PHYSICAL REVIEW B VOLUME 51, NUMBER 22 1 JUNE 1995-II

Elementary excitations of $S = 1$ antiferromagnetic Heisenberg chains with bond alternation

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(Received 12 December 1994)

A world-line quantum Monte Carlo method is employed to study the elementary excitations of $S = 1$ antiferromagnetic Heisenberg chains with bond alternation described by the Hamiltonian, $\mathcal{H} = J\sum_i[1-(-1)^i\delta]\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}$. Imaginary-time correlation functions of this system at low enough temperatures exhibit almost single-exponential decay and thus the lowest excitation spectrum can be successfully extracted from them. As δ increases from 0 to 1, the system encounters a continuous phase transition at $\delta \simeq 0.25$, where the energy (E)–momentum (q) relation is fitted well to the form $E(q) = (v^2\sin^2 q+\Delta^2)^{1/2}$ with the effective light velocity $v = 2.46\pm0.08$ and the energy gap Δ which vanishes in the long chain limit. The central charge c at the massless critical point is estimated to be 1.02 ± 0.09, which suggests the universality class of the Gaussian model.

I. INTRODUCTION

The one dimensional quantum Heisenberg antiferromagnets have been a fascinating subject since the Haldane conjecture.[1] Haldane predicted that the spin-S antiferromagnetic Heisenberg chain

$$\mathcal{H} = J\sum_i \boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1} \tag{1.1}$$

is in a massive phase if S is an integer and in a massless phase if S is a half-odd integer, identifying the model (1.1) with the O(3) nonlinear σ model[2] in the large-S limit. Affleck[3] further applied this identity to the bond-alternating chain

$$\mathcal{H} = J\sum_i \left[1-(-1)^i\delta\right]\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}\,, \tag{1.2}$$

and showed that (1.2) is in the massless critical phase only in the case where the topological angle of the model, $\theta \equiv 2\pi S(1-\delta)$, is equal to $(2k+1)\pi$ with an integer k. According to his argument, as δ increases from -1 to 1, the system (1.2) encounters $2S$ massless points (here, let us call it the Affleck-Haldane conjecture). The $S = 1/2$ system, which exhibits a massless excitation spectrum[4] at the Heisenberg point and is widely believed to be spontaneously dimerized,[5–12] coincides with the Affleck-Haldane conjecture not only qualitatively but also quantitatively. For $S = 1$, on the other hand, various numerical approaches, such as exact diagonalization methods,[13–15] a sequence transformation method,[16] quantum Monte Carlo methods,[17–21] a quantum transfer-matrix method,[22] and a renormalization-group method,[23] have revealed that there exists an energy gap between the ground state and the first excited state at the pure Heisenberg point. However, studies on the dimerized chain (1.2) seem to be still in their earlier stage. With a series expansion technique, Singh and Gelfand[24] detected a continuous phase transition from the Haldane phase to the dimer phase for the model (1.2). They estimated the transition point δ_c to be 0.25 ± 0.03, which, as expected, deviates from the expression in the large-S limit, $\delta_c = 1-1/2S$. Their estimate has recently been reconfirmed by a density-matrix renormalization-group method[25] and a quantum Monte Carlo method.[26] Kato and Tanaka[25] gave a more precise estimate of the critical point, $\delta_c = 0.25\pm0.01$, demonstrating that the system is massless at $\delta = \delta_c$. On the other hand, the present author[26] visualized the ground-state spin correlation as a function of δ and confirmed collapse of the chain-end states with an $S = 1/2$ effective moment[27,28] for $\delta \geq \delta_c$.

Now we have a reliable estimate of δ_c itself for $S = 1$. Under such circumstances, we take further interest in the ground-state properties and the excitation spectrum of the system around the critical point. As for the ground-state properties, such as the spin correlation, the chain-end states and the hidden antiferromagnetic order,[29] we present them elsewhere.[26,30] We here study the elementary excitations. Low-lying excitations of the the non-alternating $S = 1$ chains have already been vigorously studied.[20,31–39] In particular, Takahashi[20] succeeded with a Monte Carlo technique in obtaining the lowest energy with arbitrary momentum q and made a prediction that the low-momentum ($q \simeq 0$) excited state is a scattering state of two excitations with momenta near π. This picture of low-lying excitations was supported by a quantitative approach[32,33,36] and qualitative discussions,[23,40] and is now widely accepted. In the trivial case with perfect dimerization $\delta = 1$, on the other hand, all the excitation bands are dispersionless and no excited state is a scattering state of the elementary excitations. Thus we calculate the lowest energies as a function of q in the region $0 < \delta < 1$ including the fascinating point $\delta = \delta_c$.

The criticality at $\delta = \delta_c$ is also an interesting subject. Singh and Gelfand[24] found in their series-expansion study on the bilinear biquadratic Hamiltonian

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$$\mathcal{H} = J\sum_i \left[1-(-1)^i\delta\right]\left[(\boldsymbol{S}_i,\boldsymbol{S}_{i+1})_\lambda - \beta(\boldsymbol{S}_i,\boldsymbol{S}_{i+1})_\lambda^2\right] , \tag{1.3}$$

where

$$(\boldsymbol{A},\boldsymbol{B})_\lambda = \lambda(A^xB^x + A^yB^y) + A^zB^z , \tag{1.4}$$

that the transition point $\delta = \delta_c$ of the model (1.2) is a multicritical point in the δ-λ plane at $\beta = 0$ of the model (1.3), where the so-called Haldane, dimer, Ising, and XY phases meet. Although they discussed in detail the criticality of the phase boundaries, no definite conclusion was obtained in the vicinity of the multicritical point due to the ill behavior of the series. A recent numerical study[25] has estimated the conformal anomaly parameter c (the central charge in the Virasoro algebra[41]) at the critical point to be 1.0 ± 0.15. In this article, we independently give an estimate of c at the critical point with the effective light velocity directly obtained from the excitation spectrum.

Here we employ a world-line quantum Monte Carlo approach[39] which has been successfully applied to a study of the dispersion relation of an $S = 1$ quantum spin chain. In Sec. II, this method is explained and its reliability is confirmed. Results are presented in Sec. III. Section IV is devoted to summary and discussion.

II. METHOD

We treat the $S = 1$ bond-alternating Hamiltonian (1.2) with the periodic boundary condition. Because of the translational symmetry, there is a translation operator $\mathcal{T}$ satisfying

$$[\mathcal{H},\mathcal{T}] = 0 , \quad \mathcal{T}^N = \mathcal{I} , \tag{2.1}$$

where $\mathcal{I}$ is the identity operator and N is the length of the system scaled by that of the unit cell. Therefore $\mathcal{H}$ and $\mathcal{T}$ have coeigenvectors classified by the momentum k:

$$\mathcal{H}\,|l;k\rangle = E_l(k)\,|l;k\rangle , \tag{2.2}$$

$$\mathcal{T}\,|l;k\rangle = e^{ik}\,|l;k\rangle , \tag{2.3}$$

where $|l;k\rangle$ and $E_l(k)$ are the l-th eigenvector and eigenvalue in the k momentum space and

$$\begin{aligned} &E_1(k) \le E_2(k) \le \cdots , \\ &k = \frac{2\pi m}{La} , \; m = -\frac{N}{2}+1, -\frac{N}{2}+2, \ldots, \frac{N}{2} , \end{aligned} \tag{2.4}$$

where L is the length of the system scaled by the lattice constant a.

Let us define an imaginary-time correlation function $S(q,\tau)$ as

$$S(q,\tau) = \langle e^{\mathcal{H}\tau}O_q e^{-\mathcal{H}\tau}O_{-q}\rangle_{MC} , \tag{2.5}$$

where

$$O_q = \frac{1}{N}\sum_{j=1}^{N} O_j e^{iqj} \tag{2.6}$$

with an arbitrary local operator O_j and $\langle\cdots\rangle_{MC}$ denotes a Monte Carlo average of the quantity at a given temperature T. We here take for O_j an S_j^z-linear operator, which commutes with the Hamiltonian. In world-line quantum Monte Carlo simulations,[42] the imaginary time τ takes a finite set of evenly spaced values between 0 and $\beta/2$, where $\beta = (k_BT)^{-1}$ with the Boltzmann constant k_B. $S(q,\tau)$ is evaluated by calculating O_q at two Trotter layers separated by $(n/\beta)\tau$, where n is the Trotter number used. The dynamical structure factor $S(q,\omega)$, which is related to $S(q,\tau)$ via

$$S(q,\tau) = \int_0^\infty S(q,\omega)e^{-\omega\tau}d\omega , \tag{2.7}$$

is, in principle, obtained by continuing $S(q,\tau)$ to real frequencies. Although the analytic continuation is generally unfeasible, there is a recent proposition[43] to overcome the difficulty which has been successfully applied to several quantum systems.[44,45] This fascinating approach, which is a combination of world-line quantum Monte Carlo and maximum-entropy[46] methods, is also powerful for Haldane systems and in fact gave a fine explanation[44] of a neutron scattering experiment[47] for $\mathrm{Ni(C_2H_8N_2)_2NO_2ClO_4}$.[48]

However, we here consider another treatment for $S(q,\tau)$. We can represent $S(q,\tau)$ in terms of the complete vector set $|l;k\rangle$ as

$$S(q,\tau) = \frac{\sum_{l,k}\langle l;k|e^{-\beta\mathcal{H}}e^{\mathcal{H}\tau}O_q e^{-\mathcal{H}\tau}O_{-q}|l;k\rangle}{\sum_{l,k}\langle l;k|e^{-\beta\mathcal{H}}|l;k\rangle} . \tag{2.8}$$

Noting that

$$\mathcal{T}O_q|l;k\rangle = e^{i(k-q)}O_q|l;k\rangle , \tag{2.9}$$

we obtain the following expression:

$$S(q,\tau) = \frac{\sum_{l,l',k} e^{-\beta E_l(k)}|\langle l;k|O_q|l';k+q\rangle|^2 e^{-\tau[E_{l'}(k+q)-E_l(k)]}}{\sum_{l,k} e^{-\beta E_l(k)}} . \tag{2.10}$$

Therefore we expect that $S(q,\tau)$ is approximately evaluated as

$$S(q,\tau) = \sum_l |\langle \mathrm{GS}|O_q|l;q\rangle|^2 e^{-\tau[E_l(q)-E_G]}, \qquad (2.11)$$

at low enough temperatures, where $|\mathrm{GS}\rangle \equiv |1;0\rangle$ and $E_G \equiv E_1(0)$ are the ground state and the ground-state energy. We here note that the matrix elements $\langle \mathrm{GS}|O_q|l;q\rangle$ do not depend on temperature but are definitely determined once the model Hamiltonian is given. Equation (2.11) suggests that the lowest energies as a function of q can be straightforwardly extracted from the large-τ $S(q,\tau)$ data. When the lowest-energy states are the lower edge of the continuum, $S(q,\omega)$ for them is generally expected to take the largest values. However, this is not the case when the lowest-energy states form an isolated band separated from the continuum above it, as is seen in the present $S=1$ Haldane system. White and Huse[23] illustrated the spectrum of low-lying states for the $S=1$ chain and proposed that the isolated lowest magnon band disappears into the two magnon continuum near momentum 0.3π. Recently, Takahashi[38] has confirmed this picture by calculating $S(q,\omega)$ as a series of δ-function peaks. According to his result, any ratio of $|\langle \mathrm{GS}|S^z_q|l;q\rangle|^2_{l\geq 2}$ to $|\langle \mathrm{GS}|S^z_q|l;q\rangle|^2_{l=1}$ in the region $q \gtrsim 0.3\pi$ is not larger than 0.015. Thus, with a straightforward procedure, we could extract the elementary excitation spectrum from Monte Carlo data of $S(q,\tau)$ at a sufficiently low temperature.

We demonstrate in the following our method in the case that $\delta = 0$, where the present result can be compared with the previous ones.[20,34,38] Here the operator O_j is necessarily defined as S^z_j. The chain length L, which is equal to N in this case, and the Trotter number n are set equal to 32 and 200, respectively. We have used such a large Trotter number as to guarantee enough acceptance ratio for the Monte Carlo flips and as to observe the large-τ decay of $S(q,\tau)$. We have calculated $S(q,\tau)$ in the subspace with $\sum_i S^z_i = 0$ at $(\beta J)^{-1} = 0.02$ and 0.04, and have confirmed that quantitatively almost the same data are obtained at the two temperatures. Hence we take these temperatures to be low enough to justify the approximation (2.11). In Fig. 1(a) and Fig. 1(b), we plot $S(q,\tau)$ versus τ at various values of q in natural and logarithmic scales, respectively. $S(q,\tau)$ shows, with fine accuracy, single-exponential decay except in the small-τ region where there are small but non-negligible contributions of the higher-lying states. Therefore $-\partial \ln[S(q,\tau)]/\partial\tau$ evaluated at the tail of decay is expected to give the lowest excitation energy as a function of q, $E_1(q) - E_G$, with good accuracy. We show in Fig. 2 the elementary excitation spectrum thus obtained (•) with the previous result[20] (○) obtained by the projector Monte Carlo method, where the lattice constant a which is now equal to the length of the unit cell is set equal to unity. The present data are in good agreement with the previous result within the numerical errors which mainly come from ambiguity in estimating the slopes in Fig. 1(b), rather than the inaccuracy of the Monte Carlo data themselves. In the small-q region, relevant contributions of the second excited states[38] seem to bring about the small uncertainty in our data.

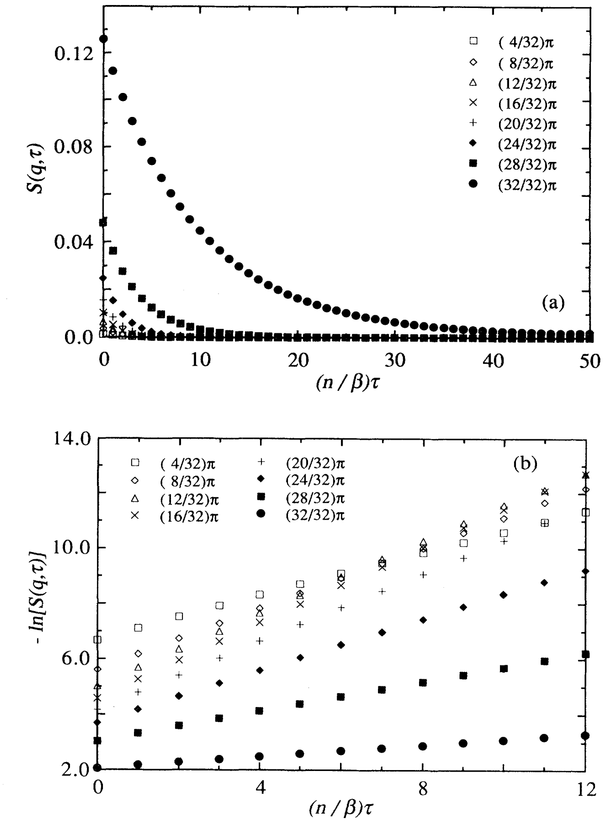

FIG. 1. Bare (a) and logarithmic (b) plots of $S(q,\tau)$ versus τ at various values of q for the $L=32$ chain, where $\delta = 0$, $(\beta J)^{-1} = 0.02$, and $n = 200$. Here the values of qa are given with the corresponding symbols.

Now let us consider the $\delta \neq 0$ cases, where $L = 2N$ and the first Brillouin zone is reduced to the range $-\pi/2a < k \leq \pi/2a$. Due to the dimerization of the system, two in-

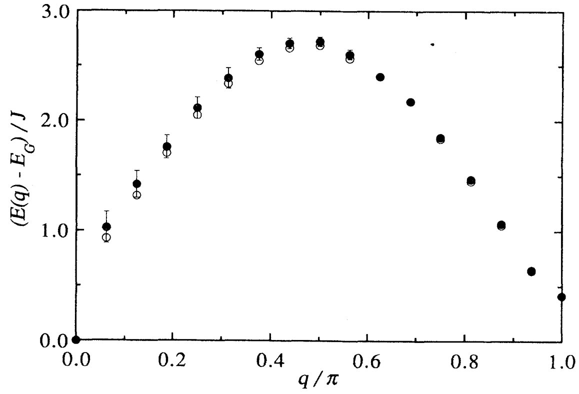

FIG. 2. Elementary excitations of the ground state as a function of q in the subspace with $\sum_i S^z_i = 0$, where $L = 32$ and $\delta = 0$. The present result is indicated by •, while ○ represents the previous result obtained by Takahasi with the projector Monte Carlo method.

dependent operators can be taken for O_j. We here define them as $S^z_{2j-1} \pm S^z_{2j}$. In both the cases, we have calculated $S(q,\tau)$ in the subspace with $\sum_i S^z_i = 0$ for $L = 32$ and 64, $n = 200$, $(\beta J)^{-1} = 0.02$, and $0.10 \leq \delta \leq 0.80$. The system with L sites has the smallest energy gaps at the transition point that vanishes in the $L \to \infty$ limit with L^{-1}-linear dependence.[25] Since the gaps at the transition point for $L = 32$ and 64 are about $0.19J$ and $0.09J$ (Sec. III), respectively, the present temperature $(\beta J)^{-1} = 0.02$ is considered low enough to study the elementary excitations. In order to evaluate $S(q,\tau)$, we have carried out 6×10^5 Monte Carlo steps at each value of δ, where the first 5×10^4 steps were discarded as the initial transient stage. $S(q,\tau)$ was averaged over all the Trotter layers so that the numerical error is held to a minimum. Due to the huge Trotter number, the CPU time needed for each calculation (in the case that $L = 32$) at a fixed value of δ amounted to several hours with the supercomputer and several days with the workstations. The numerical precision in the final results (the dispersion relations) is about two digits, where the ambiguity mainly comes from the estimation of $-\partial \ln[S(q,\tau)]/\partial\tau$. The results obtained are presented in the next section. We set the lattice constant a equal to unity and use the reduced zone scheme in the following.

III. RESULTS

We show in Fig. 3 excitation energies as a function of q of the $L = 32$ chain obtained from $S(q,\tau)$'s with $O_j = S^z_{2j-1} + S^z_{2j}$ (○) and $O_j = S^z_{2j-1} - S^z_{2j}$ (×) cal-

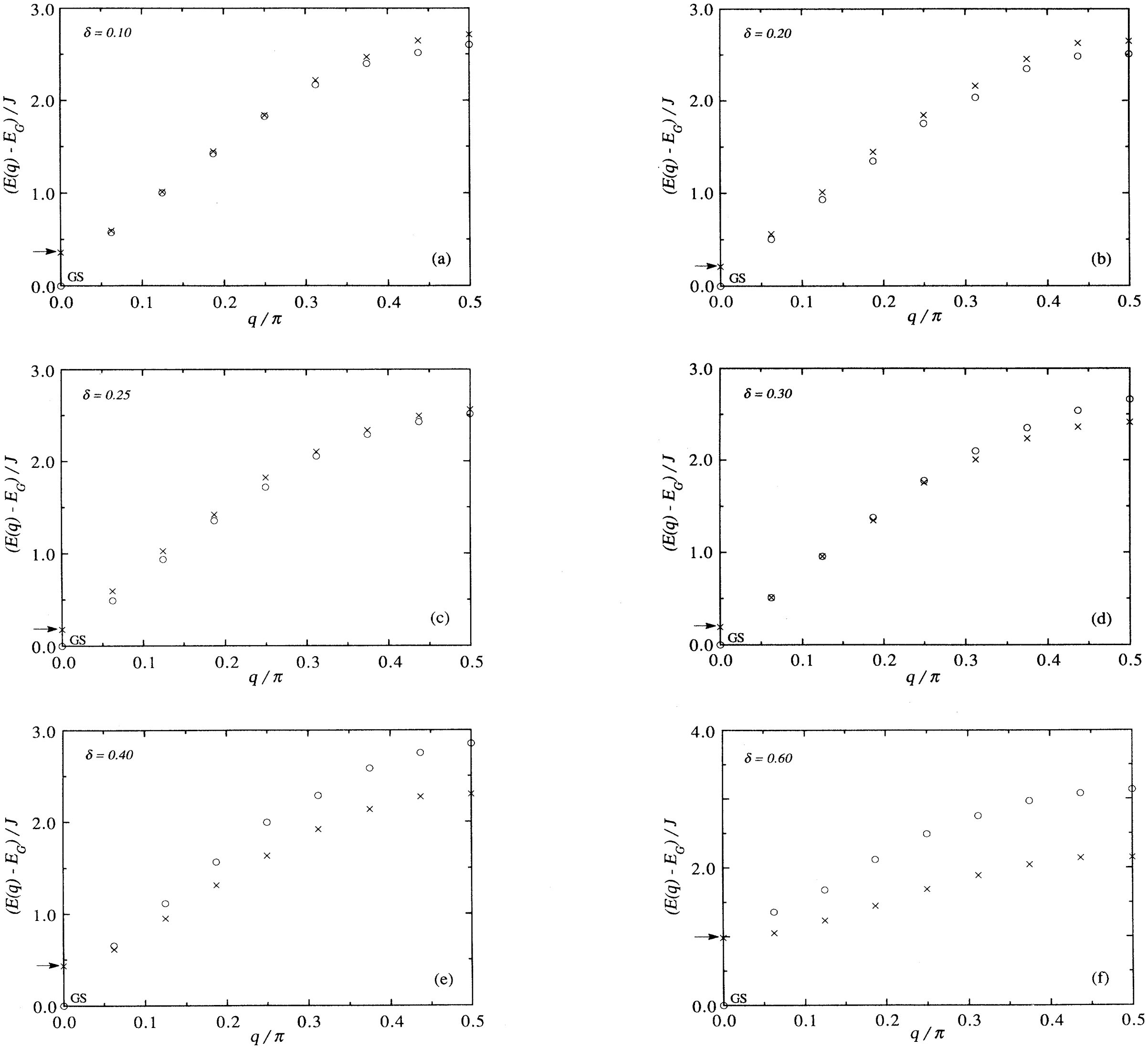

FIG. 3. Excitation energies as a function of q of the $L = 32$ chain obtained from $S(q,\tau)$'s with $O_j = S^z_{2j-1} + S^z_{2j}$ (○) and $O_j = S^z_{2j-1} - S^z_{2j}$ (×) calculated in the subspace with $\sum_i S^z_i = 0$, at $\delta = 0.10$ (a), 0.20 (b), 0.25 (c), 0.30 (d), 0.40 (e), and 0.60 (f). Here GS denotes the ground state and the arrow indicates the gap between the ground state and the first excited state independently obtained by estimating the lowest energies in the subspaces with $\sum_i S^z_i = 0$ and 1.

culated in the subspace with $\sum_i S_i^z = 0$. When dimerization is introduced, the states with wave vectors q and $\pi - q$ are coupled with each other and split into bonding and antibonding states. We find that for $\delta < 0.25$ (the Haldane phase) the scattering matrices $O_j = S_{2j-1}^z + S_{2j}^z$ and $O_j = S_{2j-1}^z - S_{2j}^z$ extract energy eigenvalues of the bonding and antibonding states, respectively, and vice versa for $\delta > 0.25$ (the dimer phase). This fact can be a consequence of level crossing at the transition point $\delta = 0.25$. It has in fact been reported[25] that the low-lying level structures for $\delta < 0.25$ and $\delta > 0.25$ are different. The first excited state is now located at $q = 0$ (the zone center). We have independently calculated the energy gaps between the ground state and the first excited state by estimating the lowest energies in the subspaces with $\sum_i S_i^z = 0$ and 1 and have shown them by arrows in Fig. 3. The two independent estimates coincide well. In the Haldane-phase region, the overall dispersion curve almost remains unchanged although it shifts downward with increase of δ. Therefore, even with bond alternation, the low-lying excitations may be considered the scattering states of the domain walls[20] in the hidden antiferromagnetic ordering[29] which exists as long as the system is in the Haldane phase.[30] In the dimer-phase region, on the other hand, the elementary excitations are roughly described by a triplet pair in the disordered state composed of local singlet pairs. Since the formation energy of a localized triplet pair on the strongly coupled bond is $(1+\delta)J$, the triplet pair is stabilized by its delocalization in the vicinity of the zone center, while it is less stable in the vicinity of the zone boundaries. The upper bands in Figs. 3 (d)–3(f) can be attributed to the scattering states of the two triplet pairs, rather than a quintuplet pair as the elementary excitation, due to the relatively large formation energy of the quintuplet pair and the symmetry property of the operator $O_j = S_{2j-1}^z + S_{2j}^z$. This simple picture of low-lying excitations may be valid so long as δ is not so large. In the trivial case with $\delta = 1.0$, the excitations are completely dispersionless and their energies are simply multiples of $2J$, where the formation energies of the triplet and quintuplet pairs are given by $2J$ and $6J$, respectively.

In Fig. 4(a) we show the δ dependence of the elementary excitations as a function of q for $L = 32$. There is a momentum around $q = 0.3\pi$ where the δ dependence of the elementary excitations is very weak. For $\delta > 0.25$, the δ dependence of the elementary excitations with a fixed momentum is monotonic except in the vicinity of $q = 0.3\pi$. Let us focus our attention on the energy gap between the ground state and the first excited state which is found at $q = 0$. The gap takes a minimum value at $\delta = 0.25$, which is consistent with the continuous phase transition at $\delta = 0.25$.[24–26] Kato and Tanaka[25] have demonstrated, with excellent numerical accuracy, that the gap vanishes in the $L \to \infty$ limit at the critical point. We have also confirmed that the size dependences of the gap at $\delta \neq 0$ are fitted well to the form L^{-2}, while at $\delta = 0.25$ the gap goes to zero with slower convergence, that is, the L^{-1}-linear dependence which is predicted by the finite-size scaling[49,50] based on the conformal field theory.[51]

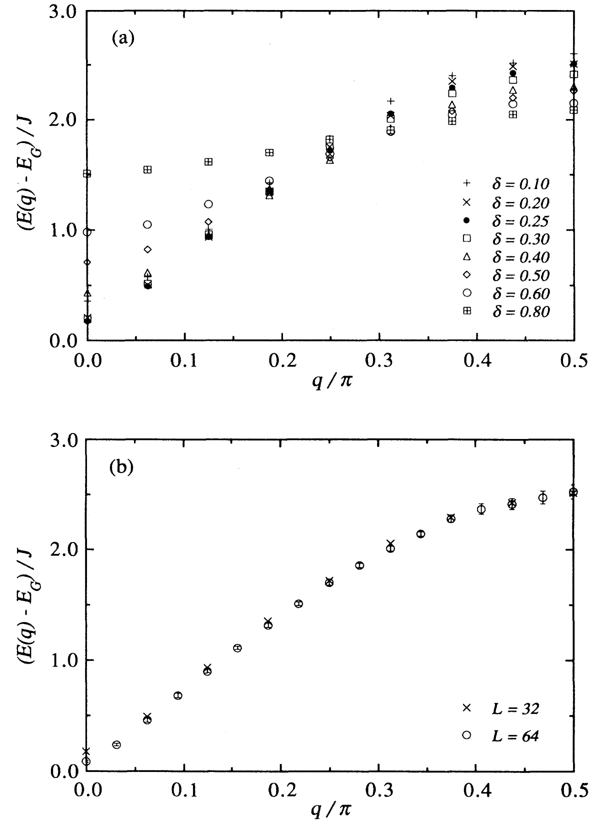

FIG. 4. (a) Elementary excitations of the ground state as a function of q at various values of δ for the $L = 32$ chain. (b) Elementary excitations of the ground state as a function of q at the critical point $\delta = 0.25$ for the $L = 32$ ($\times$) and $L = 64$ ($\circ$) chains, where the attached error bars are ones for the $L = 64$ result.

We show in Fig. 4(b) the elementary excitations as a function of q at $\delta = 0.25$ for $L = 32$ ($\times$) and $L = 64$ ($\circ$). The overall q dependences of the excitations of the two chains are quantitatively almost the same except for the energy gap at $q = 0$ and thus can be considered to describe well the property in the thermodynamic limit. Both the curves are fitted well to the form $(v^2 \sin^2 q + \Delta^2)^{1/2}$, where v is the effective light velocity of the system and Δ is the energy gap between the ground state and the first excited state which goes to zero in the thermodynamic limit. Here v is estimated to be 2.47 ± 0.06 for $L = 32$ and 2.46 ± 0.08 for $L = 64$. Taking account of the divergence of the correlation length at the critical point, we expect Δ of the finite periodic chain with L sites to be roughly evaluated by

$$\Delta = \frac{v}{\xi} \simeq \frac{2v}{L} . \tag{3.1}$$

This phenomenological relation gives, with the above-estimated values of v, $\Delta = 0.15$ for $L = 32$ and $\Delta = 0.08$ for $L = 64$, which are in fairly good agreement with the numerical observations shown in Fig. 4(b).

Finally in this section, let us evaluate the conformal anomaly at the critical point. Conformal invariance of

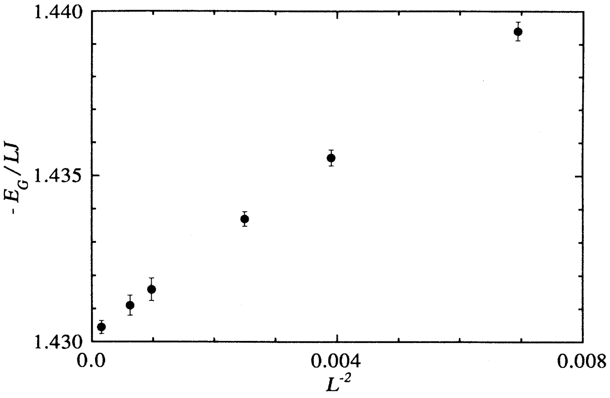

FIG. 5. Chain-length dependence of the ground-state energy of the periodic chain at the critical point $\delta = 0.25$.

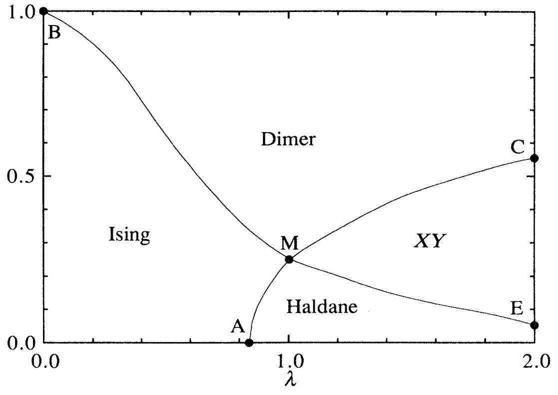

FIG. 6. A ground-state phase diagram of the bilinear biquadratic Hamiltonian (1.3) obtained by Singh and Gelfand with a series-expansion method.

the system gives the finite-size scaling form[49,50] of the ground-state energy of the periodic chain as

$$\frac{E_G}{L} = \varepsilon - \frac{\pi c v}{6L^2}, \qquad (3.2)$$

where ε is the ground-state energy density in the bulk and c is the central charge, which may be used to label different universality classes.[52,53] Equation (3.2) relates the finite-size correction to the ground-state energy to the conformal anomaly parameter. In Fig. 5 we plot Monte Carlo estimates of the ground-state energies of the periodic chains versus chain length at the critical point $\delta = 0.25$. We find that the scaling form (3.2) holds with good accuracy in Fig. 5. The central charge c is estimated to be 1.02 ± 0.08 for $L = 32$ and 1.02 ± 0.09 for $L = 64$, which are consistent with the previous result 1.0 ± 0.15.[25]

IV. SUMMARY AND DISCUSSION

We have made clear the elementary excitations of the $S = 1$ antiferromagnetic Heisenberg chains with bond alternation. The continuous phase transition at $\delta = 0.25$ (Refs. 24–26) was reconfirmed, where the energy gap takes a minimum value. The critical excitation spectrum is fitted well to the form $(v^2 \sin^2 q + \Delta^2)^{1/2}$ with $v = 2.46 \pm 0.08$ and Δ which vanishes in the long-chain limit. In the dimer-phase region $\delta > 0.25$, the elementary excitations monotonically move toward the trivial flat band with the excitation energy $2J$.

The criticality at the transition point is in the universality class with the central charge $c = 1$, that is, in the universality class of the Gaussian fixed line.[54] As mentioned in Sec. I, the transition point which appears in the present study is a multicritical point[24] of the extended system described by the Hamiltonian (1.3). The phase diagram in the δ-λ plane at $\beta = 0$ obtained by Singh and Gelfand[24] with a series-expansion method is shown in Fig. 6, where the point M is the $\delta = 0.25$ transition point of the present model. According to their study, the criticality all along the line AMB, except possibly in the vicinity of the point M, is in the universality class of the two dimensional Ising model ($c = 1/2$). They also suggested that the critical line MC is XY-like ($c = 1$). Unfortunately they gave no definite conclusion in the vicinity of the point M and along the line ME due to the ill behavior of the series. Now here is the complementary and fascinating result that the critical point M is described in terms of a conformally invariant field theory with $c = 1$. All the results we have suggest a possibility that the critical point M may be equivalent to the free fermion point[55] of the critical Ashkin-Teller model,[54,56,57] where the model degenerates into two uncoupled copies of the critical Ising model. We hope that the present study will motivate, from the above point of view, further studies on the critical exponents along the line EMC.

The present method may be generally applied to a wide range of low-dimensional quantum systems although their quantum mechanical properties control numerical accuracy in the final results. It is expected that the present method with the advantage of applicability to large systems and the diagonalization method[38] which has successfully been applied to $S = 1$ quantum spin chains will cooperatively contribute to understanding of the low-lying excitation mechanisms of various systems.

ACKNOWLEDGMENTS

The author would like to express his special thanks to Professor H. Akai and Professor K. Higashijima for helpful discussions and suggestions. The author is also grateful to Professor S. Miyashita, Professor M. Takahashi, and Dr. Y. Kato for valuable discussions. Numerical calculations were performed on FACOM VP2600/10 at the Supercomputer Center of Kyoto University, and on DEC 3000/600 AXP and HP-UX 9000/730 at Osaka University. The present work is supported in part by a Grant-in-Aid for Encouraged Researches (06740289) from the Ministry of Education, Science and Culture.

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