Coupled-cluster approximation for a spin-1 Heisenberg antiferromagnet with anisotropic exchange interaction and easy-plane single-ion anisotropy

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In this paper we have applied the coupled-cluster method to investigate the ground state of the spin-1 Heisenberg antiferromagnet with anisotropic exchange interaction and easy-plane single-ion anisotropy. A coupled-cluster approximation up to the second level has been performed to evaluate the ground-state energy and staggered magnetization for various lattices such as linear chain, honeycomb, square, simple cubic, and body-centered-cubic lattice. The convergence of our results is fairly rapid, and thus the coupled-cluster method seems to be a practical tool for calculating ground-state energy of a spin system since only the first few levels of approximation will be needed in actual practice.

I. INTRODUCTION

In the past few decades the magnetic properties of anisotropic antiferromagnets have been widely studied both theoretically and experimentally.[1] Here the anisotropy means either anisotropic exchange interactions or single-ionic-type anisotropy. Despite the apparent simplicity of the system, exact results are scarce. For instance, in the case of the isotropic spin-$\frac{1}{2}$ Heisenberg antiferromagnet, the exact ground state is known for the linear chain only, whereas beyond one dimension the exact nature of the ground state remains unknown.[2,3] Recently, interest has been further intensified by the discovery of high-temperature superconductivity and Anderson's suggestion that there is a possible connection between the ground state of the high-temperature superconducting materials and the two-dimensional spin-$\frac{1}{2}$ antiferromagnet.[4,5] Exhaustive investigations have been made on the magnetic properties of the spin-$\frac{1}{2}$ system but thorough studies of the spin-1 system are still lacking. Most recent studies on the spin-1 system have been performed on finite-size linear chains using the Lanczos method and Monte Carlo simulation technique.[6-8] This is mainly due to Haldane's conjecture concerning the qualitative difference between integer-spin and half-integer-spin antiferromagnetic Heisenberg models in one dimension[9] as well as the fact that the one-dimensional spin-1 antiferromagnetic Heisenberg models have been realized experimentally.[10] Besides, as far as we know, systematic analytical studies of the spin-1 system for various lattices are quite rare, especially recent ones.[11-16] Therefore, it is the purpose of this paper to investigate the ground-state properties of the spin-1 anisotropic Heisenberg antiferromagnet for various lattices using the coupled-cluster method. In addition to the anisotropic exchange interaction, the effect of the single-ion anisotropy will be considered as well. Single-ion anisotropies can have a fundamental influence on the magnetic behavior of a magnetic system, and prevail in almost all physical systems with spin greater than one-half. Because of the complexities caused by the single-ion anisotropy term, the mean-field approximation is commonly used in calculations of the thermodynamic quantities. However, in the mean-field approximation the quantum fluctuations have been neglected. Thus, it is of interest to go beyond the mean-field approximation and include the quantum fluctuations systematically.

The coupled-cluster method has proved to be a very useful technique in quantum many-body theory, and has been applied to a wide range of physical systems in nuclear physics, quantum chemistry, and relativistic quantum field theory.[17] Its main advantages are its automatic avoidance of unphysical divergences in the thermodynamic limit and its systematic ability to be taken to arbitrary accuracy. The coupled-cluster method can be used to calculate ground-state and excited-state energies, and also such other physical quantities as correlation functions and density matrices. The basic ideas of the coupled-cluster method rely on the fact that the exact ground state of a many-body Hamiltonian H can always be expressed as

$$|\Psi\rangle = \exp(S)|\Phi_0\rangle \ , \tag{1}$$

with $|\Phi_0\rangle$ being an appropriate "starting wave function" which is not orthogonal to the exact ground state. The corresponding Schrödinger equation,

$$H|\Psi\rangle = E_0|\Psi\rangle \ , \tag{2}$$

can then be written as

$$\mathcal{H}|\Phi_0\rangle \equiv \exp(-S)H\exp(S)|\Phi_0\rangle = E_0|\Phi_0\rangle \ , \tag{3}$$

where

$$\exp(-S)H\exp(S) = H + [H,S] + \tfrac{1}{2}[[H,S],S] + \cdots \ . \tag{4}$$

Since $|\Phi_0\rangle$ is normalized, we may write

$$E_0=\langle\Phi_0|\mathcal{H}|\Phi_0\rangle=\langle\Phi_0|\exp(-S)H\exp(S)|\Phi_0\rangle\ , \tag{5}$$

and by projecting Eq. (3) onto the states $|\Phi_n\rangle$ which are orthogonal to $|\Phi_0\rangle$, we obtain

$$\langle\Phi_n|\mathcal{H}|\Phi_0\rangle=\langle\Phi_n|\exp(-S)H\exp(S)|\Phi_0\rangle=0\ . \tag{6}$$

This orthogonality condition yields a series of nonlinear coupled equations, each of which contains a finite number of terms. The correlation operator S is determined by solving these equations. Once S is known, the ground-state energy and wave function can be obtained readily. Hence, the problem of finding the ground-state energy and wave function of the many-body system is reduced to computing the operator S. Nevertheless, this is a very formidable task, and some approximation scheme has to be used to solve the coupled equations. Bishop and Kümmel have prescribed the so-called sub-n coupled-cluster approximation in which the operator $S\equiv S_1+S_2+S_3+\cdots$, where $S_1,S_2,S_3,\ldots$ contain products of one, two, three,... raising operators, respectively, is truncated at the S_n level.[17] For the lattice problem, the strict breakdown into sub-n is not very useful since some effects at sub-4 are substantially larger than certain effects at sub-2; it is better to keep all reasonable terms inside a compact cluster than to include sub-2 terms where the two particles are far apart. In the following we shall apply a successive coupled-cluster approximation scheme, which was recently proposed by Roger and Hetherington,[18] to investigate the ground state of the spin-1 anisotropic antiferromagnetic Heisenberg model. This approximation scheme has been successfully applied to quantum spin systems and the Hubbard model on a square lattice.[18–22]

The general outline of this paper is as follows. In the next section we apply the successive coupled-cluster approximation (up to the second level) to the spin-1 antiferromagnetic Heisenberg model for various lattices such as the linear chain (lc), honeycomb (hc), square (sq), simple cubic (sc), and body-centered-cubic (bcc) lattices. Numerical results are also discussed. We then consider the easy-plane spin-1 antiferromagnet in Sec. III. This system represents a simple, but nontrivial, system with single-ion anisotropy, and has a phase transition at $T=0$. Finally, a conclusion is presented in Sec. IV.

II. SPIN-1 ANTIFERROMAGNET WITH ANISOTROPIC EXCHANGE INTERACTION

A. Theory

The Hamiltonian of the spin-1 antiferromagnetic Heisenberg model with anisotropic exchange interaction is given by

$$\begin{aligned}H&=\frac{J}{2}\sum_{(i,j)}\{S_i^zS_j^z+R\,(S_i^xS_j^x+S_i^yS_j^y)\}\\&=\frac{J}{2}\sum_{(i,j)}S_i^zS_j^z+\frac{JR}{4}\sum_{(i,j)}(S_i^+S_j^-+S_i^-S_j^+)\ ,\end{aligned} \tag{7}$$

where the spin raising and lowering operators are defined by $S^{\pm}\equiv S^x\pm iS^y$. Here J is a positive quantity representing the antiferromagnetic exchange interaction strength, R is the anisotropy parameter varying between 0 and 1, and $\sum_{(i,j)}$ denotes the summation over all nearest-neighbor pairs. Anticipating antiferromagnetism, we may rewrite the Hamiltonian by performing a rotation of the spin quantization axis at each site of one sublattice ("down" sublattice) into the direction of the local mean field. After the transformation the Hamiltonian becomes

$$\begin{aligned}H&=H_0+H_1\\&=-\frac{J}{2}\sum_{(i,j)}S_i^zS_j^z-h\sum_i S^z+\frac{JR}{4}\sum_{(i,j)}(S_i^+S_j^++S_i^-S_j^-)\ .\end{aligned} \tag{8}$$

Note that a source term $-h\sum_i S^z$ has been added to the Hamiltonian so that an estimate of the staggered magnetization of the system can be obtained. In this new basis, the Hamiltonian H_0 is just the Hamiltonian of the spin-1 ferromagnetic Ising model in an external magnetic field, and its ground state $|\phi_0\rangle$ is well known, i.e., the state with all spins "up": $|\phi_0\rangle\equiv\prod_{i=1}^{N}|+1\rangle_i$. It is, therefore, natural to choose the state $|\phi_0\rangle$ as our trial starting state of the successive coupled-cluster approximation for the Hamiltonian H. In fact, we believe that, when R is small, the state $|\phi_0\rangle$ should be pretty close to the exact ground state.

In order to incorporate the quantum fluctuations due to H_1, we now apply a successive coupled-cluster approximation as follows. With $|\phi_0\rangle$ as our starting state, we simply choose the correlation operator S to be zero for the zeroth level of the successive coupled-cluster approximation. Using this trivial correlation operator S, we obtain

$$\exp(-S)H\exp(S)|\phi_0\rangle=\left\{E_0+\frac{JR}{2}\sum_{(i,j)}L_{21}^iL_{21}^j\right\}|\phi_0\rangle\ , \tag{9}$$

where

$$E_0=-N\left[\frac{Jz}{2}+h\right] \tag{10}$$

with z being the coordination number. Here we have introduced the use of the local standard basis operators, which are defined, in terms of the eigenstates of S^z

$$|1\rangle=|+1\rangle,\quad |2\rangle=|0\rangle,\quad |3\rangle=|-1\rangle\ , \tag{11}$$

as

$$L_{mn}=|m\rangle\langle n|,\quad m,n=1,2,3\ . \tag{12}$$

These operators obey the commutation relation

$$[L_{kl}^i,L_{mn}^j]=\delta_{ij}(\delta_{lm}L_{kn}^i-\delta_{kn}L_{ml}^i)\ , \tag{13}$$

where the superscripts i and j are the lattice-site indices. Any operator can be written as a linear combination of these L operators:

$$O=\sum_{m,n}\langle m|O|n\rangle L_{mn}\ ; \tag{14}$$

in particular, the spin operators S^z and $S^{\pm}$ are expressed as

$$S^z=L_{11}-L_{33},\quad S^{+}=\sqrt{2}(L_{12}+L_{23})\ ,\quad S^{-}=\sqrt{2}(L_{21}+L_{32})\ . \tag{15}$$

The ground-state energy is given by $E_0|_{h=0}=-NJz/2$ with the remaining terms of Eq. (9) being neglected at this level. This is just the expectation value of H with respect to the state $|\phi_0\rangle$. Also, an estimate of the staggered magnetization can be found to be $M\equiv -N^{-1}\partial E_0/\partial h|_{h=0}=1$. All these imply that at the zeroth level of approximation the coupled-cluster method does not give any improvement at all, and thus we need to go to higher levels of the coupled-cluster approximation. In the next level of approximation, we also include in S the terms necessary to cancel the remaining terms of Eq. (9):

$$S=\alpha\sum_{(i,j)}L^i_{21}L^j_{21}\ . \tag{16}$$

This operator simply represents the simultaneous excitation of a pair of nearest-neighbor spins. With this correlation operator it can be found that

$$\exp(-S)H\exp(S)|\phi_0\rangle=\{E_0+FS+\cdots\}|\phi_0\rangle\ , \tag{17}$$

where

$$E_0=-N\left[\frac{Jz}{2}(1-2R\alpha)+h\right] \tag{18}$$

$$\alpha F=\frac{JR}{2}+[J(2z-1)+2h]\alpha+2JR\left[\frac{A}{z}-2(2z-1)\right]\alpha^2\ . \tag{19}$$

Here the quantity A is defined as

$$A=\sum_{(i,j)}\sum_{k(j)}\sum_{l(k)}\sum_{m(l)}\delta_{im}\ , \tag{20}$$

and its numerical values for various lattices are

$$A=\begin{cases}6 & \text{for lc}\\ 15 & \text{for hc}\\ 36 & \text{for sq}\\ 90 & \text{for sc}\\ 216 & \text{for bcc}\end{cases}\ .$$

By setting F to be zero, a quadratic equation of the parameter α is obtained, which can be easily solved to give two roots. The admissible solution is given by

$$\alpha=-\left[\left\{\frac{[J(2z-1)+2h]z}{4JR[A-2z(2z-1)]}\right\}^2-\frac{z}{4[A-2z(2z-1)]}\right]^{1/2}-\frac{[J(2z-1)+2h]z}{4JR[A-2z(2z-1)]}\ . \tag{21}$$

With the remaining terms of Eq. (17) being neglected, this then enables us to obtain the ground-state energy

$$E_0|_{h=0}=-NJz(1-2R\alpha)/2|_{h=0}$$

and staggered magnetization $M=1-JzR(\partial\alpha/\partial h)|_{h=0}$ readily. It is obvious that, provided the parameter α is not zero, there is considerable improvement beyond the zeroth-level results (see Table I).

Although we have made improvement beyond the zeroth-level results, there are still remaining terms in the expansion of $\exp(-S)H\exp(S)|\phi_0\rangle$ in the first level of the coupled-cluster approximation. One may then intend to include all the remaining terms of the first-level approximation into the correlation operator S. However, this will require us to manipulate a huge number of terms, and thus an alternate approach is badly needed. The simplest way is just to include the extra terms generated from $\{H+[H,S]\}|\phi_0\rangle$ in the first-level approximation into the new correlation operator. Accordingly, for the square, simple cubic, and body-centered-cubic lattices, the operator S consists of four terms and is given by

$$S=\sum_{n=1}^{4}S_n\ , \tag{22}$$

where

$$S_1=\alpha_1\sum_{(i,j)}L^i_{21}L^j_{21},\quad S_2=\alpha_2\sum_{(i,j)}L^i_{31}L^j_{31}\ ,\quad S_3=\alpha_3\sum_{(i,j,k)}^{D}L^i_{21}L^j_{31}L^k_{21},\quad S_4=\alpha_4\sum_{(i,j,k)}^{L}L^i_{21}L^j_{31}L^k_{21}\ ; \tag{23}$$

on the other hand, for the honeycomb lattice there is no such term as S_3 whereas the term S_4 does not exist in the case of the linear chain. Here the terms S_1 and S_2 denote simultaneous excitations of a pair of nearest-neighbor spins, while S_3 and S_4 are simultaneous excitations of a triplet placed in a straight line and an L-shaped configuration as shown in Fig. 1, respectively. (Note that for the body-centered-cubic lattice we have omitted another type of simultaneous excitation of a triplet forming a different L configuration [see Fig. 1(d)], because we believe that this type of excitation contributes less in comparison with the other two.) After some straightforward, though tedious, calculations similar to those in the first-level approximation, we obtain a set of four nonlinear coupled algebraic equations of the parameters α_i for each of the square, simple cubic, and body-centered-cubic lattices as well as three equations for both the linear chain and honeycomb lattices (see the Appendix). These nonlinear coupled equations have no closed-form solutions in general and need to be solved numerically. At this second level of coupled-cluster approximation the ground-state energy per site is given by

$$\frac{E_0}{N}=-\frac{Jz}{2}(1-2R\alpha_1)-h \tag{24}$$

in the limit $h\to 0$, which in turn readily yields an estimate of the staggered magnetization $M=1-JzR(\partial\alpha_1/\partial h)|_{h=0}$ (see Table I). Detailed numerical results will be discussed in the next section.

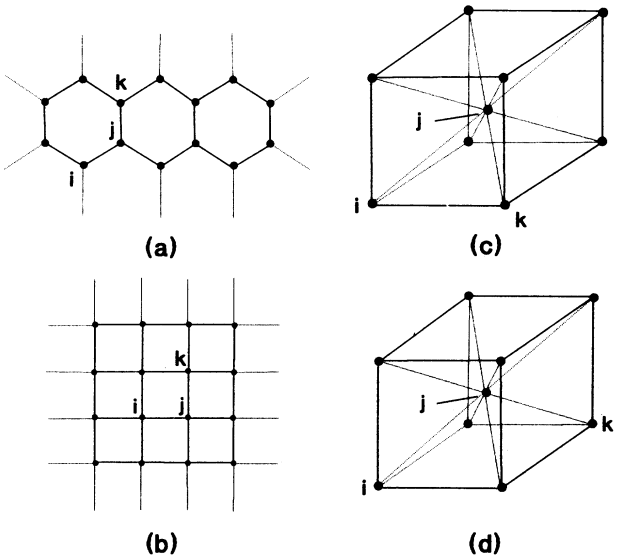

FIG. 1. Configurations of the L-shaped operator in different lattices: (a) hc; (b) sq and sc; (c) bcc; and (d) bcc. [Note that the one in (d) is different from that in (c).]

B. Numerical results and discussions

In Table I the numerical results of ground-state energy and staggered magnetization for various lattices with different R are tabulated. From the numerical data of ground-state energy it is observed that for small values of R a convergent pattern is found. This is actually not surprising because our starting state $|\phi_0\rangle$ is supposed to be pretty close to the exact ground state when R is small. For larger values of R the convergence appears to be slower due to the quantum fluctuations. Since the quantum fluctuations will be more dominant in low dimension, we may expect to obtain better results for higher dimensions. In fact, this can easily be seen by inspecting the numerical data for large R. Although the results converge more slowly when R is large, the estimates of the ground-state energy should still be reasonably close to the exact results. To see this more explicitly, we now compare our results for the case of isotropic exchange interaction with those obtained by other methods. Using a 64-site linear chain, Liang estimated the exact ground-state energy per spin to be $-1.402J$ for the one-dimensional case.[6] Our first- and second-level coupled-cluster approximations give the values $-1.2638J$ and $-1.3294J$, respectively. Obviously our results are in fairly good agreement with the exact result, even though the starting state $|\phi_0\rangle$ is actually a rather poor starting state in this case. The ground-state energies for various lattices obtained by other methods are listed in Table II. It can be seen that our results are consistent with these, especially in the three-dimensional case. For a further comparison we also tabulate the ground-state energies of the case with anisotropic exchange interaction for various lattices evaluated by Davis[15] and Arai *et al.*[16] in Table III. It is clear that our results agree with theirs pretty well over the whole range of anisotropy parameter R. This suggests that the first few levels of coupled-cluster approximation have already recovered a large portion of

TABLE I. (a) Ground-state energy per site in units of J; (b) Staggered magnetization. For each lattice, the result of the first-level approximation is listed on the left and that of the second-level on the right.

R	lc		hc		sq		sc		bcc	
					(a)					
0	−1	1	−1.5	−1.5	−2	−2	−3	−3	−4	−4
0.1	−1.0033	−1.0033	−1.5030	−1.5030	−2.0029	−2.0029	−3.0027	−3.0027	−4.0027	−4.0027
0.2	−1.0132	−1.0134	−1.5119	−1.5120	−2.0114	−2.0115	−3.0109	−3.0109	−4.0107	−4.0107
0.3	−1.0292	−1.0302	−1.5265	−1.5271	−2.0255	−2.0258	−3.0244	−3.0246	−4.0240	−4.0241
0.4	−1.0508	−1.0538	−1.5466	−1.5481	−2.0450	−2.0461	−3.0432	−3.0439	−4.0426	−4.0429
0.5	−1.0774	−1.0844	−1.5716	−1.5753	−2.0697	−2.0723	−3.0672	−3.0688	−4.0664	−4.0671
0.6	−1.1083	−1.1216	−1.6012	−1.6084	−2.0993	−2.1046	−3.0962	−3.0995	−4.0955	−4.0969
0.7	−1.1429	−1.1652	−1.6349	−1.6475	−2.1336	−2.1431	−3.1300	−3.1359	−4.1298	−4.1324
0.8	−1.1807	−1.2148	−1.6722	−1.6923	−2.1723	−2.1879	−3.1685	−3.1784	−4.1692	−4.1736
0.9	−1.2211	−1.2697	−1.7128	−1.7426	−2.2149	−2.2391	−3.2114	−3.2270	−4.2137	−4.2206
1	−1.2638	−1.3294	−1.7562	−1.7982	−2.2613	−2.2967	−3.2585	−3.2817	−4.2632	−4.2736
					(b)					
0	1	1	1	1	1	1	1	1	1	1
0.1	0.9978	0.9978	0.9988	0.9988	0.9992	0.9992	0.9995	0.9995	0.9996	0.9996
0.2	0.9915	0.9910	0.9953	0.9952	0.9968	0.9967	0.9980	0.9980	0.9986	0.9986
0.3	0.9816	0.9793	0.9898	0.9891	0.9928	0.9925	0.9956	0.9955	0.9968	0.9968
0.4	0.9693	0.9626	0.9825	0.9805	0.9875	0.9866	0.9923	0.9919	0.9943	0.9942
0.5	0.9553	0.9409	0.9739	0.9694	0.9810	0.9788	0.9881	0.9872	0.9912	0.9909
0.6	0.9407	0.9147	0.9643	0.9559	0.9735	0.9690	0.9832	0.9814	0.9874	0.9868
0.7	0.9259	0.8851	0.9543	0.9402	0.9651	0.9571	0.9776	0.9744	0.9829	0.9819
0.8	0.9115	0.8533	0.9440	0.9226	0.9562	0.9432	0.9714	0.9661	0.9778	0.9761
0.9	0.8978	0.8207	0.9337	0.9035	0.9468	0.9273	0.9647	0.9565	0.9721	0.9693
1	0.8849	0.7887	0.9236	0.8833	0.9371	0.9094	0.9576	0.9455	0.9658	0.9616

TABLE II. Ground-state energy per site in units of J from other methods for isotropic spin-1 antiferromagnet.

Method	lc	hc	sq	sc	bcc
Anderson (spin wave, Ref. 11)	−1.363		−2.316	−3.291	
Kubo (spin wave, Ref. 12)	−1.369		−2.3284	−3.2982	−4.2972
Fisher (Variational method, Ref. 13)	−1.3333	−1.8	−2.2857	−3.2727	−4.2667
Bullock (perturbation, Ref. 14)	−1.3594		−2.3164	−3.2901	−4.2868
Davis (perturbation, Ref. 15)	−1.3567		−2.3126	−3.2916	−4.2908
Arai and Goodman (cumulant expansion, Ref. 16)	−1.3759		−2.3110	−3.2892	−4.2868

the ground-state energy.

In addition, a closer look at the form of the ground-state energy in Eq. (18) for the case of isotropic exchange interaction suggests to us to make a more direct comparison with the results of linear spin-wave theory.[11] According to linear spin-wave theory, the ground-state energy takes the form

$$E_0^{\mathrm{LSW}} = -\tfrac{1}{2}JzN\left\{1+\frac{\gamma}{z}\right\}, \tag{25}$$

where the parameter γ lies between 0 and 1. The corresponding value of γ in our first-level coupled-cluster approximation is $\tilde{\gamma} \equiv -2z\alpha$. For large z, or equivalently

$$\xi \equiv |4[A-2z(2z-1)]/[z(2z-1)^2]| < 1 ,$$

the parameter α can be expressed as

$$\alpha = -\frac{1}{2(2z-1)}\left\{1-\frac{\xi}{4}+\frac{\xi^2}{8}+\cdots\right\}. \tag{26}$$

Thus, the lowest-order estimation of $\tilde{\gamma}$ is ≈ -0.5. In Table IV we tabulate the values of γ and $\tilde{\gamma}$ for various z. It is clear that γ and $\tilde{\gamma}$ are in pretty good agreement, at least for large z. This seems to suggest that, within the first level of coupled-cluster approximation, we are able to recover the results of linear spin-wave theory, at least for large z. Accordingly, the successive coupled-cluster approximation seems to be a practical tool for calculating the ground-state energy of a spin system, since only the first few levels of approximation will be needed in actual practice.

Nevertheless, our estimates of the staggered magnetization are less satisfactory in comparison to those of ground-state energy. In particular, for large R and small z no sign of convergence is in sight within the first two levels of coupled-cluster approximation. For instance, in the case of the linear chain with isotropic exchange interaction, the finite-size numerical calculations show that the ground state is disordered with a correlation length of 6.2 lattice spacings, whereas the second-level approximation still produces a rather large value of staggered magnetization. Hence, in order to obtain more definite estimates of staggered magnetization, it is necessary to go to higher levels of coupled-cluster approximation.

In summary, we have applied the coupled-cluster method to investigate the ground state of the spin-1 Heisenberg antiferromagnet with anisotropic exchange interaction. Coupled-cluster approximation up to the second level has been performed to evaluate the ground-state energies for various lattices. A detailed comparison has shown good agreement between our results and those obtained by other methods. The convergence of our results is fairly rapid, and becomes better as the coordination number increases or the anisotropy parameter of exchange interaction decreases. In addition, since our choice of the Néel state as the starting state is dictated primarily by our desire to use a calculationally manageable starting state and may not be a good one at all, especially for the isotropic case, one may improve the convergence of the successive coupled-cluster approximation by using a better starting state, e.g., a Gutzwiller-type trial wave function.

TABLE III. Ground-state energy per site in units of J from other methods for anisotropic spin-1 Heisenberg antiferromagnet. [For each lattice, the result by Davis (Ref. 15) is listed on the left while that by Arai and Goodman (Ref. 16) on the right.]

R	lc		sq		sc		bcc	
0	−1	−1	−2	−2	−3	−3	−4	−4
0.1	−1.0033	−1.0033	−2.0029	−2.0029	−3.0027	−3.0027	−4.0027	−4.0027
0.2	−1.0134	−1.0130	−2.0115	−2.0115	−3.0109	−3.0109	−4.0107	−4.0107
0.3	−1.0302	−1.0303	−2.0259	−2.0259	−3.0247	−3.0247	−4.0242	−4.0242
0.4	−1.0541	−1.0544	−2.0464	−2.0464	−3.0441	−3.0441	−4.0432	−4.0432
0.5	−1.0851	−1.0860	−2.0730	−2.0730	−3.0692	−3.0692	−4.0680	−4.0680
0.6	−1.1235	−1.1255	−2.1062	−2.1062	−3.1004	−3.1003	−4.0988	−4.0986
0.7	−1.1696	−1.1735	−2.1462	−2.1461	−3.1378	−3.1376	−4.1360	−4.1355
0.8	−1.2238	−1.2308	−2.1936	−2.1932	−3.1819	−3.1813	−4.1800	−4.1789
0.9	−1.2860	−1.2979	−2.2488	−2.2480	−3.2330	−3.2317	−4.2314	−4.2292
1	−1.3567	−1.3759	−2.3126	−2.3110	−3.2916	−3.2892	−4.2908	−4.2868

TABLE IV. Values of γ and $\tilde{\gamma}$ for different lattices.

	lc	hc	sq	sc	bcc
γ	0.726		0.632	0.582	0.584
$\tilde{\gamma}$	0.528	0.512	0.523	0.517	0.526

III. EASY-PLANE SPIN-1 ANTIFERROMAGNET WITH ANISOTROPIC EXCHANGE INTERACTION

A. Theory

The Hamiltonian of the easy-plane spin-1 antiferromagnet with anisotropic exchange interaction is given by

$$H=D\sum_i (S_i^x)^2+\frac{J}{2}\sum_{(i,j)}\{S_i^zS_j^z+R(S_i^xS_j^x+S_i^yS_j^y)\}$$
$$=D\sum_i (S_i^x)^2+\frac{J}{2}\sum_{(i,j)} S_i^zS_j^z+\frac{JR}{4}\sum_{(i,j)}(S_i^+S_j^-+S_i^-S_j^+)\ , \tag{27}$$

where the spin raising and lowering operators are defined by $S^{\pm}\equiv S^x\pm iS^y$. D is a positive quantity representing the strength of the single-ion anisotropy, J is the antiferromagnetic exchange integral, R, which varies between 0 and 1, measures the anisotropy of the exchange interaction, and $\sum_{(i,j)}$ denotes the summation over all nearest-neighbor pairs. The single-ion anisotropy term describes the fluctuations along the x axis and forces the spins to lie in the yz plane, namely, the easy plane. (Of course, there is no such effect in a spin-$\frac{1}{2}$ system.) For convenience, we may rewrite the Hamiltonian by performing a rotation of the spin quantization axis at each site of one sublattice ("down" sublattice) into the direction of the local mean field. After the transformation the Hamiltonian becomes

$$H=D\sum_i (S_i^x)^2-\frac{J}{2}\sum_{(i,j)} S_i^zS_j^z$$
$$+\frac{JR}{4}\sum_{(i,j)}(S_i^+S_j^++S_i^-S_j^-)-h\sum_i S_i^z\ . \tag{28}$$

Note that a source term $-h\sum_i S^z$ has been added to the Hamiltonian so that an estimate of the staggered magnetization of the system can be obtained. This Hamiltonian can be split into three parts, namely, H_0, H_1, and H_2:

$$H=H_0+H_1+H_2\ , \tag{29}$$

where

$$H_0=\sum_i \mathcal{H}_0^i=D\sum_i (S_i^x)^2-\tilde{h}\sum_i S_i^z+N\epsilon_0\ , \tag{30}$$

$$H_1=\frac{JR}{4}\sum_{(i,j)}(S_i^+S_j^++S_i^-S_j^-)\ , \tag{31}$$

$$H_2=-\frac{J}{2}\sum_{(i,j)}(S_i^z-\langle S^z\rangle)(S_j^z-\langle S^z\rangle)\ , \tag{32}$$

with $\tilde{h}=h+Jz\langle S^z\rangle$, $\epsilon_0=(Jz/2)\langle S^z\rangle^2$, and z being the coordination number. H_0 is the mean-field Hamiltonian which includes all single-ion potentials and a self-consistent field term extracted from the two-ion interaction potential, whereas H_1 and H_2 represent the quantum fluctuations. The self-consistent field is characterized by a parameter $\langle S^z\rangle$ which minimizes the free energy of the system. In the mean-field approximation, H_1 and H_2 are ignored, and $\mathcal{H}_0$ can be diagonalized exactly, yielding the eigenvalues

$$\epsilon_1=\frac{D}{2}-\left[\left[\frac{D}{2}\right]^2+\tilde{h}^2\right]^{1/2}+\epsilon_0\ , \tag{33}$$

$$\epsilon_2=D+\epsilon_0\ , \tag{34}$$

$$\epsilon_3=\frac{D}{2}+\left[\left[\frac{D}{2}\right]^2+\tilde{h}^2\right]^{1/2}+\epsilon_0\ , \tag{35}$$

and eigenstates

$$|\epsilon_1\rangle=\cos(\theta)|1\rangle-\sin(\theta)|-1\rangle\ , \tag{36}$$

$$|\epsilon_2\rangle=|0\rangle\ , \tag{37}$$

$$|\epsilon_3\rangle=\sin(\theta)|1\rangle+\cos(\theta)|-1\rangle\ , \tag{38}$$

where $|1\rangle$, $|0\rangle$, and $|-1\rangle$ are eigenstates of the operator S^z and the mixing angle θ is given by $\tan(2\theta)=D/(2\tilde{h})$. The ground-state energy per site and staggered magnetization are given by

$$E_0/N=\begin{cases}\dfrac{D}{2}\left[1-\dfrac{D}{2D_c}\right]-\dfrac{D_c}{4} & \text{for } D\le D_c\ ,\\ 0 \text{ for } D>D_c\ ,\end{cases}$$

$$M=\langle S^z\rangle=\begin{cases}\left[1-\left[\dfrac{D}{D_c}\right]^2\right]^{1/2} & \text{for } D\le D_c\ ,\\ 0 \text{ for } D>D_c\ ,\end{cases}$$

where D_c is the critical D and equals $2Jz$ in the mean-field approximation. So, there exists the critical value D_c above which long-range ordering disappears. This behavior of the system is due to the quantum-mechanical nature of the system and does not occur in classical spin systems. When D is very small, the mean-field Hamiltonian $\mathcal{H}_0$ for each single site is approximately given by $-\tilde{h}S^z$. The ground state can then be approximated by the state $|1\rangle$, implying that the mixing angle θ is very small, and the staggered magnetization $\langle S^z\rangle$ is thus very close to unity. On the other hand, when D is very large, $\mathcal{H}_0\simeq D(S^x)^2$. Obviously, the eigenstates for this Hamiltonian are the eigenstates of the spin operator S^x. For the ground state, we should choose the eigenstate with eigenvalue zero; that is, the ground state should be the state $(|1\rangle-|-1\rangle)/\sqrt{2}$, which means that $\theta=\pi/4$. Thus $\langle S^z\rangle$ tends to zero for very large values of D. As a consequence, the increase of the mixing angle and decrease of the staggered magnetization with increasing D are expected, and the phase transition can be easily understood.

In the mean-field approximation, the results are independent of the lattice structure and the anisotropy pa-

rameter R, and this is because we have ignored entirely the quantum fluctuations which play an essential role in determination of D_c and the critical behavior of the system. In order to incorporate the quantum fluctuations, we apply the successive coupled-cluster approximation to the system. Following the approximation scheme discussed in Sec. II, we first need to choose a suitable trial state $|\phi_0\rangle$ to start our coupled-cluster calculations. A natural choice is the ground state of the mean-field Hamiltonian H_0; that is, we choose

$$|\phi_0\rangle=\prod_{i=1}^{N}|\epsilon_1\rangle_i \ . \tag{39}$$

For the zeroth level of the successive coupled-cluster approximation, we simply choose the correlation operator S to be zero. Using this trivial correlation factor, we obtain

$$\exp(-S)H\exp(S)|\phi_0\rangle=\left\{E_0+F_1\sum_i L_{31}^i+F_2\sum_{(i,j)}L_{21}^iL_{21}^j+F_3\sum_{(i,j)}L_{31}^iL_{31}^j\right\}|\phi_0\rangle \ , \tag{40}$$

where

$$E_0/N=\epsilon_0+\epsilon_1-\frac{Jz}{2}[\cos(2\theta)-\langle S^z\rangle]^2 \ , \tag{41}$$

$$F_1=-Jz\sin(2\theta)[\cos(2\theta)-\langle S^z\rangle] \ , \tag{42}$$

$$F_2=\frac{JR}{2} \ , \tag{43}$$

$$F_3=-\frac{J}{2}\sin^2(2\theta) \ . \tag{44}$$

Here we have introduced the use of the local standard basis operators, which are defined in terms of the energy eigenstates of $\mathcal{H}_0$ as

$$L_{mn}\equiv|\epsilon_m\rangle\langle\epsilon_n| \ . \tag{45}$$

Any operator can be written as a linear combination of these L operators:

$$O=\sum_{m,n}\langle\epsilon_m|O|\epsilon_n\rangle L_{mn} \ ; \tag{46}$$

in particular, the spin operators S^z and $S^{\pm}$ are expressed as

$$S^z=\cos(2\theta)(L_{11}-L_{33})+\sin(2\theta)(L_{13}+L_{31}) \ , \tag{47}$$

$$S^+=\sqrt{2}[\cos(\theta)(L_{12}+L_{23})-\sin(\theta)(L_{21}-L_{32})] \ , \tag{48}$$

$$S^-=\sqrt{2}[\cos(\theta)(L_{21}+L_{32})-\sin(\theta)(L_{12}-L_{23})] \ . \tag{49}$$

The ground-state energy E_0 is given by $N(\epsilon_0+\epsilon_1)$ with the remaining terms of Eq. (40) being neglected at this level. This is just the mean-field result; in other words, at the zeroth-level approximation the coupled-cluster method does not give any improvement at all, and thus we need to go to higher levels of the coupled-cluster approximation.

In the next level of approximation, we include in S the terms necessary to cancel the remaining terms of Eq. (20):

$$S=S_1+S_2+S_3=\alpha_1\sum_i L_{31}^i+\alpha_2\sum_{(i,j)}L_{21}^iL_{21}^j+\alpha_3\sum_{(i,j)}L_{31}^iL_{31}^j \ . \tag{50}$$

The first term represents single-spin excitation whereas the other two terms denote simultaneous excitations of a pair of nearest-neighbor spins. With this S, it can be found that

$$\exp(-S)H\exp(S)|\phi_0\rangle=E_0|\phi_0\rangle+G_1S_1|\phi_0\rangle+G_2S_2|\phi_0\rangle+G_3S_3|\phi_0\rangle+\cdots \ , \tag{51}$$

where

$$E_0/N=\epsilon_0+\epsilon_1-\tfrac{1}{2}Jz[\cos(2\theta)-\langle S^z\rangle]^2-Jz\alpha_3\sin^2(2\theta)+JzR\alpha_2-Jz\alpha_1\sin(2\theta)[\cos(2\theta)-\langle S^z\rangle]-\tfrac{1}{2}Jz\alpha_1^2\sin^2(2\theta) \ , \tag{52}$$

$$\alpha_1G_1=(\epsilon_3-\epsilon_1)\alpha_1-Jz\sin(2\theta)[\cos(2\theta)-\langle S^z\rangle]+Jz\alpha_1[2\cos^2(2\theta)-\sin^2(2\theta)-2\langle S^z\rangle\cos(2\theta)]$$
$$+2Jz\alpha_3\sin(2\theta)[\langle S^z\rangle z-(z-2)\cos(2\theta)]+\tfrac{1}{2}Jz\alpha_1^2[6\sin(2\theta)\cos(2\theta)-2\langle S^z\rangle\sin(2\theta)]$$
$$-2Jz(z-2)\alpha_1\alpha_3\sin^2(2\theta)-2JzR\alpha_1\alpha_2+Jz\alpha_1^3\sin^2(2\theta) \ , \tag{53}$$

$$\alpha_2G_2=\tfrac{1}{2}JR+2(\epsilon_2-\epsilon_1)\alpha_2+J\alpha_1^2\alpha_2(2z-1)\sin^2(2\theta)+JR\alpha_3+J\alpha_2\cos(2\theta)[(2z-1)\cos(2\theta)-2\langle S^z\rangle z]$$
$$+\tfrac{1}{2}JR\alpha_1^2+JR\alpha_2^2\left[(4-8Z)+\frac{2A}{z}\right]+2J(2z-1)\alpha_2\alpha_3\sin^2(2\theta)$$
$$+J\alpha_1\alpha_2[2(2z-1)\cos(2\theta)\sin(2\theta)-2\langle S^z\rangle z\sin(2\theta)] \ , \tag{54}$$

$$\alpha_3 G_3 = -\tfrac{1}{2}J\sin^2(2\theta)+2(\epsilon_3-\epsilon_1)\alpha_3+JR\alpha_2+2J\alpha_1\sin(2\theta)\cos(2\theta)$$
$$-4J\alpha_3\cos(2\theta)[\langle S^z\rangle z-(z-1)\cos(2\theta)]-(4z-2)JR\alpha_2\alpha_3+J\alpha_1^2[\sin^2(2\theta)-2\cos^2(2\theta)]$$
$$+J\left[(8z-4)-\frac{2A}{z}\right]\alpha_3^2\sin^2(2\theta)+JR\alpha_1^2\alpha_2-2J\alpha_1^3\sin(2\theta)\cos(2\theta)+4J(z-1)\alpha_1^2\alpha_3\sin^2(2\theta)$$
$$+4J\alpha_1\alpha_3[2(z-1)\sin(2\theta)\cos(2\theta)-\langle S^z\rangle z\sin(2\theta)]-\tfrac{1}{2}J\alpha_1^4\sin^2(2\theta)\ . \tag{55}$$

Here the quantity A is defined in Eq. (20). By setting the G_i's to be zero, we obtain a set of three nonlinear coupled algebraic equations of the parameters α_i for each lattice. These nonlinear coupled equations have no closed-form solutions in general, and need to be solved numerically under the self-consistency condition of the staggered magnetization M,

$$M\equiv\langle S^z\rangle=-\frac{1}{N}\lim_{h\to 0}\frac{\partial E_0(h,\langle S^z\rangle)}{\partial h}\ . \tag{56}$$

Once the α_i's and M are found, the ground-state energy $E_0|_{h=0}$ can be obtained readily. It is obvious that, provided the parameters α_i are not zero, there is considerable improvement beyond the zeroth-level results.

Next, in the second-level approximation we include the extra terms generated from $\{H+[H,S]\}|\phi_0\rangle$ in the first-level approximation into the new correlation operator. Accordingly, for the square, simple cubic, and body-centered-cubic lattices, the operator S consists of thirteen terms and is given by

$$S=\sum_{n=1}^{13}S_n\ , \tag{57}$$

where

$$S_1=\alpha_1\sum_i L_{31}^i,\ S_2=\alpha_2\sum_{(i,j)}L_{21}^iL_{21}^j,\ S_3=\alpha_3\sum_{(i,j)}L_{31}^iL_{31}^j\ ,$$
$$S_4=\alpha_4\sum_{(i,j)}^{(2)}L_{21}^iL_{21}^j,\ S_5=\alpha_5\sum_{(i,j)}^{(2)}L_{31}^iL_{31}^j\ ,$$
$$S_6=\alpha_6\sum_{(i,j,k)}^{L}L_{21}^iL_{21}^jL_{31}^k,\ S_7=\alpha_7\sum_{(i,j,k)}^{L}L_{21}^iL_{31}^jL_{21}^k\ ,$$
$$S_8=\alpha_8\sum_{(i,j,k)}^{L}L_{31}^iL_{31}^jL_{31}^k,\ S_9=\alpha_9\sum_{(i,j)}^{(3)}L_{21}^iL_{21}^j\ , \tag{58}$$
$$S_{10}=\alpha_{10}\sum_{(i,j)}^{(3)}L_{31}^iL_{31}^j,\ S_{11}=\alpha_{11}\sum_{(i,j,k)}^{D}L_{21}^iL_{21}^jL_{31}^k\ ,$$
$$S_{12}=\alpha_{12}\sum_{(i,j,k)}^{D}L_{21}^iL_{31}^jL_{21}^k,\ S_{13}=\alpha_{13}\sum_{(i,j,k)}^{D}L_{31}^iL_{31}^jL_{31}^k\ ;$$

on the other hand, for the honeycomb lattice there are no such terms as S_{11}, S_{12}, and S_{13}, whereas the terms S_6, S_7, and S_8 do not exist in the case of the linear chain. Here $\sum_{(i,j)}^{(2)}$ and $\sum_{(i,j)}^{(3)}$ denote the summations over the second-nearest-neighbor and third-nearest-neighbor pairs (in terms of the Euclidean distance), respectively. In the summation $\sum_{(i,j,k)}^{(D)}$, the sites i, j, and k are placed in a straight line, while in $\sum_{(i,j,k)}^{(L)}$ the three sites are in an L configuration as shown in Fig. 1. These terms with three local standard basis operators denote the simultaneous excitations of three spins. (Note that for the body-centered-cubic lattice we have omitted another type of simultaneous excitation of a triplet forming a different L configuration [see Fig. 1(d)], because we believe that this type of excitation contributes less in comparison with the other two.) After some straightforward, though tedious, calculations similar to those in the first-level approximation, we obtain a set of 13 nonlinear coupled algebraic equations of the parameters α_i for each of the square, simple cubic, and body-centered-cubic lattices, as well as ten equations for both the linear chain and honeycomb lattices. As in the first-level approximation, one needs to resort to numerical methods to solve these equations under the self-consistency condition of the staggered magnetization in Eq. (56). Then, these parameters α_i will in turn give the ground-state energy and staggered magnetization of the system. Detailed numerical results will be discussed in the next section.

B. Numerical results and discussions

As mentioned above, the sets of nonlinear coupled-cluster equations in both levels have no closed-form solutions and need to be solved numerically to determine the parameters α_i for different values of $D/2J_z$. With these numerical solutions we are able to calculate the ground-state energy and staggered magnetization as functions of $D/2Jz$. The first-level numerical results for different lattices such as the linear chain, honeycomb, square, simple cubic, and body-centered-cubic lattices are shown in Figs. 2 and 3. In Table V(a) the values of D_c for these lattices are tabulated. Clearly the quantum fluctuations have induced substantial deviations from the mean-field result, which depend on the coordination number z and anisotropy parameter R: the larger the z is, the smaller the deviation is; whereas on the other hand, the deviation varies directly with R. One can also observe that the first-level estimates of the staggered magnetization are all lower than those obtained from the mean-field theory. This is expected because the quantum fluctuations are acting against the alignment of the spins, and thus reduce the staggered magnetization. Consequently, the first-level estimates of the D_c for each of the lattices are smaller than the mean-field result.

In Figs. 2 and 3 numerical results of the second level of coupled-cluster approximation are also shown, and the values of D_c are tabulated in Table V(b). These second-level results are qualitatively very similar to those of the

first level, though quantitatively quite different. In the second level the estimates of the staggered magnetization are again all lower than those given in the first level, but the corrections are comparatively smaller than before, in particular, for small values of D. This seems to suggest that the results at small D converge faster than those close to D_c, where quantum fluctuations are supposed to be most severe and higher levels of approximation are needed to account for them. Comparing the graphs of the ground-state energy and staggered magnetization, we can also observe that the ground-state energy does not change much from the first level to the second level, whereas the staggered magnetization has a comparatively more dramatic correction, especially in the region close to D_c. This is expected because, being a derivative of the ground-state energy, the staggered magnetization is a more sensitive quantity than the energy itself. Thus, in order to have better estimates of the staggered magnetization and critical point D_c, one needs to go to higher levels of coupled-cluster approximation.

Furthermore, it should be noted that in both levels of approximation there appears a small hump in each curve of staggered magnetization for $R \neq 0$. The exact positions of these humps for each level are listed in Table VI. This

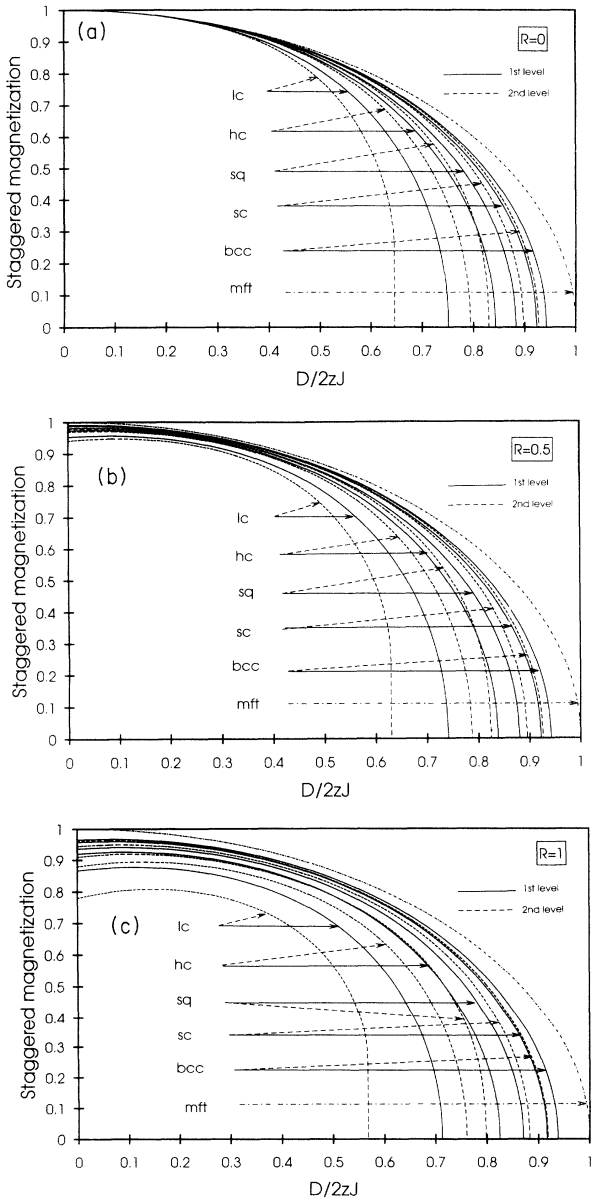

FIG. 2. Staggered magnetization as a function of the crystal field to exchange interaction ratio for different lattices: (a) $R=0$, (b) $R=0.5$, and (c) $R=1$. The dash-dotted, solid, and dashed curves denote the mean-field, first-level, and second-level results, respectively.

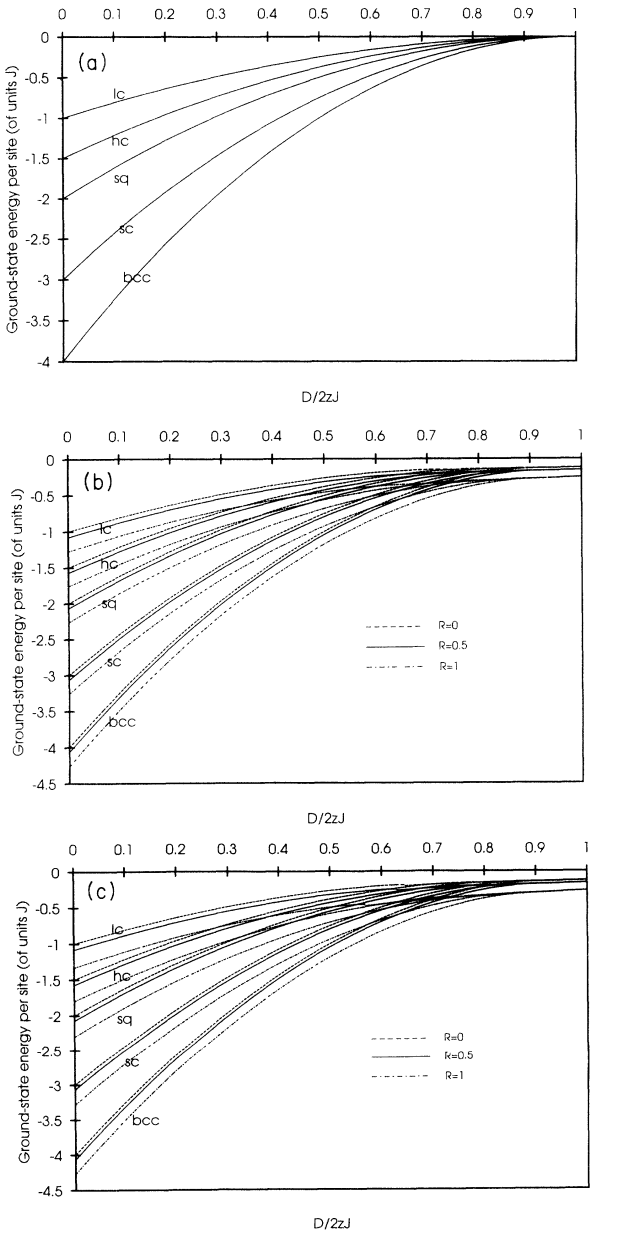

FIG. 3. Ground-state energy per site as a function of the crystal field to exchange interaction ratio for different lattices: (a) mean-field, (b) first-level, and (c) second-level results. The dashed, solid, and dash-dotted curves denote the results of $R=0$, $R=0.5$, and $R=1$, respectively.

TABLE V. Values of $D_c/2zJ$ for different lattices in the (a) first-level approximation, and (b) second-level approximation.

Lattice	$R=0$	$R=0.5$	$R=1$
	(a)		
lc	0.751	0.741	0.713
hc	0.843	0.838	0.825
sq	0.883	0.880	0.871
sc	0.923	0.922	0.917
bcc	0.943	0.942	0.938
	(b)		
lc	0.646	0.630	0.568
hc	0.794	0.787	0.761
sq	0.830	0.824	0.798
sc	0.898	0.895	0.884
bcc	0.928	0.926	0.919

interesting feature cannot be found in the mean-field theory, and also depends on the parameters z and R. While the hump is most prominent in the case of the linear chain with isotropic exchange interaction, it almost disappears in the case of a body-centered-cubic lattice with a very small R. In addition, as we go from the first level to the second level, the humps become more prominent, especially for low-dimensional systems with isotropic exchange interaction. However, we have not yet understood the physical picture behind this unexpected appearance of a small hump in the curve of staggered magnetization. Finally, we would like to point out that, in order to ensure the humps are not just artifacts of the coupled-cluster method and they do really reflect the physics of the system, we have applied an independent method, namely the connected-moments expansion, to investigate the system as well, and the humps do appear in this independent analysis.[23]

In summary, we have investigated the ground state of an easy-plane spin-1 antiferromagnet using the coupled-cluster method. The mean-field approximation is commonly used in calculations of thermodynamic quantities for such systems because of the complexities caused by the single-ion anisotropy term. However, in the mean-field approximation quantum fluctuations are entirely neglected. Here a successive coupled-cluster approximation up to the second level has been performed to evaluate the ground-state energy, staggered magnetization, and critical point D_c for various lattices. Although the coupled-cluster method is not a variational method and the estimates of the ground-state energy at each level of approximation are not necessarily upper bounds of the energy, the method does systematically improve its estimation of the energy by including the correlations of quantum fluctuations as we go to higher and higher levels of approximation. According to our calculations, the first couple of levels of the coupled-cluster approximation has already recovered a large portion of the ground-state energy. Hence the coupled-cluster method seems to be a practical tool for calculating the ground-state energy of a spin system, since only the first few levels of approximation will be needed in actual practice. In addition, the present calculations clearly show the failure of the mean-field approximation in predicting the behavior of the system both quantitatively and qualitatively, for instance, the appearance of a hump in the curve of staggered magnetization. It is found that the correlations of quantum fluctuations do play a major role in determining the critical behavior of the system.

TABLE VI. Coordinates of the hump for different lattices in the (a) first-level approximation, and (b) second-level approximation. Here the first coordinate is $D/2zJ$ while the second one is the staggered magnetization.

Lattice	$R=0$	$R=0.5$	$R=1$
		(a)	
lc	(0,1)	(0.073,0.956)	(0.112,0.877)
hc	(0,1)	(0.047,0.975)	(0.091,0.925)
sq	(0,1)	(0.036,0.982)	(0.086,0.940)
sc	(0,1)	(0.023,0.988)	(0.064,0.960)
bcc	(0,1)	(0.017,0.991)	(0.057,0.968)
		(b)	
lc	(0,1)	(0.090,0.947)	(0.148,0.807)
hc	(0,1)	(0.055,0.971)	(0.127,0.894)
sq	(0,1)	(0.040,0.980)	(0.104,0.919)
sc	(0,1)	(0.025,0.988)	(0.082,0.949)
bcc	(0,1)	(0.018,0.991)	(0.060,0.964)

IV. CONCLUSIONS

In this paper we have applied the coupled-cluster method to investigate the ground state of the spin-1 Heisenberg antiferromagnet with anisotropic exchange interaction and easy-plane single-ion anisotropy. Coupled-cluster approximation up to the second level has been performed to evaluate the ground-state energy and staggered magnetization for various lattices such as the linear chain, honeycomb, square, simple cubic, and body-centered-cubic lattices. The convergence of our results is fairly rapid, and becomes better as the coordination number increases or the anisotropy parameter of the exchange interaction decreases. According to our calculations, the first couple of levels of the coupled-cluster approximation have already recovered a large portion of the ground-state energy. Hence the coupled-cluster method seems to be a practical tool for calculating the ground-state energy of a spin system, since only the first few levels of approximation will be needed in actual practice.

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APPENDIX

In this Appendix, the coupled equations for different lattices in the second level are displayed.

1. Linear chain

$$\alpha_1 F_1 = \frac{J}{2}R + (3J+2h)\alpha_1 - 6JR\alpha_1^2 + JR\alpha_2 + 2JR\alpha_3 = 0 ,$$

$$\alpha_2 F_2 = JR\alpha_1 + 4(J+h)\alpha_2 - 6JR\alpha_1\alpha_2 = 0 ,$$

$$\alpha_3 F_3 = 2JR\alpha_1 + 4(J+h)\alpha_3 - 8JR\alpha_1\alpha_3 = 0 .$$

2. Honeycomb

$$\alpha_1 F_1 = \frac{J}{2}R + (5J+2h)\alpha_1 - 10JR\alpha_1^2 + JR\alpha_2 + 4JR\alpha_4 = 0 ,$$

$$\alpha_2 F_2 = JR\alpha_1 + 4(2J+h)\alpha_2 - 10JR\alpha_1\alpha_2 = 0 ,$$

$$\alpha_4 F_4 = 2JR\alpha_1 + 4(2J+h)\alpha_4 - 14JR\alpha_1\alpha_4 = 0 .$$

3. Square, simple cubic, and body-centered cubic

$$\alpha_1 F_1 = \frac{J}{2}R + [J(2z-1)+2h]\alpha_1 + 2JR\left[\frac{A}{z} - 2(2z-1)\right]\alpha_1^2 + JR\alpha_2 + BJR\alpha_3 + CJR\alpha_4 = 0 ,$$

$$\alpha_2 F_2 = JR\alpha_1 + 4[J(z-1)+h]\alpha_2 - 2JR(2z-1)\alpha_1\alpha_2 = 0 ,$$

$$\alpha_3 F_3 = 2JR\alpha_1 + 4[J(z-1)+h]\alpha_3 - 2JR(5z-D)\alpha_1\alpha_3 + EJR\alpha_1\alpha_4 = 0 ,$$

$$\alpha_4 F_4 = 2JR\alpha_1 + 4[J(z-1)+h]\alpha_4 - 2JR(5z-G)\alpha_1\alpha_4 + HJR\alpha_1\alpha_2 + IJR\alpha_1\alpha_3 = 0 ,$$

where A, B, C, D, E, G, H, and I are values listed in the following table:

	A	B	C	D	E	G	H	I
sq	36	2	4	10	8	10	4	4
sc	90	2	8	14	16	18	4	4
bcc	216	2	6	18	12	22	12	4

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