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Cluster-effective-field approximations in frustrated quantum spin systems: CAM analysis of Néel-dimer transition in the $S = \frac{1}{2}$ frustrated XXZ chain at the ground state

Yoshihiko Nonomura and Masuo Suzuki
Department of Physics, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan

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Abstract. How to impose boundary conditions is crucial to finite-cluster calculations of quantum spin systems, but only open-boundary clusters have been used in cluster-effective-field approximations up to now. In the present paper, periodic-boundary clusters are also considered for the formulation of cluster-effective-field approximations in frustrated quantum spin systems. Namely, the open-boundary-condition double-cluster approximation (OBC-DCA) and the periodic-boundary-condition double-cluster approximation (PBC-DCA) are applied to the one-dimensional $S = \frac{1}{2}$ frustrated XXZ model at the ground state. These two approximations are compared using the coherent-anomaly method (CAM). Within the limitation of cluster sizes in exact-diagonalization calculations, the PBC-DCA can reproduce the true phase boundary of the Néel-dimer transition. On the other hand, the OBC-DCA severely underestimates the existence of magnetic orders as quantum fluctuation is increased. These findings suggest that previous cluster-effective-field studies based on open-boundary clusters should be reconsidered.

1. Introduction

Recently two-dimensional frustrated quantum spin systems have been intensively studied. Especially, the following J_1–J_2 model on a square lattice,

$$\mathcal{H} = J_1 \sum_{\text{n.n.}} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\text{n.n.n.}} \boldsymbol{S}_k \cdot \boldsymbol{S}_l \qquad S = \tfrac{1}{2} \tag{1.1}$$

has attracted many authors, because its ground-state properties seem to be closely related to the mechanism of high-temperature superconductivity. The Néel order (figure 1(a)) exists for $J_1 \gg J_2$ [1], and the collinear order (figure 1(b)), a special case of the classical four-sublattice Néel order, is stabilized for $J_1 \ll J_2$ [2]. The main interest here is to study whether these classical magnetic orders survive against quantum fluctuations in the vicinity of the classical frustration point, $J_2 = 0.5J_1$. Although numerous studies [3–11] have already been made, a definite conclusion has not yet been obtained. For example, an exact-diagonalization study up to the 6×6 cluster [8] claims that there is no magnetic long-range order between $J_2 \approx 0.4J_1$ and $J_2 \approx 0.65J_1$. On the other hand, a very recent quantum Monte Carlo simulation up to the 8×8 cluster [9] suggests that the Néel order survives at least up to the vicinity of $J_2 = 0.5J_1$. Such large differences originate from a slight variance of the extrapolation scheme of finite-cluster data, which means that this problem is still very subtle.

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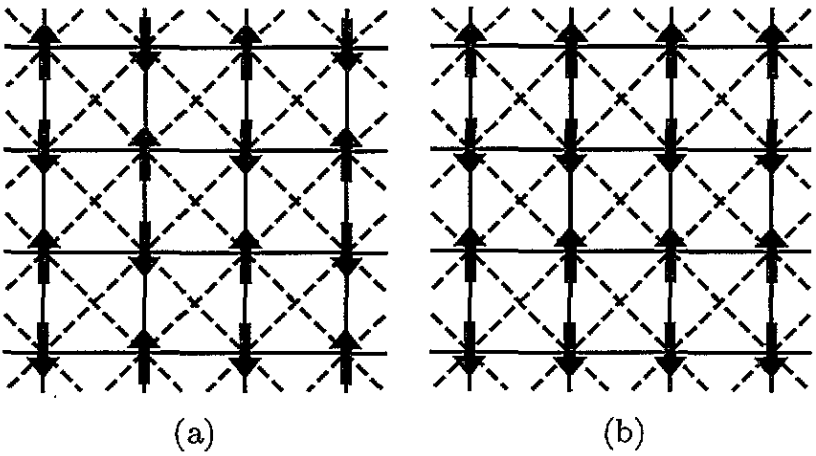

Figure 1. Classical long-range orders in the J_1–J_2 model: (a) the Néel order, (b) the collinear order.

The cluster-effective-field approximation can be a powerful tool in such a difficult situation, because it usually gives an upper limit of the critical point. An approximation has already been proposed by Gelfand *et al* [10] in order to enforce their series-expansion results [10, 11]. They calculated up to an 18-spin cluster in the open-boundary conditions, and concluded that the classical magnetic orders are destroyed between $J_2 \approx 0.4J_1$ and $J_2 \approx 0.65J_1$, which is also consistent with the result in [7]. However, as was pointed out by the present authors [12], the results obtained from cluster-effective-field approximations are sensitive to boundary conditions in quantum antiferromagnets. Therefore, when we apply these approximations to an unknown problem, such as the J_1–J_2 model, we should first confirm the validity of the approximations in a well known model. Such a test study is the main purpose of the present paper.

Here we consider the simplest model with quantum frustration—the *one-dimensional* $S = \frac{1}{2}$ XXZ model with a next-nearest-neighbour interaction. Two kinds of approximations are applied to this model. One is the one-dimensional version of the approximation of Gelfand *et al* and the other is a new type of approximation using *periodic-boundary* clusters. As a criterion of a 'good' approximation, not only qualitative plausibility but also quantitative correctness are required: a suitable approximation should reproduce the true phase diagram when it is combined with the coherent-anomaly method (CAM) [13, 14]. In section 2, ground-state properties of the present model and its coherent anomaly are briefly reviewed. In section 3, some basic features of the double-cluster approximation (DCA) [15, 16] are summarized at first, and two different formulations of the DCA are shown explicitly, using open- and periodic-boundary clusters. In section 4, numerical results based on the two approximations are given, and they are compared using CAM. The Néel-dimer phase boundary is evaluated, and the origin of differences between the results obtained by these two approximations are discussed on the basis of the behaviour of correlation functions in finite clusters. The estimation of the critical exponent γ is also mentioned here. In section 5, these descriptions are summarized and a conclusion of the present study is given.

2. The model and its coherent anomaly

In order to find a suitable cluster-effective-field approximation for frustrated quantum spin systems and to test its validity, we consider here ground-state properties of the following antiferromagnetic one-dimensional model,

$$\mathcal{H} = \sum_i [J_{xy}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_z S_i^z S_{i+1}^z] + g \sum_i [J_{xy}(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y) + J_z S_i^z S_{i+2}^z] - H_{st} \sum_i (-1)^{i-1} S_i^z \qquad S = \tfrac{1}{2} . \tag{2.1}$$

This model has already been solved exactly at $g = 0$ [17] and at $g = \frac{1}{2}$ [18]. Especially, at the latter point, its ground state is perfectly dimerized. Since the motivation of the present study is the magnetic orders in the J_1–J_2 model, here we only consider the Ising region ($J_{xy} \leqslant J_z$). In this region, the ground state of the present model has the Néel order at $g = 0$ [17] and there occurs a second-order phase transition between the Néel phase and the dimer phase at a certain critical point g_c^*, as the frustration parameter g is varied from 0 to $\frac{1}{2}$. One reason why we utilize this model in the present paper is that its ground-state properties have already been very well studied [19–22], since it is the simplest frustrated quantum spin system. Another is that quantum fluctuation is strongest in one-dimensional systems. Therefore, an approximation which gives a satisfactory result even in this model is expected to be suitable for application to two-dimensional systems, such as the J_1–J_2 model.

Recently Tonegawa, Harada and Kaburagi estimated [21] a phase diagram of its ground state using the phenomenological renormalization-group and finite-size scaling methods [23], and Nomura and Okamoto showed [22] another phase diagram on the basis of a mapping onto the quantum sine-Gordon model [19] and using a level-crossing behaviour of low-energy excitations. These two results coincide quantitatively with one another in the Ising region. Their phase diagram will be shown later, together with the present results (figures 5 and 7).

Now we turn to a review of the coherent-anomaly method (CAM) [13, 14]. In the present paper, cluster-effective-field approximations are formulated on the ground that the staggered magnetization is regarded as the order parameter. Namely, in the present formulation the Néel phase corresponds to the 'ordered phase', and the dimer phase corresponds to the 'disordered phase'. Then the zero-field staggered susceptibility

$$\chi_{st} \equiv \frac{1}{N} \sum_{i=1}^{N} (-1)^{i-1} \left. \frac{\partial}{\partial H_{st}} \langle S_i^z \rangle_g \right|_{H_{st}=0} \tag{2.2}$$

shows the following classical singularity

$$\chi_{st} \sim \bar{\chi} \left| \frac{g_c}{g - g_c} \right| \qquad \text{and} \qquad \bar{\chi} \equiv \frac{1}{g_c} \left. \frac{d\chi_{st}}{dg} \right|_{g=g_c} \tag{2.3}$$

in the vicinity of its approximate critical point g_c. If we consider a suitable series of approximations (for example, the series obtained by gradual enlargement of clusters), the critical coefficient $\bar{\chi}$ is expected to be scaled [13] as

$$\bar{\chi} \sim \text{const.} \times \left| \frac{g_c^*}{g_c - g_c^*} \right|^{\gamma - 1} \qquad \text{for} \qquad g_c \to g_c^* \tag{2.4}$$

and both the true critical point g_c^* and the true critical exponent γ can be estimated.

3. Formulation of cluster-effective-field approximations

Recently a new class of cluster-effective-field approximations, namely the double-cluster approximation (DCA) [15, 16], was found in the context of the application of the CAM. This approximation is a natural extension of the constant-coupling approximation [24], and it shows a good scaling behaviour [16] when combined with CAM. Namely, the approximate critical points rapidly converge to the true one, and the critical coefficients are scaled by formula (2.4) without any serious size-dependent correction. In the present paper, we consider two kinds of approximations, both of which are based on the DCA.

3.1. Basic aspects of the DCA

Before actual formulations of the DCA in the present model, some basic features of this approximation [16] are reviewed here for later convenience. In DCA, two different clusters A and B (here $N_A < N_B$ is assumed) are utilized, and the same effective field $H_{\rm eff}$ is applied to their boundary spins. The effective Hamiltonian of an N_I-spin cluster ($I = A$ or B) is given by

$$\mathcal{H}_{N_I}^{\rm eff} = \mathcal{H}_{N_I}^{\rm cl} - \sum_{j\in\text{boundary}} \epsilon_j S_j^z \tag{3.1}$$

where $\mathcal{H}_{N_I}^{\rm cl}$ represents the cluster Hamiltonian and ϵ_j denotes the weight (including signs) of effective fields on the boundary spins. The consistency condition is required as

$$\langle S_0^z\rangle_{\rm g}^A = \langle S_0^z\rangle_{\rm g}^B \tag{3.2}$$

where $\langle\cdots\rangle_{\rm g}^I$ stands for the ground-state average in the cluster I, and S_0^z represents the characteristic spin of each cluster, for example, the central one. The approximate critical point $g_{\rm c}$ is obtained from the linear response of the condition (3.2) for the effective field, namely

$$\mathcal{F}_A(g) = \mathcal{F}_B(g) \quad \text{and} \quad \mathcal{F}_I(g) \equiv \sum_{j\in\text{boundary}} \epsilon_j \langle S_0^z; S_j^z\rangle_{\rm g}^I \tag{3.3}$$

where $\mathcal{F}_I(g)$ is called the 'feedback function', and $\langle A; B\rangle_{\rm g}^I$ denotes the 'ground-state canonical correlation function' [14] in the cluster I defined by

$$\langle A; B\rangle_{\rm g} \equiv \sum_{n\neq g} \langle g|A|n\rangle\langle n|B|g\rangle \frac{2}{E_n - E_g} \,. \tag{3.4}$$

We start from the following scaling form of correlation functions of $(1+1)$-dimensional systems in the the disordered phase:

$$\langle S_0^z; S_r^z\rangle_{\rm g} \sim \frac{e^{-r/\xi}}{r^{\eta-1}} \,. \tag{3.5}$$

Note that this scaling form differs slightly from the conventional one,

$$\langle S_0^z S_r^z\rangle_{\rm g} \sim \frac{e^{-r/\xi}}{r^{\eta}} \,, \tag{3.6}$$

because after the Suzuki–Trotter decomposition [25], the correlation function (3.5) is expressed as the summation of all the (3.6)-type correlation functions along the Trotter direction. Then the feedback function of an N-spin chain is found to be scaled [16] as

$$\mathcal{F}(g; N) \sim N^{1-\eta} f(N/\xi) \tag{3.7}$$

where f stands for a scaling function determined by the application scheme of effective fields and boundary conditions of relevant clusters. The exponent η is always less than unity [19] along the Néel-dimer transition line of the present model, and the inequality $\mathcal{F}_A(g_c^*) < \mathcal{F}_B(g_c^*)$ is satisfied at each transition point g_c^*. On the other hand, for $g \gg g_c^*$, the opposite inequality $\mathcal{F}_A(g) > \mathcal{F}_B(g)$ holds because correlation functions decay exponentially in this region. In short, the feedback functions of clusters A and B behave as in figure 2. The crossing point of the two curves $\mathcal{F}_A(g)$ and $\mathcal{F}_B(g)$ gives the approximate critical point g_c, which approaches the true one g_c^* from the disordered phase.

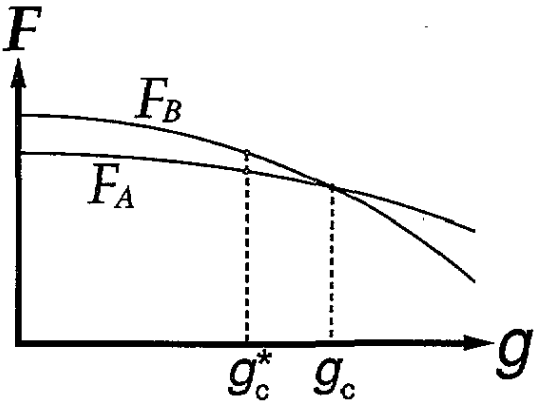

Figure 2. A schematic behaviour of feedback functions in the DCA.

3.2. Open-boundary condition DCA *(*OBC–DCA*)*

Following previous studies and using the DCA [14, 15], we first consider two different *open-boundary* clusters. Not only the effective field $H_{\rm eff}$ which originates from the nearest-neighbour interaction but also the effective field $-gH_{\rm eff}$ from the next-nearest-neighbour interaction are applied to the edge spins, and $-gH_{\rm eff}$ is also applied to the spins within one site from the edges (figure 3). This formulation is nothing but a one-dimensional version of the approximation proposed by Gelfand *et al* [10] for the J_1–J_2 model.

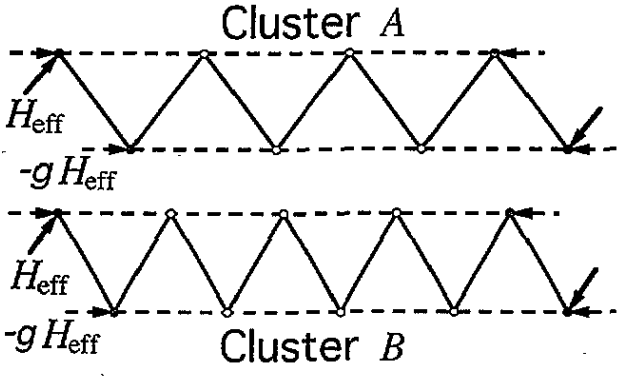

Figure 3. The application scheme of the effective fields in the OBC-DCA.

The effective Hamiltonian of an N_I-spin cluster is given by

$$\mathcal{H}_{N_I}^{\text{eff}} = \sum_{i=1}^{N_I-1}\left[J_{xy}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_z S_i^z S_{i+1}^z\right]$$
$$+g\sum_{i=1}^{N_I-2}\left[J_{xy}(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y) + J_z S_i^z S_{i+2}^z\right]$$
$$-H\sum_{i=1}^{N_I}(-1)^{i-1}S_i^z - H_{\text{eff}}\left[S_1^z + (-1)^{N_I-1}S_{N_I}^z\right]$$
$$-(-gH_{\text{eff}})\left[S_1^z - S_2^z + (-1)^{N_I-2}S_{N_I-1}^z + (-1)^{N_I-1}S_{N_I}^z\right] \tag{3.8}$$

and the required consistency condition is

$$\frac{1}{N_A}\sum_{i=1}^{N_A}(-1)^{i-1}\langle S_i^z\rangle_g^A = \frac{1}{N_B}\sum_{i=1}^{N_B}(-1)^{i-1}\langle S_i^z\rangle_g^B\,. \tag{3.9}$$

Although such a treatment of frustration can be justified in classical spin systems, it is not certain whether this approximation is also valid in quantum spin systems or not.

3.3. Periodic-boundary condition DCA *(*PBC–DCA*)*

Periodic-boundary clusters are used in this cluster-effective-field approximation. The Weiss-like approximation is not suitable for the CAM fitting because of serious size-dependent corrections [26]. The Bethe-like approximation cannot be formulated under the PBC, because all the spins are equivalent under this boundary condition. Thus the DCA is essential for the application of the CAM to PBC clusters.

The effective Hamiltonian of an N_I-spin cluster is given by

$$\mathcal{H}_{N_I} = \sum_{i=1}^{N_I}\left[J_{xy}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_z S_i^z S_{i+1}^z\right] + g\sum_{i=1}^{N_I}\left[J_{xy}(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y) + J_z S_i^z S_{i+2}^z\right]$$
$$-H\sum_{i=1}^{N_I}(-1)^{i-1}S_i^z - H_{\text{eff}}S_1^z \tag{3.10}$$

where $S_{N_I+1}^{\alpha} = S_1^{\alpha}$ and $S_{N_I+2}^{\alpha} = S_2^{\alpha}$ ($\alpha = x, y, z$). The required consistency condition is formally the same as shown in (3.9). This approximation has already been used in the study of the $S = \frac{1}{2}$ XXZ chain [12].

Since there is no real 'boundary' in PBC clusters, the application scheme of effective fields is not so complicated as in the OBC–DCA. Here we have only to apply H_{eff} on a certain spin (figure 4) in order to break the up–down symmetry. Since only the vicinity of the critical point is treated in the CAM, all we have to consider here is the linear response of the order parameter for infinitesimal effective and external fields. Namely, we calculate nothing but canonical correlation functions of finite clusters. Thus, we need not worry about the 'physical meaning' of this boundary condition.

4. Numerical results and discussion

In OBC clusters, we have calculated up to the 18-spin cluster here. This maximum size is smaller than the ones used in previous finite-cluster studies [21, 22], because translational symmetry cannot be used in OBC clusters and some dozens of repeating diagonalization

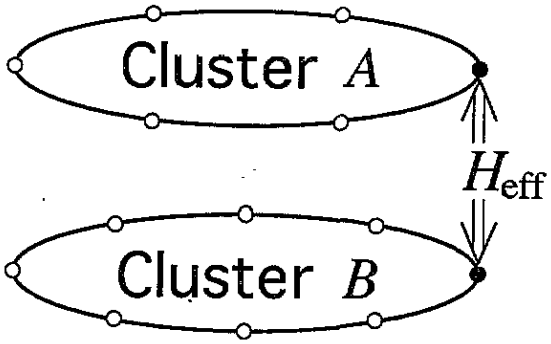

Figure 4. The application scheme of the effective field in the PBC-DCA.

calculations are necessary for the estimation of the approximate critical points. On the other hand, in PBC clusters, translational symmetry can be used [12], and larger clusters can be easily treated. However, since the purpose of the present paper is the comparison of the OBC-DCA and the PBC-DCA, the maximum size of PBC clusters is also limited here to 18 spins. As will be shown later, this cluster size is large enough for the present purpose.

At first, we show the raw data of the approximate critical points $\{g_c\}$ for all the calculated values of J_{xy}/J_z (figure 5). In each value of J_{xy}/J_z, g_c approaches the true value g_c^* from the disordered phase in the PBC-DCA, and from the ordered phase in the OBC-DCA. The latter behaviour is not consistent with the phenomenological derivation of the coherent anomaly explained in 3.1. Moreover, as J_{xy} approaches J_z, the discrepancy between g_c and g_c^* becomes larger and larger in the OBC-DCA, as is shown in figure 5. For $J_{xy} > 0.834J_z$, the approximate critical point obtained from the OBC-DCA becomes negative [12] even in the 16–18 approximation. In addition, the cluster-size dependence of g_c is much smaller in the OBC-DCA than in the PBC-DCA near the Heisenberg point.

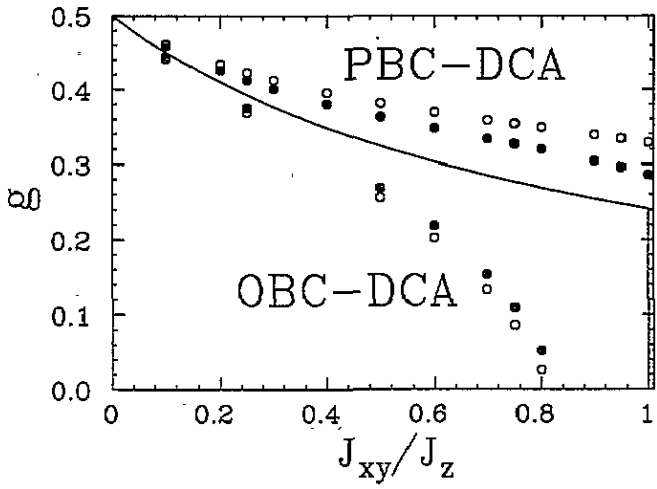

Figure 5. The approximate critical points obtained from the OBC-DCA and the PBC-DCA. The data below the Néel-dimer phase boundary (solid line) [22] correspond to the former, and the ones above that line correspond to the latter. The open circles stand for the 8–10 approximations and the full circles stand for the 16–18 approximations.

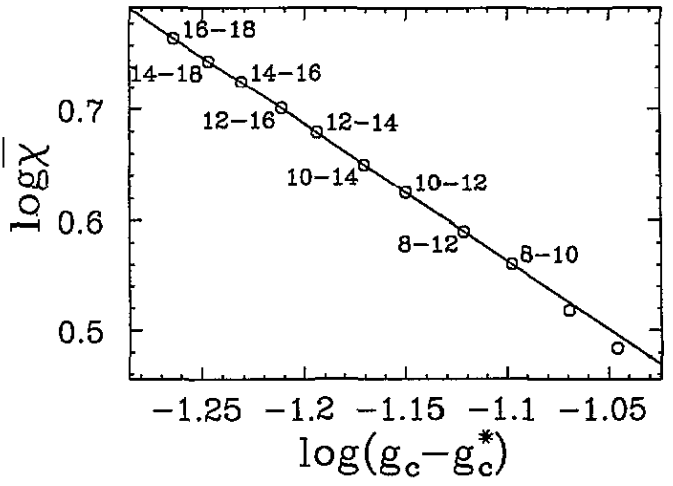

Figure 6. An example of the coherent anomaly of $\bar{\chi}$ in the PBC-DCA. Log $\bar{\chi}$ is plotted versus $\log(g_c - g_c^*)$ for $J_{xy} = 0.25J_z$.

Next, we estimate the true critical point g_c^* using the CAM. In the PBC-DCA, we make a least-squares fitting for the critical coefficients $\{\bar{\chi}\}$ defined by (2.3) using the scaling form (2.4). An example of the fitting is shown in figure ?? in the case of $J_{xy} = 0.25J_z$. The critical coefficients $\{\bar{\chi}\}$ are scaled by (2.4) very well even from a rather low-level, namely the 8–10 approximation. In the OBC-DCA, the least-squares fitting can be made similarly as in the PBC-DCA, though the coherent anomaly of the approximation is not justified [16] when $g_c < g_c^*$. Moreover, in this approximation, the value of g_c becomes smaller and smaller as J_{xy} approaches J_z, and the definition of $\bar{\chi}$ in (2.3) is not appropriate in this parameter region. Then we re-define $\bar{\chi}$ by $d\chi_{st}/dg|_{g=g_c}$ for $J_{xy} \geqslant 0.5J_z$.

The phase diagrams estimated by the CAM are given in figure 7 together with the result by Nomura and Okamoto (NO) [22]. The phase boundaries obtained from the two

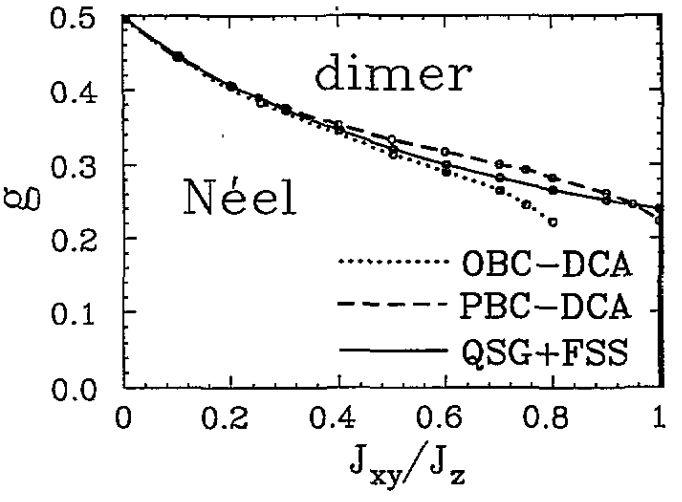

Figure 7. The phase diagrams obtained from the PBC-DCA (broken line), the OBC-DCA (dashed line), and the properties of low-energy excitations (solid line) [22, 28].

approximations coincide quantitatively with the NO result as long as the ratio J_{xy}/J_z is small, because g_c itself is very close to g_c^* in this region. The estimates of g_c^* obtained from the OBC–DCA tend to be smaller and smaller than the NO ones as the ratio J_{xy}/J_z grows larger. If the original definition (2.3) of $\bar{\chi}$ is used even for $J_{xy} \geqslant 0.5J_z$, this discrepancy becomes much worse. On the other hand, the PBC–DCA overestimates the Néel order by at most a few per cent in comparison with the NO result for $J_{xy} \geqslant 0.5J_z$. Although this slight discrepancy is not improved so much when calculations are extended up to the 22–24 approximation, such a tendency of overestimation is natural in cluster-effective-field approximations, and this tendency changes to underestimation in the vicinity of the Heisenberg point, namely for $J_{xy} \geqslant 0.95J_z$. This behaviour corresponds to the Néel-spin fluid transition at the Heisenberg point. Consequently, the PBC–DCA can be regarded as a good approximation in the whole parameter region.

Of course, if we consider an infinite cluster, boundary conditions should not affect the results. However, since the size of clusters is limited in exact-diagonalization studies, the extrapolated results may depend on boundary conditions of the relevant clusters. The remaining question is that the undesired behaviour of the OBC–DCA may not be due to the open-boundary condition itself, but due to the present treatment of frustration effects. Then the centre-to-boundary correlation function of an N-spin cluster with respect to the Néel order,

$$\mathcal{F}_{cb}(g; N) \equiv ((-1)^{N/2-1} S_{N/2}; (S_1^z + (-1)^{N-1} S_N^z))_g \tag{4.1}$$

is calculated in OBC clusters (figures 8(a)–(c)) and in PBC clusters (figures 8(d)–(f)) for various anisotropy parameters. Although the correlation functions given by PBC clusters behave as is explained in section 3.1, those given by OBC clusters do not. Figures 8(a)–(c) clearly demonstrate that the behaviour of the approximate critical points in the OBC–DCA originates from the principal character of correlation functions in OBC clusters, and that mere modifications of the application scheme of effective fields or the consistency conditions cannot improve the undesired behaviour of the OBC–DCA.

In the CAM fitting based on the scaling form (2.4), the critical exponent γ of χ_{st} is also estimated simultaneously. This exponent is related [19, 27] with other exponents with respect to the z-component correlation function, namely ν and $\eta_{\text{Néel}}$, as

$$\gamma = \nu(2 - \eta_{\text{Néel}}) = \frac{2 - \eta_{\text{Néel}}}{2(1 - \eta_{\text{Néel}})} . \tag{4.2}$$

The exponent $\eta_{\text{Néel}}$ is unity at the Heisenberg point $J_{xy} = J_z$, and ν and γ diverge there. This behaviour corresponds to a Kosterlitz–Thouless-type transition at this point. On the other hand, $\eta_{\text{Néel}}$ approaches $\frac{1}{2}$ as J_{xy} goes to zero, where $\nu = 1$ and $\gamma = 3/2$. Quite recently Nomura and Okamoto numerically estimated [28] the exponent $\eta_{\text{Néel}}$ in the intermediate region between these two limits on the basis of the conformal field theory. Unfortunately, the present estimate of γ is not consistent with the one obtained from Nomura and Okamoto's results. The reason may be the following: when J_{xy}/J_z is small, the variance of the approximate critical points g_c is very small and the CAM fitting is difficult. On the other hand, when J_{xy}/J_z is large, the Néel order is weakened by quantum fluctuations, the scaling region of this order becomes narrow and the present cluster sizes are not large enough for the estimation of critical exponents. In order to confirm this argument, we make a series of fittings using the data of g_c^* estimated by Nomura and Okamoto [22, 28]. As given in figure 9, the estimate of γ is consistent with the value obtained from the relation (4.2) for $J_{xy}/J_z \leqslant 0.3$, and these two values clearly separate as quantum fluctuations are increased, in accordance with a discrepancy of the estimates of g_c^* (figure 7). In short, the CAM scaling

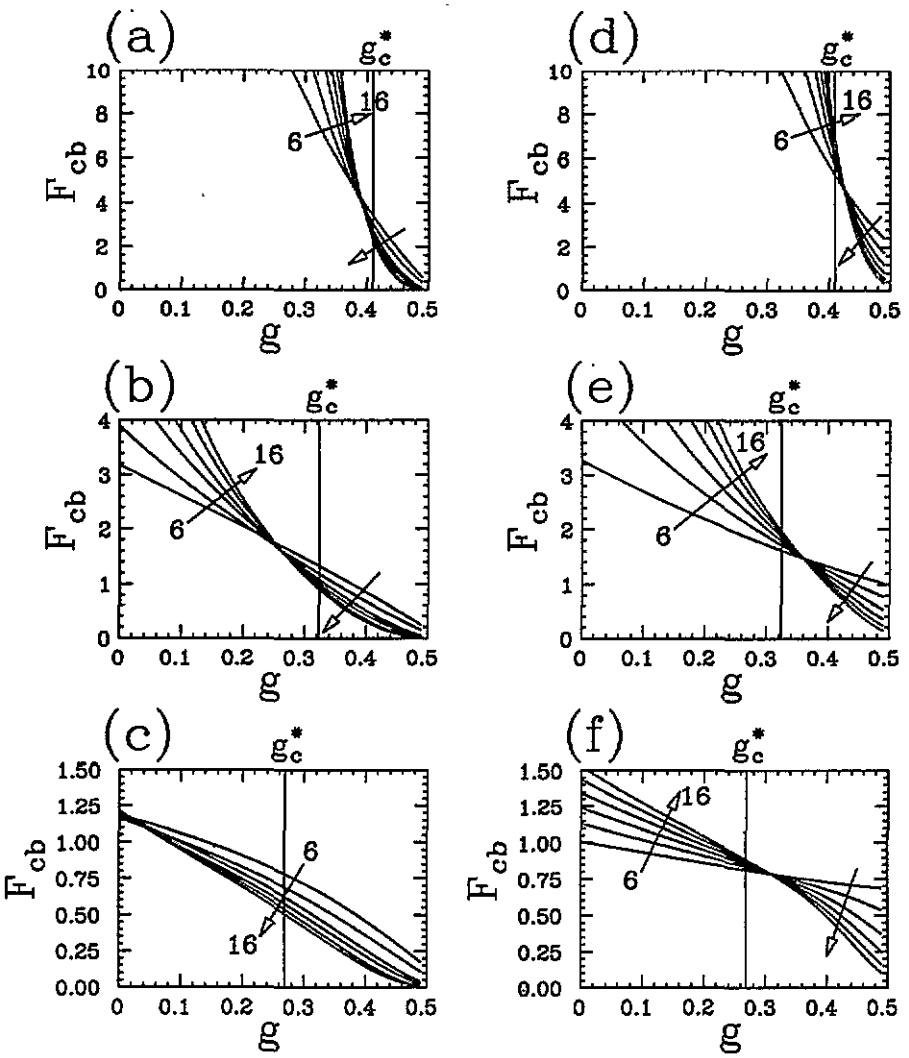

Figure 8. The centre-to-boundary correlation functions in OBC and PBC clusters: (a) $J_{xy} = 0.2J_z$, OBC; (b) $J_{xy} = 0.5J_z$, OBC; (c) $J_{xy} = 0.8J_z$, OBC; (d) $J_{xy} = 0.2J_z$, PBC; (e) $J_{xy} = 0.5J_z$, PBC; (f) $J_{xy} = 0.8J_z$, PBC.

relation (2.4) is satisfied, even in the present model, *self-consistently*, namely, this relation holds well as long as the critical point g_c^* can be estimated accurately using itself.

5. Summary and conclusion

In the present paper we have considered the effect of boundary conditions on the formulation of cluster-effective-field approximations in frustrated quantum spin systems. Since the maximum cluster size to be used in exact-diagonalization calculations is limited, the effect of boundary conditions is not negligible. For the investigation of this effect, we have analysed the Néel-dimer transition of the one-dimensional $S = \frac{1}{2}$ frustrated XXZ model

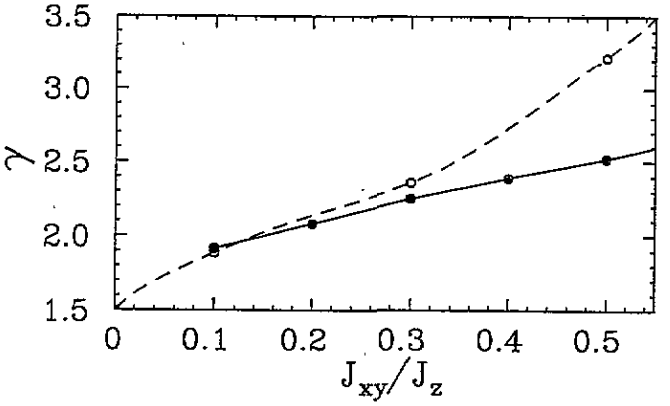

Figure 9. The critical exponent γ obtained from the PBC-DCA (full circles) and from the CFT (open circles) [28]. In the former estimation, the values of the critical points given in [22] and [28] are assumed. The solid and dashed lines are drawn only for convenience.

at the ground state, using the OBC-DCA and the PBC-DCA, with the aid of the CAM. Within the calculation up to the 18-spin (partly 24-spin) cluster, the approximate critical points obtained from the PBC-DCA approach the true one as the enlargement of clusters, and this approximation has reproduced the true phase diagram in the whole parameter region when it is combined with the CAM. On the other hand, the OBC-DCA tends to underestimate the Néel order more and more as the system approaches the Heisenberg point, and such a large discrepancy of the critical point still remains even after the CAM fitting. These facts suggest that the previous studies of the J_1–J_2 model based on cluster-effective-field approximations should be reconsidered, because they are formulated using open-boundary clusters. In fact, when we make similar calculations with the J_1–J_2 model using periodic-boundary clusters, the result of approximations changes qualitatively. Details of this study will be reported [29] elsewhere, together with an extension of cluster-effective-field approximations to non-magnetic order parameters.

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