Density-matrix renormalization-group study of the spin-1/2 XXZ antiferromagnet on the Bethe lattice

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Ground-state properties of a spin-1/2 XXZ antiferromagnet on the Bethe lattice with three nearest neighbors are investigated; especially, the nature of the phase transition driven by the anisotropy is examined. In actual calculations, we employ the density-matrix renormalization-group method which is so far used in the studies on the one-dimensional quantum systems; its applicability to the higher-dimensional system is thus exhibited in our calculations. Numerical data on local spin correlations imply that the model undergoes the first-order phase transition at the Heisenberg point $J_{xy}=J_z$ and the ground state is conjectured to be in the Ising-like ordered phase (the ordered phase in XY plain) for $J_{xy}<J_z$ ($J_{xy}>J_z$). We also compare our results with those for other systems, say, the XXZ model on the square lattice to discuss a possible type of symmetry breaking. [S0163-1829(96)02821-4]

So far, the ground-state properties of the quantum antiferromagnets are of interest in both theoretical and experimental researches of magnetism. Especially, after the discovery of the high-T_c superconductors, the spin-1/2 Heisenberg antiferromagnet on the square lattice which is accepted as the proper model corresponding to the undoped materials has been extensively investigated. Generally speaking, since exact solutions are not available and some powerful techniques cannot be used except for one-dimensional systems, numerical approaches, e.g., the quantum Monte Carlo simulations[1–3] and the exact diagonalization method,[4,5] have been frequently employed for the investigations of higher-dimensional systems. However, fully convincing calculations are not always possible due to the limitations on the computer ability.

In solid-state physics, the Bethe lattice has been successfully used as an effective instrument for the periodic and the nonperiodic systems because it has often presented their simple treatments; theoretical models on the Bethe lattice may be expected to describe the realistic two- and three-dimensional systems to some extent.[6]

In this paper, we discuss the ground-state properties of the spin-1/2 XXZ antiferromagnet on the Bethe lattice:

$$\mathscr{H}=2\sum_{\langle l,m\rangle} J_{xy}(S_l^xS_m^x+S_l^yS_m^y)+J_zS_l^zS_m^z \qquad (1)$$

($J_{xy},J_z>0$) by employing the density-matrix renormalization-group (DMRG) method;[7] the purpose is twofold: the properties of the phase transition caused by the anisotropy J_z/J_{xy} are clarified and a possible type of the symmetry breaking is discussed through the comparison with other systems, e.g., the XXZ antiferromagnet on the square lattice.[2–5] At the same time, we shall propose a new application of the DMRG method which enables us to treat a quantum system not in one dimension; the applicability to the present higher-dimensional system is to be clarified through our calculations.

Before starting with the description of the DMRG calculation procedure, let us see the structure of the Bethe lattice on which quantum systems are located. As is well known, the Bethe lattice is defined as a group of infinite points each connected to q neighbors such that no closed loops exist [see Fig. 1(a)]. This type of graph is also known as a Cayley tree and possesses the features of both one and infinite dimensions: Since $V(n)$, a number of points within a distance of n steps from a point, is given as $[q(q-1)^{n-}2]/(q-2)$, the lattice dimension defined by $D=\lim_{n\to\infty}[\ln V(n)/\ln n]$ is infinite. On the other hand, any two points on the lattice are connected by a unique path (indeed, the $q=2$ case is reduced to a one-dimensional chain). As we shall see below, this single connectivity may allow us to adapt the DMRG algorithm straightforwardly. And then, we finally describe the infinite system as shown in Fig. 1(b), where four filled double circles indicate the renormalized-effective blocks representing the parts of the original infinite system.

The DMRG method which was proposed by White[7] has achieved great improvements in the efficiency of the numerical renormalization-group calculation by utilizing the information of the reduced density matrix for *the physical system* combined with *the environment*. As a result, the convergency of the data against the number of states (m) kept in the DMRG transformation is remarkably accelerated. However, the scope of the applicable systems is limited to the one-

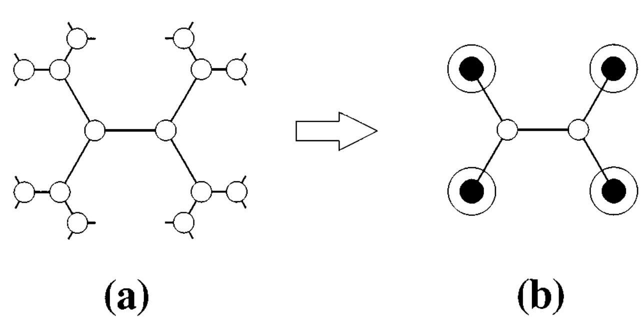

FIG. 1. The original Bethe lattice ($q=3$) (a) is renormalized and finally reduced to the six-block system (b). Four filled double circles represent the renormalized blocks to be obtained.

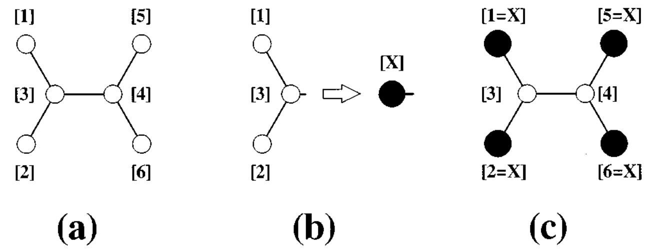

FIG. 2. The schematic representation of the DMRG calculation for the quantum systems on the Bethe lattice ($q=3$). The starting six-site system (a), the RG process (b), and the whole system in the next step (c).

dimensional quantum systems[8] due to the technical problem; the extension of the algorithm for higher-dimensional systems has been desired. Here, we shall see that the single connectivity between *the physical system* and *the environment* might be crucial for the implementation of the DMRG calculations; at least, the Bethe lattice fulfills this topological condition as well as the one-dimensional case.

The schematic representation of the DMRG calculation for the quantum systems on the Bethe lattice ($q=3$) is given in Fig. 2. We start with the six-site system shown as Fig. 2(a). Each site/block is described by the bases which are classified by a set of quantum numbers (μ) conserved under the DMRG transformation, e.g., the total S^z (S_T^z) for quantum spins and the up- and down-electron numbers (n_+^e, n_-^e) for fermions. The whole system is represented by the direct product of bases for each block: $|\{\mu\}\rangle = |\mu_6\rangle \otimes |\mu_5\rangle \otimes |\mu_4\rangle \otimes |\mu_3\rangle \otimes |\mu_2\rangle \otimes |\mu_1\rangle$, where $\{\mu\} = (\mu_1, \mu_2, ..., \mu_6)$. In actual calculations, we do not know expressions of these bases, but only store the representation matrices for the block Hamiltonian: H_B and spin components: S_l^+, S_l^z or fermion operators: $c_{l\sigma}, n_{l\sigma}$, which have a block form indexed by μ. To calculate *the target state* (usually the ground state of the whole system) using the Lanczos method, we should multiply the representation matrix of the whole Hamiltonian constructed from a direct product of matrices of the six blocks. Here, it should be noted that when calculating the electron-hopping term between [4] and [6], for example (we hereafter denote the jth block as $[j]$), we should properly take the fermion anticommuting nature into account:

$$\langle \{\overline{\mu}\} | c_{6\sigma}^\dagger c_{4\sigma} | \{\mu\} \rangle = (-1)^{n_5^e} [c_{6\sigma}^\dagger]_{\overline{\mu_6}, \mu_6} \otimes \mathbf{1}_{\mu_5} \otimes [c_{4\sigma}]_{\overline{\mu_4}, \mu_4} \otimes \mathbf{1}_{\mu_3} \otimes \mathbf{1}_{\mu_2} \otimes 1_{\mu_1}, \tag{2}$$

where $n_5^e \equiv n_{5+}^e + n_{5-}^e$ is the total electron number of a given μ_5 subspace and $\mathbf{1}_\mu$ is a $d(\mu) \times d(\mu)$ unit matrix [$d(\mu)$ is the dimension of μ subspace].

As the same manner with the one-dimensional case, the RG part is defined by the projection:[9] the bases describing the left-block [1], [2], and [3] are truncated using the orthogonal matrix which is constructed from the eigenvectors belonging to the largest m eigenvalues of the reduced density matrix. And then, the renormalized new block $[X]$ is obtained [Fig. 2(b)]. We again construct the six-block system as shown in Fig. 2(c) by replacing [1], [2], [5], and [6] in Fig. 2(a) with $[X]$, and repeat the same procedures until the system becomes sufficiently large.

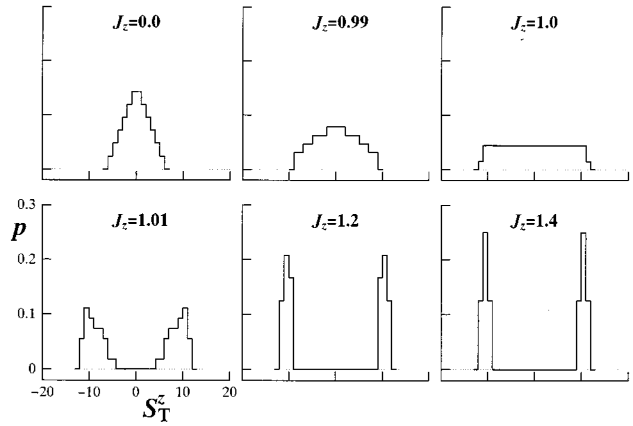

FIG. 3. The normalized distribution function of the numbers of bases classified by the total S^z: $p(S_T^z, J_z)$. The x axis is the value of S_T^z. We exhibit the data for the largest 63-site block.

Now, suppose that n_R is the renormalization level (the number of iterations), the numbers of sites in the whole system and the sites belonging to the boundary are given as $N_q(n_R) = 2[(q-1)^{n_R+2} - 1]/(q-2)$ and $M_q(n_R) = 2(q-1)^{n_R+1}$, respectively. So, unlikely to regular lattices, the ratio of boundary sites does not become smaller even in the thermodynamic limit. To avoid the difficulty, we will follow the definition of the Bethe *lattice*: the measurements of physical quantities are performed on the center part of the whole system, e.g., the local spin correlations between [3] and [4], and identically with the usual lattices, these sites are regarded to be equivalent.[10]

In the following, we summarize our numerical results on the ground state of the XXZ model; the energy is measured in units of J_{xy}, and thus J_z is an anisotropy parameter. The DMRG calculation was repeated $n_R=5$ times (so, up to 254-site systems were treated). The truncation error was estimated using the eigenvalues of the reduced density matrix: $Q(m, J_z) \equiv 1 - P(m, J_z)$, which strongly depends upon the number of states m and J_z (see Ref. 8). When $J_z \geqslant 1.1$, $m \simeq 30$ is enough to realize $Q < 10^{-7}$ and in the region near the XY point ($J_z \leqslant 0.6$), the truncation error is moderate against m. However, the states up to $m \sim 70$ are required to keep $Q < 5 \times 10^{-3}$ for the systems near the Heisenberg point.

In Fig. 3, the distribution function of the numbers of bases classified by S_T^z: $p(S_T^z) \equiv d(S_T^z)/m$ is presented for various J_z values (for the largest 63-site block). A single peak observed in the XY region becomes broader and the width seems to diverge with approaching the Heisenberg point where the length of the total-spin S is a good quantum number. The Lieb-Mattis theorem says that the ground state of the $s=1/2$ antiferromagnetic Heisenberg model on a bipartite lattice is in the sector of $S=|N_A - N_B|/2$, where N_A (N_B) is the number of sites belonging to the A sublattice (B sublattice).[11] In the present case, the true ground state of the 63-site block possesses $S=21/2$ and it has thus $(2S+1)$-fold degeneracy concerning about S_T^z. Therefore, the flat distribution of the bases against S_T^z is thought to be a reflection of the symmetry at the Heisenberg point. On the other hand, the distribution shows a double-peak structure in the Ising re-

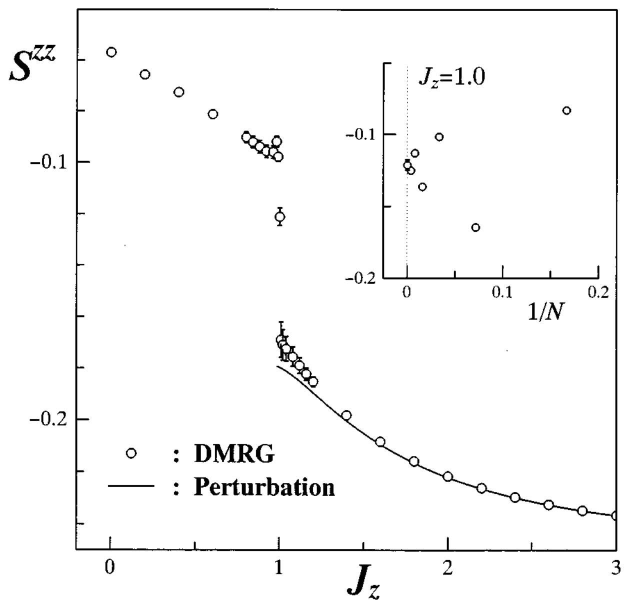

FIG. 4. The longitudinal spin correlation function $S^{zz}(J_z)$ estimated from the finite-size-system data using a least-squares-fitting procedure. The inset exhibits the system-size dependence of S^{zz} and the extrapolated data at $J_z=1$. The solid line shows the result of the perturbation expansion from the Ising limit.

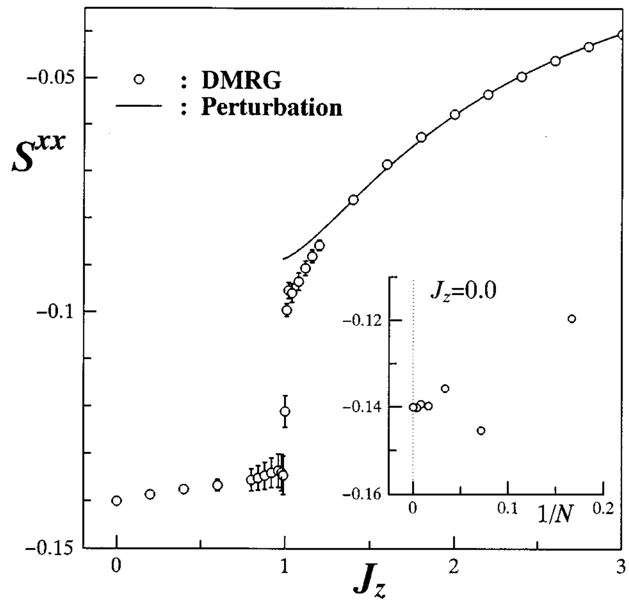

FIG. 5. The transverse spin correlation function $S^{xx}(J_z)$ estimated from the finite-size-system data using a least-squares-fitting procedure. The inset exhibits the system-size dependence of S^{xx} and the extrapolated value at $J_z=0$. The solid line shows the result of the perturbation expansion from the Ising limit.

gion; this may exhibit the formation of the Néel order because the peak positions $S_T^z=\pm 21/2$ are corresponding to the magnetizations of the twofold degenerate Néel states.

As mentioned above, we could not calculate the long-distance properties such as the Néel-order parameters and the long-range correlation functions which are the most proper quantities indicating the symmetry breaking property.[2] However, the singularity accompanied with the phase transition should be reflected in an anomalous behavior of the ground-state energy per bond $E_g(J_z)$ or its derivatives. Further, they are directly related with the measurable local spin correlation functions by the Feynman-Hellman theorem:

$$S^{xx}(J_z)\equiv\langle\Psi|S^x_{[3]}S^x_{[4]}|\Psi\rangle=\frac{1}{4}\left[E_g(J_z)-J_z\,\frac{\partial E_g(J_z)}{\partial J_z}\right], \tag{3}$$

$$S^{zz}(J_z)\equiv\langle\Psi|S^z_{[3]}S^z_{[4]}|\Psi\rangle=\frac{1}{2}\,\frac{\partial E_g(J_z)}{\partial J_z}. \tag{4}$$

Thus, some significant insights into the magnetic phase diagram may be obtained from the measurements on these quantities. In Figs. 4 and 5, we present the results on the local spin correlations. The original data exhibit the staggered dependence on the system size (as shown in the insets in these figures). We thus extrapolated these two sequences of data independently with the use of a least-squares-fitting procedure, and then by taking a weighted average of them, the infinite system size data have been evaluated. For the finite system, the Peron-Frobenius theorem guarantees that the ground state of the present system is unique and the energy level crossing does not occur in the whole parameter range.[11] However, the level crossing may occur in the thermodynamic limit. Actually, from these figures, we can recognize the phase transition at the Heisenberg point, where the symmetry of the ground state should be changed. When we define the order of the ground-state phase transition on the basis of the singularity in $E_g(J_z)$, the jump observed in these figures is naturally recognized as a sign of the first order.

In the Ising region ($J_z \gg 1$), the perturbation results on the quantum antiferromagnets have been available;[12] the expressions on the local spin correlations are given as follows:

$$S^{xx}(J_z)=-\frac{1}{8J_z}+\frac{7}{192J_z^3}+\cdots\ ,$$

$$S^{zz}(J_z)=-\frac{1}{4}+\frac{1}{8J_z^2}-\frac{7}{128J_z^4}+\cdots\ .$$

The results are drawn with the solid lines in these figures. We can see that the DMRG data agree well with the perturbation results at $J_z>1$; this coincidence indicates that the system possesses the long-range order (LRO) in the z direction, and the phase may continue just to the Heisenberg point.

Before inquiring into the data in the XY region ($J_z \ll 1$), we briefly refer to the previously obtained results on the spin-1/2 XY ferromagnets on the two-dimensional lattices. It has been conjectured that the longitudinal nearest-neighbor correlation is nearly lattice independent: $qS^{zz}(0)\sim -0.16$, -0.15, and -0.16 for the honeycomb, square and triangular lattices, respectively.[13] This sort of universal behavior may be naturally expected as a resultant of LRO. Indeed, the existence of LRO was exactly proved for the square lattice,[14] while it is difficult to draw a definite conclusion for the triangular lattice case based on the finite size data.[15] Now, our result on the XY antiferromagnet on the Bethe lattice (the sign of the coupling is irrelevant in this case) is $qS^{zz}(0) \sim -0.17$, which is considerably close to the above universal value. We thus think that the XY antiferromagnet on the Bethe lattice may have LRO in XY plain. At the same time, the above conjecture may be valid not only for two-dimensional systems, but its origin should lie in more general effects of the quantum XY model. Since no singular behavior is observed except for the Heisenberg point, the supposed ordered state may continue up to $J_z = 1$.

At this stage, we shall conjecture the magnetic phase diagram: the ground state shows LRO in the z-direction (in xy plain) for $J_z > 1$ ($0 < J_z < 1$). From the observation of the jump in $S^{zz}(J_z)$, we think that the order parameter is finite at the Heisenberg point, which changes its direction by an infinitesimal symmetry-breaking field. Seemingly, these results agree well with those for the XXZ model on the square lattice in many points: the same magnetic phase diagram has been confirmed and the order parameters were evaluated by various methods.[1–4] More directly, by employing the quantum Monte Carlo method, Barnes *et al.* have reported the discontinuous behavior of the first derivative of $E_g(J_z)$ at the Heisenberg point.[3]

In conclusion, we have investigated the ground-state phase transition of the spin-1/2 XXZ antiferromagnet on the Bethe lattice ($q = 3$). The density-matrix renormalization-group method which has been used in the studies of the one-dimensional quantum systems was extended and applied to the present higher-dimensional system. As a result, its applicability was confirmed and the following conclusions have been obtained: The model undergoes the first-order phase transition at the Heisenberg point and the system may be in the Ising-like ordered ground state (the ordered state in XY plain) for $J_{xy} < J_z$ ($J_{xy} > J_z$), which is a quite similar situation to the closely investigated XXZ antiferromagnet on the square lattice. However, we should remind the reader that the definitive conclusion on the magnetic phase diagram should be drawn with calculating the order parameters in both Ising and the XY regions, which is left as a future problem.

The applications of the DMRG method to the other quantum systems on the Bethe lattice, e.g., the Hubbard model, are also interesting; we shall report the results elsewhere. At the same time, since the idea of the DMRG method is not characteristic of one-dimensional systems, the new algorithm by which we can treat the quantum systems on the square lattice, for example, is desired.[16]

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