that result. Although our approach is a variational one, the truncation of the expansion series for the matrix elements introduces error as α grows.

IV. CONCLUSIONS

Our main objective in this paper is to show a method that constitutes a valuable tool in the study of the Heisenberg model with magnetic field in one or more dimen-

sions, for spin arbitrary. Beside its precision and mathematical simplicity, the method has the important advantage of accounting for the different magnetic phases at $T=0$ and their transitions with a single trial function having a compact mathematical expression. Whenever it has been possible, our results had been compared with the existing literature, giving a good agreement. We also developed—due to our need for reliable numerical data—numerical methods for solving the one-dimensional Heisenberg Hamiltonian in the presence of a magnetic field for the $S=1$ and $S=\frac{3}{2}$ cases.

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APPENDIX: CALCULATION OF MATRIX ELEMENTS

The calculation of matrix elements for arbitrary dimension d and spin values S are not known in a closed analytical expression, except in the $d=1$, $S=\frac{1}{2}$ case. Here we show a method to obtain them as a power series in the anisotropy parameter α.

The qualities to calculate are the expressions (2.9), (2.10), and (2.11). Except for (2.10), they are of the form

$$\langle \hat{f} \rangle = \left\langle \mathcal{N} \left| \exp\left[\frac{\alpha'}{(2zS-1)} \hat{B} \right] \hat{f} \exp\left[-\frac{\alpha'}{(2zS-1)} \hat{B} \right] \right| \mathcal{N} \right\rangle , \tag{A1}$$

where $\hat{f}$ is a Hermitian operator that conserves S_z *locally*, $\hat{B}$ is the anti-Hermitian PNME ground-state operator:

$$\hat{B} = \sum_{\mathbf{R},\delta} [S^+(\mathbf{R}+\delta)S^-(\mathbf{R}) - S^+(\mathbf{R})S^-(\mathbf{R}+\delta)] ,$$

and $|\mathcal{N}\rangle$ is the Néel state.

Using the identity

$$e^{-\hat{g}}\hat{f}e^{\hat{g}} = \hat{f} + [\hat{f},\hat{g}] + \frac{1}{2!}[[\hat{f},\hat{g}],\hat{g}] + \frac{1}{3!}[[[\hat{f},\hat{g}],\hat{g}],\hat{g}] + \cdots , \tag{A2}$$

it becomes clear that if we need a series expansion to the nth power in α', then we have to calculate the nth nested commutator between $\hat{f}$ and $\hat{B}$, and in principle the reduction of that to simpler commutators between S^z and $S^{\pm}$ constitutes a formidable task. We approached this problem from another point of view: taking advantage of the characteristics of the operators involved, is easily shown that

$$\langle [\hat{f},\hat{B}] \rangle = 0 , \tag{A3}$$

$$\langle [[\hat{f},\hat{B}],\hat{B}] \rangle = 2\langle \hat{B}^2\hat{f} - \hat{B}\hat{f}\hat{B} \rangle , \tag{A4}$$

$$\langle [[[\hat{f},\hat{B}],\hat{B}],\hat{B}] \rangle = 0 , \tag{A5}$$

$$\langle [[[[\hat{f},\hat{B}],\hat{B}],\hat{B}],\hat{B}] \rangle = -2\langle 4\hat{B}^3\hat{f}\hat{B} - 3\hat{B}^2\hat{f}\hat{B}^2 - \hat{B}^4\hat{f} \rangle , \tag{A6}$$

where the mean values are taken in the Néel state.

The determination of the effect of $\hat{f}$ over the Néel state is immediate because it conserves S^z locally and in consequence its effect is to multiply the ket by a constant. Thus the nontrivial part of the work is reduced to calculate

$$[\hat{f},\hat{B}] , \quad [\hat{f},\hat{B}^2] , \quad \langle \hat{B}^2 \rangle , \text{ and } \langle \hat{B}^4 \rangle . \tag{A7}$$

After a lengthy but straightforward work in this way, one can derive the expressions (2.15, 2.17).

The case of (2.10) is different. Here we note that

$$[S^+(\mathbf{R}),\hat{B}] = -\sum_{\delta} [S^+(\mathbf{R}+\delta)S^-(\mathbf{R}) + S^+(\mathbf{R})S^-(\mathbf{R}+\delta)] \tag{A8}$$

and thus derive (2.11) with respect to α' to obtain (2.16):

$$(2Sz-1)\frac{\partial}{\partial\alpha'}\langle g(\alpha')|S^z(\mathbf{R})|g(\alpha')\rangle = \langle g(\alpha')|S^x(\mathbf{R}+\delta)S^x(\mathbf{R}) + S^y(\mathbf{R}+\delta)S^y(\mathbf{R})|g(\alpha')\rangle . \tag{A9}$$

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