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Coherent-anomaly method in zero-temperature phase transitions in quantum spin systems

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Abstract. A cluster-effective-field theory, called the double-cluster approximation, is formulated for quantum spin systems at $T = 0$. Combining this approximation with the coherent-anomaly method (CAM), critical phenomena in such systems can be analysed. To test our theory, we have estimated the critical points and critical exponents of the one-dimensional $S = \frac{1}{2}$ transverse Ising model and the one-dimensional $S = \frac{1}{2}$ XZ model. Our estimates are in good agreement with the exact solutions. These results show that the CAM approach is useful in treating zero-temperature phase transitions in quantum spin systems.

1. Introduction

Recently the ground state properties of quantum spin systems have been intensively studied, especially in antiferromagnetic systems or frustrated systems. In these systems phase transitions may even occur at $T = 0$ as a parameter of the Hamiltonian is varied. For simplicity, we consider a zero-temperature ferromagnetic quantum spin model described by the following Hamiltonian:

$$\mathcal{H} = \mathcal{H}_{\mathrm{Is}} - g\mathcal{H}_{\mathrm{qu}} \tag{1.1}$$

with a quantum interaction $\mathcal{H}_{\mathrm{qu}}$ satisfying

$$[\mathcal{H}_{\mathrm{Is}}, \mathcal{H}_{\mathrm{qu}}]_- \neq 0 \tag{1.2}$$

and

$$\mathcal{H}_{\mathrm{Is}} = -\sum_{\langle ij \rangle} S_i^z S_j^z - H \sum_i S_i^z \tag{1.3}$$

where $\sum_{\langle ij \rangle}$ denotes the sum over all the nearest-neighbour bonds. Since $\mathcal{H}_{\mathrm{Is}}$ is the Ising Hamiltonian, $\langle S^z \rangle_{\mathrm{g}}$ (the ground state average of S^z) is the order parameter of this model. It displays critical phenomena in the vicinity of a certain critical point $g = g_{\mathrm{c}}^*$. The critical exponents are defined as follows:

$$\chi \equiv \frac{\partial}{\partial H} \langle S^z \rangle_{\mathrm{g}} \bigg|_{H=0} \propto \begin{cases} \dfrac{1}{(g - g_{\mathrm{c}}^*)^{\gamma}} & \text{for } g \to g_{\mathrm{c}}^* + 0 \\ \dfrac{1}{(g_{\mathrm{c}}^* - g)^{\gamma'}} & \text{for } g \to g_{\mathrm{c}}^* - 0 \end{cases} \tag{1.4}$$

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$$m_s \equiv \langle S^z \rangle_g |_{H=0} \propto (g_c^* - g)^\beta \qquad \text{for } g \to g_c^* - 0 \tag{1.5}$$

$$m_c \equiv \langle S^z \rangle_g |_{g=g_c^*} \propto H^{1/\delta} \qquad \text{for } H \to 0 \tag{1.6}$$

$$C \equiv \frac{\partial}{\partial g} \langle \mathcal{H}_{qu} \rangle_g \propto \begin{cases} \dfrac{1}{(g-g_c^*)^\alpha} & \text{for } g \to g_c^* + 0 \\ \dfrac{1}{(g_c^*-g)^{\alpha'}} & \text{for } g \to g_c^* - 0. \end{cases} \tag{1.7}$$

Until the present time, quantum spin models of this type at $T = 0$ have often been treated by the phenomenological renormalization-group and finite-size scaling methods [1, 2]. In these methods each finite-size cluster is characterized by its linear size. Then only regular clusters (for example, on the square lattice, $2 \times 2, 3 \times 3, 4 \times 4, \ldots$ ones) can be used for the estimation of the critical point and critical exponents. Although these methods are useful in one-dimensional systems [3] and some simple two-dimensional systems [4], it is generally difficult to apply them to higher-dimensional systems, because only a few clusters are available owing to the limited memories of computers.

In the present paper we propose a new approach to treat zero-temperature phase transitions of quantum spin systems, using the coherent-anomaly method (CAM) [5, 6] proposed by one of the present authors (MS). In the CAM, non-classical critical exponents are estimated from *a series of* mean-field or effective-field approximations. Each approximation has the mean-field critical point g_c, and the approximation is characterized by the 'degree of approximation' $g_c - g_c^*$. Then not only regular clusters but also some others can be used, and more data are available for fitting in our approach than in the finite-size scaling approach. Our formulation is applicable to many other models. In order to test our theory we analyse the models which have exact solutions, namely the one-dimensional $S = \frac{1}{2}$ transverse Ising model [7, 8]:

$$\mathcal{H} = -\sum_i S_i^z S_{i+1}^z - g \sum_i S_i^x - H \sum_i S_i^z \tag{1.8}$$

and the one-dimensional $S = \frac{1}{2}$ XZ model [9, 10]:

$$\mathcal{H} = -\sum_i S_i^z S_{i+1}^z - g \sum_i S_i^x S_{i+1}^x - H \sum_i S_i^z . \tag{1.9}$$

In section 2, the CAM is reviewed briefly. In section 3, the double-cluster approximation [11–16] is formulated for quantum spin systems at $T = 0$. The mean-field critical point and critical coefficients of various thermodynamic quantities are calculated. In section 4, the critical points and critical exponents of the relevant models are estimated using the CAM. These estimates are compared with the exact solutions, and the possibilities for further applications are pointed out. In section 5, these descriptions are summarized.

2. Coherent-anomaly method (CAM)

The basic idea of the CAM [5, 6] is given as follows. When we evaluate a certain physical quantity Q in a mean-field or effective-field approximation using a certain cluster (size L), the quantity Q diverges at the mean-field critical point $g = g_c(L)$ as

$$Q(L,g) \simeq \begin{cases} \dfrac{\bar{Q}_+(L,g_c(L))}{\epsilon^{\varphi_{cl}}} & \text{for } g \to g_c(L)+0 \\ \dfrac{\bar{Q}_-(L,g_c(L))}{(-\epsilon)^{\varphi_{cl}}} & \text{for } g \to g_c(L)-0 \end{cases} \tag{2.10}$$

where

$$\epsilon \equiv (g - g_c(L))/g_c(L) \tag{2.11}$$

and φ_{cl} is the classical critical exponent. If we choose some systematically constructed series of approximations (canonical series) and take the limit $L \to \infty$, the mean-field critical point $g_c(L)$ approaches the true one g_c^* [6], and the critical coefficient $\bar{Q}_\pm(L, g_c(L))$ asymptotically diverges as

$$\bar{Q}_\pm(L,g_c(L)) \simeq \frac{\text{constant}}{|\delta(g_c(L))|^{\psi}} \tag{2.12}$$

where

$$\delta(g_c(L)) \equiv \frac{g_c(L) - g_c^*}{g_c^*}. \tag{2.13}$$

This asymptotic behaviour of the critical coefficient is called the coherent anomaly, and such behaviour can be seen in finite-L systems. Then the critical point g_c^* and the exponent ψ can be estimated from a series of approximations $\{g_c(L), \bar{Q}_\pm(L, g_c(L))\}$. The true critical exponent φ can be obtained [5, 6] from the following relationship,

$$\varphi = \varphi_{cl} + \psi. \tag{2.14}$$

These formulae cannot describe the singularity of m_c. To do that we have to formulate the CAM more generally [5]. We start from the following scaling form (the finite-degree-of-approximation scaling form) for $x \approx x_c$ and $g_c \approx g_c^*$,

$$Q(x;g_c) \simeq (x - x_c)^{-\varphi_{cl}}(g_c - g_c^*)^{-\psi} f^{(sc)}\left(\frac{x - x_c}{(g_c - g_c^*)^{\mu}}\right) \tag{2.15}$$

where x is a certain physical variable, and x_c is its critical value. If we assume that the scaling form (2.15) describes the true critical behaviour

$$Q(x) \propto (x - x_c)^{-\varphi} \qquad \text{for } x \to x_c \tag{2.16}$$

in the limit $g_c \to g_c^*$, we arrive at the coherent-anomaly relationship [5],

$$\varphi = \varphi_{cl} + \frac{\psi}{\mu}. \tag{2.17}$$

In fact, formulae (2.10)–(2.14) are the special cases of these general formulae, with $x = g$ and $\mu = 1$.

In order to evaluate m_c we should consider [5] the following asymptotic form,

$$\langle S^z \rangle_g |_{g=g_c} \simeq \delta(g_c)^{-\psi_{m_c}} H^{1/3} f_1^{(sc)} + \delta(g_c)^{-1-\psi_\chi} H f_2^{(sc)} \qquad \text{for } H \to 0 \tag{2.18}$$

which represents the singularities of m_c and χ_+ at the same time. When the asymptotic form (2.18) satisfies the scaling form (2.15) ($x = H$, $x_c = 0$), we obtain

$$\mu = \tfrac{3}{2}(1 + \psi_\chi - \psi_{m_c}) \tag{2.19}$$

and the critical exponent δ defined in the formula (1.6) is given by

$$\delta = \frac{3(1 + \psi_\chi - \psi_{m_c})}{1 + \psi_\chi - 3\psi_{m_c}}. \tag{2.20}$$

The CAM has already been applied to many problems (see the references cited in [17]), and its validity has been confirmed. However, its applications to quantum systems [12, 18, 19] are not very numerous at present. One reason is that the justification of effective fields are not so easy in quantum systems, and another is that only small clusters can be treated. As is well known, a zero-temperature D-dimensional quantum system represented by a Hamiltonian $\mathcal{H}$ is equivalent [20–22] to a $(D+1)$-dimensional system represented by the 'transfer-matrix' $e^{-\mathcal{H}}$ (an *anisotropic limit* of a classical system). Thus, our present approach is directly related to the transfer matrix CAM [14, 15, 23–25], in which good estimates can be obtained from small clusters. A similar advantage is expected in our approach. The only difference is that *isotropic* classical systems are treated in the transfer-matrix CAM.

3. Double-cluster approximation for quantum spin systems at $T = 0$

In the present section we formulate the double-cluster approximation [11–16] for quantum spin systems at $T = 0$. In order to show the calculation scheme explicitly, we treat the one-dimensional $S = \frac{1}{2}$ transverse Ising model as an example. Both an equation to determine the mean-field critical point and expressions for various critical coefficients are obtained explicitly. Generalization to the one-dimensional $S = \frac{1}{2}$ XZ model and other models is straightforward.

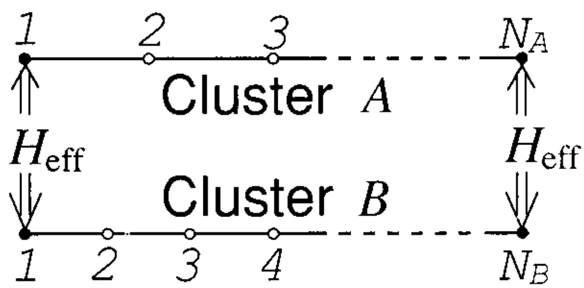

Figure 1. The way in which the effective field is applied to N_A- and N_B-spin clusters in the double-cluster approximation.

3.1. *Effective Hamiltonian and self-consistency conditions*

We investigate the one-dimensional $S = \frac{1}{2}$ transverse Ising model (1.8) using the double-cluster approximation. In this approximation we consider *two different* clusters A and B, and apply the *same* effective field $H_{\rm eff}$ to their boundary spins (figure 1). In principle, effective fields are applied not only on the boundary spins, but also on all the spins of the relevant clusters in the effective-field approximations in quantum spin systems. From a physical standpoint of view, this simplification is regarded as a first-order approximation, in which only the most important effective field is taken into account. The effective Hamiltonian of the $N_{\rm I}$-spin cluster (I $\equiv$ A or B) is given by

$$\mathcal{H}_{N_{\rm I}} = \mathcal{H}_{N_{\rm I}}^{(\rm cl)} + \mathcal{H}_{N_{\rm I}}^{(\rm ext)} + \mathcal{H}_{N_{\rm I}}^{(\rm eff)} \tag{3.1}$$

with

$$\mathcal{H}_{N_I}^{(\rm cl)} = -\sum_{i=1}^{N_{\rm I}-1} S_i^z S_{i+1}^z - g\sum_{i=1}^{N_{\rm I}} S_i^x \tag{3.2}$$

$$\mathcal{H}_{N_{\rm I}}^{(\rm ext)} = -H\sum_{i=1}^{N_{\rm I}} S_i^z \tag{3.3}$$

$$\mathcal{H}_{N_{\rm I}}^{(\rm eff)} = -H_{\rm eff}(S_1^z + S_{N_{\rm I}}^z). \tag{3.4}$$

The required self-consistency condition is

$$\frac{1}{N_{\rm A}}\sum_{i=1}^{N_{\rm A}}\langle S_i^z\rangle_{\rm g}^{\rm A} = \frac{1}{N_{\rm B}}\sum_{i=1}^{N_{\rm B}}\langle S_i^z\rangle_{\rm g}^{\rm B} \tag{3.5}$$

where $\langle\cdots\rangle_{\rm g}^{\rm I}$ denotes the ground state average in the system represented by $\mathcal{H}_{N_{\rm I}}$. This is a kind of effective-field approximation, and derivation of its coherent anomaly has been given by the present authors and N Hatano [26] in a more general form.

When g is larger than a critical value g_c, the solution of equation (3.5) is always $H_{\rm eff} = 0$ for $H = 0$. On the other hand, when g is smaller than $g_{\rm c}$, equation (3.5) has a non-zero solution even for $H = 0$. It corresponds to the spontaneous symmetry breaking of the system. In order to calculate the value of $H_{\rm eff}$, we have to solve this nonlinear equation directly. However, if we are only interested in critical phenomena, it is enough for us to treat the system in the vicinity of the mean-field critical point $g = g_{\rm c}$. In this region the external field H and the effective field $H_{\rm eff}$ are taken to be infinitesimal. Then it is possible to expand equation (3.5) with respect to H and $H_{\rm eff}$, which is nothing but the perturbation expansion of the order parameter with respect to H and $H_{\rm eff}$.

Following the standard perturbation theory, the ground state of $\mathcal{H}_{N_{\rm I}}$ is expressed as a power series of H and $H_{\rm eff}$, and consequently the order parameter of the cluster I is given by

$$\frac{1}{N_{\rm I}}\sum_{i=1}^{N_{\rm I}}\langle S_i^z\rangle_{\rm g}^{\rm I} = H_{\rm eff}\frac{1}{N_{\rm I}}\sum_{n\neq g}\langle g|S_{\rm t}^z|n\rangle^{\rm I}\langle n|S_{\rm b}^z|g\rangle^{\rm I}\frac{2}{E_n^{\rm I} - E_g^{\rm I}}$$
$$+ H_{\rm eff}^3\left\{\frac{1}{N_{\rm I}}\sum_{n\neq g}\sum_{m\neq g}\sum_{l\neq g}(\langle g|S_{\rm t}^z|n\rangle^{\rm I}\langle n|S_{\rm b}^z|m\rangle^{\rm I}\langle m|S_{\rm b}^z|l\rangle^{\rm I}\langle l|S_{\rm b}^z|g\rangle^{\rm I}\right.$$

$$+ \langle n|S_{\rm t}^z|m\rangle^{\rm I}\langle m|S_{\rm b}^z|g\rangle^{\rm I}\langle g|S_{\rm b}^z|l\rangle^{\rm I}\langle l|S_{\rm b}^z|n\rangle^{\rm I})$$

$$\times \frac{2}{(E_n^{\rm I}-E_g^{\rm I})(E_m^{\rm I}-E_g^{\rm I})(E_l^{\rm I}-E_g^{\rm I})}$$

$$- \frac{1}{N_{\rm I}}\sum_{n\neq g}\sum_{m\neq g}\langle g|S_{\rm t}^z|n\rangle^{\rm I}\langle n|S_{\rm b}^z|g\rangle^{\rm I}\langle g|S_{\rm b}^z|m\rangle^{\rm I}\langle m|S_{\rm b}^z|g\rangle^{\rm I}$$

$$\times\left[\frac{2}{(E_n^{\rm I}-E_g^{\rm I})^2(E_m^{\rm I}-E_g^{\rm I})}+\frac{2}{(E_n^{\rm I}-E_g^{\rm I})(E_m^{\rm I}-E_g^{\rm I})^2}\right]\Bigg\}$$

$$+ H\frac{1}{N_{\rm I}}\sum_{n\neq g}\langle g|S_{\rm t}^z|n\rangle^{\rm I}\langle n|S_{\rm t}^z|g\rangle^{\rm I}\frac{2}{E_n^{\rm I}-E_g^{\rm I}}+\cdots \tag{3.6}$$

$$\equiv P^{\rm I}H_{\rm eff}+Q^{\rm I}H_{\rm eff}^3+R^{\rm I}H+\cdots \tag{3.7}$$

where $\sum_{n\neq g}$ denotes the sum over all the excited states, and

$$S_{\rm b}^z \equiv S_1^z + S_{N_{\rm I}}^z \tag{3.8}$$

$$S_{\rm t}^z \equiv \sum_{i=1}^{N_{\rm I}} S_i^z . \tag{3.9}$$

Here, $|g\rangle^{\rm I}$ is the ground state of $\mathcal{H}_{N_{\rm I}}^{(\rm cl)}$, and $|n\rangle^{\rm I}$ is the nth excited state of $\mathcal{H}_{N_{\rm I}}^{(\rm cl)}$. The parameters $E_g^{\rm I}$ and $E_n^{\rm I}$ are the energies of $|g\rangle^{\rm I}$ and $|n\rangle^{\rm I}$, respectively. In this calculation we have used the facts that the ground state of $\mathcal{H}_{N_{\rm I}}$ is not degenerate and that the unperturbed ground state average of the order parameter $\frac{1}{N_{\rm I}}\sum_{i=1}^{N_{\rm I}}\langle g|S_i^z|g\rangle^{\rm I}$ and the terms proportional to $H_{\rm eff}^2$, $HH_{\rm eff}$ and H^2 vanish because of the symmetry of the system.

3.2. Calculation of critical coefficients

The mean-field critical point and various critical coefficients are calculated as follows, just as in the transfer-matrix CAM [14, 15, 23–25]:

(i) *Mean-field critical point.* In this approximation equation (3.5) should be satisfied, no matter how small the value of $H_{\rm eff}$ is. In such a case the higher-order terms of formula (3.6) can be neglected. Thus, inversely, the mean-field critical point $g_{\rm c}$ is determined as the solution of the following equation,

$$P^{\rm A} = P^{\rm B}. \tag{3.10}$$

(ii) *Susceptibility for $g > g_{\rm c}$.* Above the critical point only the linear terms of equation (3.5) should be considered, and the susceptibility just above the critical point is given by

$$\chi^{\rm I} = \frac{\partial}{\partial H}\left(\frac{1}{N_{\rm I}}\sum_{i=1}^{N_{\rm I}}\langle S_i^z\rangle_{\rm g}^{\rm I}\right)_{H=0} = R^{\rm I} + P^{\rm I}\left.\frac{\partial H_{\rm eff}}{\partial H}\right|_{H=0} . \tag{3.11}$$

The derivative $\partial H_{\text{eff}}/\partial H|_{H=0}$ in (3.11) can be determined from the condition (3.5), namely $\chi^{\text{A}} = \chi^{\text{B}}$. Thus, we obtain

$$(R^{\text{A}} - R^{\text{B}}) + (P^{\text{A}} - P^{\text{B}}) \left.\frac{\partial H_{\text{eff}}}{\partial H}\right|_{H=0} = 0. \tag{3.12}$$

Then χ^{I} is given by

$$\chi^{\text{I}} = R^{\text{I}} - \frac{P^{\text{I}}(R^{\text{A}} - R^{\text{B}})}{P^{\text{A}} - P^{\text{B}}} \tag{3.13}$$

and the denominator of the second term of the right-hand side vanishes at $g = g_c$. It corresponds to the classical singularity, i.e. $\gamma_{\text{cl}} = 1$.

Finally, the susceptibility at $g = g_c + 0$ is given by

$$\chi^{\text{I}} = \bar{\chi}^{\text{I}}_{+} \left(\frac{g_c}{g - g_c}\right)^{\gamma_{\text{cl}}} \qquad \gamma_{\text{cl}} = 1 \tag{3.14}$$

$$\bar{\chi}^{\text{I}}_{+} = -\frac{1}{g_c} \frac{P^{\text{I}}(R^{\text{A}} - R^{\text{B}})}{\text{d}(P^{\text{A}} - P^{\text{B}})/\text{d}g|_{g=g_c}} \tag{3.15}$$

where $\bar{\chi}^{\text{A}}_{+} = \bar{\chi}^{\text{B}}_{+}$ because of the condition (3.10). The explicit expression of the denominator of $\bar{\chi}^{\text{I}}_{+}$ is given in the appendix. Practically, this value can be calculated precisely enough by numerical differentiation.

(iii) *Spontaneous magnetization.* The spontaneous magnetization m^{I}_{s} appears below the critical point, because the effective field H_{eff} takes a non-vanishing value. In order to determine the value of H_{eff} at $g = g_c - 0$, we have to consider up to third-order terms in equation (3.5) and set $H = 0$. We obtain

$$(P^{\text{A}} - P^{\text{B}})H_{\text{eff}} + (Q^{\text{A}} - Q^{\text{B}})H^{3}_{\text{eff}} = 0 \tag{3.16}$$

or

$$H_{\text{eff}} = (g_c - g)^{1/2} \left[\frac{\text{d}(P^{\text{A}} - P^{\text{B}})/\text{d}g|_{g=g_c}}{Q^{\text{A}} - Q^{\text{B}}}\right]^{1/2}. \tag{3.17}$$

Then the spontaneous magnetization is given by

$$m^{\text{I}}_{s} = \bar{m}^{\text{I}}_{s} \left(\frac{g_c - g}{g_c}\right)^{\beta_{\text{cl}}} \qquad \beta_{\text{cl}} = \tfrac{1}{2} \tag{3.18}$$

$$\bar{m}^{\text{I}}_{s} = g_c^{1/2} P^{\text{I}} \left[\frac{\text{d}(P^{\text{A}} - P^{\text{B}})/\text{d}g|_{g=g_c}}{Q^{\text{A}} - Q^{\text{B}}}\right]^{1/2} \tag{3.19}$$

where $\bar{m}^{\text{A}}_{s} = \bar{m}^{\text{B}}_{s}$ because of the condition (3.10).

(iv) *Susceptibility for $g < g_c$.* Although the susceptibility just below the critical point is given by the same formula as (3.11), the value of $\partial H_{\text{eff}}/\partial H|_{H=0}$ is different from the one given by equation (3.12) because of $H_{\text{eff}} \neq 0$. i.e.

$$(R^{\text{A}} - R^{\text{B}}) + [(P^{\text{A}} - P^{\text{B}}) + 3(Q^{\text{A}} - Q^{\text{B}})H^{2}_{\text{eff}}] \left.\frac{\partial H_{\text{eff}}}{\partial H}\right|_{H=0} = 0 \tag{3.20}$$

or

$$\left.\frac{\partial H_{\mathrm{eff}}}{\partial H}\right|_{H=0} = -\frac{R^{\mathrm{A}} - R^{\mathrm{B}}}{(P^{\mathrm{A}} - P^{\mathrm{B}}) + 3(Q^{\mathrm{A}} - Q^{\mathrm{B}})H_{\mathrm{eff}}^2} = -\frac{1}{2}\frac{1}{g_{\mathrm{c}} - g}\frac{R^{\mathrm{A}} - R^{\mathrm{B}}}{\mathrm{d}(P^{\mathrm{A}} - P^{\mathrm{B}})/\mathrm{d}g|_{g=g_{\mathrm{c}}}} \tag{3.21}$$

where we have used the expression (3.17).

Finally, the susceptibility at $g = g_{\mathrm{c}} - 0$ is given by

$$\chi^{\mathrm{I}} = \bar{\chi}_-^{\mathrm{I}}\left(\frac{g_{\mathrm{c}}}{g_{\mathrm{c}} - g}\right)^{\gamma'_{\mathrm{cl}}} \qquad \gamma'_{\mathrm{cl}} = 1 \tag{3.22}$$

$$\bar{\chi}_-^{\mathrm{I}} = \tfrac{1}{2}\bar{\chi}_+^{\mathrm{I}} \tag{3.23}$$

where $\bar{\chi}_-^{\mathrm{A}} = \bar{\chi}_-^{\mathrm{B}}$.

(v) *Critical magnetization.* At the critical point we have to consider up to third-order terms of equation (3.5). Since $P^{\mathrm{A}} - P^{\mathrm{B}} = 0$, we obtain

$$H_{\mathrm{eff}} = \left[-\frac{R^{\mathrm{A}} - R^{\mathrm{B}}}{Q^{\mathrm{A}} - Q^{\mathrm{B}}}\right]^{1/3} H^{1/3}. \tag{3.24}$$

Then the critical magnetization is given by

$$m_{\mathrm{c}}^{\mathrm{I}} = \bar{m}_{\mathrm{c}}^{\mathrm{I}} H^{1/\delta_{\mathrm{cl}}} \qquad \delta_{\mathrm{cl}} = 3 \tag{3.25}$$

$$\bar{m}_{\mathrm{c}}^{\mathrm{I}} = P^{\mathrm{I}}\left[-\frac{R^{\mathrm{A}} - R^{\mathrm{B}}}{Q^{\mathrm{A}} - Q^{\mathrm{B}}}\right]^{1/3} = [\bar{\chi}_+^{\mathrm{I}}(\bar{m}_{\mathrm{s}}^{\mathrm{I}})^2]^{1/3} \tag{3.26}$$

where $\bar{m}_{\mathrm{c}}^{\mathrm{A}} = \bar{m}_{\mathrm{c}}^{\mathrm{B}}$.

(vi) *'Specific heat' for $g > g_{\mathrm{c}}$.* Here C^{I} is called the 'specific heat' for convenience, because it is analogous to the specific heat of the corresponding two-dimensional model. Above the critical point the ground state of each cluster is $|g\rangle^{\mathrm{I}}$, and we obtain

$$C_+^{\mathrm{I}} = \frac{1}{N_{\mathrm{I}}}\frac{\mathrm{d}}{\mathrm{d}g}\langle g|S_{\mathrm{t}}^x|g\rangle^{\mathrm{I}} = \frac{1}{N_{\mathrm{I}}}\sum_{n\neq g}\langle g|S_{\mathrm{t}}^x|n\rangle^{\mathrm{I}}\langle n|S_{\mathrm{t}}^x|g\rangle^{\mathrm{I}}\frac{2}{E_n^{\mathrm{I}} - E_g^{\mathrm{I}}} \tag{3.27}$$

with

$$S_{\mathrm{t}}^x \equiv \sum_{i=1}^{N_{\mathrm{I}}} S_i^x. \tag{3.28}$$

In this calculation we have used the following relationship,

$$\frac{\mathrm{d}}{\mathrm{d}g}|g\rangle^{\mathrm{I}} = \sum_{n\neq g}|n\rangle^{\mathrm{I}}\langle n|S_{\mathrm{t}}^x|g\rangle^{\mathrm{I}}\frac{1}{E_n^{\mathrm{I}} - E_g^{\mathrm{I}}} \tag{3.29}$$

which is derived in the appendix.

4. Estimation of non-classical critical exponents and discussion

In the present section we list the data from various approximations and analyse them using the CAM. The values of the critical points and critical exponents of the relevant models are estimated by a least-squares fitting. These estimates are compared with the exact solutions, and further discussion is given.

4.1. One-dimensional $S = \frac{1}{2}$ transverse Ising model

Although there are many kinds of approximations according to choices of N_A and N_B, we consider the $\Delta N \equiv N_B - N_A = 1$ or 2 approximations here. The $\Delta N = 1$ series of approximations are consistent with the phenomenological derivation of the coherent anomaly of the double-cluster approximation [26], which is based on the assumption that the sizes of the two clusters are close to each other. In the $\Delta N = 2$ series of approximations, the relevant two clusters have the same character, namely in both clusters the numbers of spins are *odd* or *even*. The values of g_c and various critical coefficients of the $\Delta N = 1, N_A = 1$–8 and $\Delta N = 2, N_A = 1$–7 approximations are given in table 1.

Table 1. The mean-field critical point and critical coefficients of the one-dimensional $S = \frac{1}{2}$ transverse Ising model.

N_A	N_B	g_c	$\bar{\chi}_+$	$\bar{m}_s$	$\bar{m}_c$	C_+^A	C_+^B
1	2	0.638371	1.3134	1.0947	1.1632	0.0000	0.0970
1	3	0.615713	1.5134	1.1164	1.2706	0.0000	0.1654
2	3	0.592684	1.7821	1.2689	1.4210	0.1174	0.1834
2	4	0.581452	1.9716	1.3291	1.5158	0.1233	0.2408
3	4	0.570039	2.2052	1.4099	1.6366	0.2036	0.2546
3	5	0.563272	2.3862	1.4634	1.7225	0.2102	0.3031
4	5	0.556406	2.5994	1.5309	1.8264	0.2724	0.3141
4	6	0.551867	2.7735	1.5794	1.9054	0.2786	0.3560
5	6	0.547267	2.9727	1.6380	1.9980	0.3295	0.3650
5	7	0.544006	3.1410	1.6825	2.0717	0.3353	0.4017
6	7	0.540704	3.3298	1.7349	2.1561	0.3785	0.4094
6	8	0.538243	3.4932	1.7762	2.2254	0.3837	0.4420
7	8	0.535755	3.6737	1.8238	2.3033	0.4212	0.4486
7	9	0.533832	3.8328	1.8624	2.3689	0.4259	0.4780
8	9	0.531889	4.0066	1.9062	2.4417	0.4591	0.4838

We have made a least-squares fitting for various combinations of approximations. For the estimation of γ, β and δ we have assumed the simple CAM scaling form (2.15) and neglected higher-order correction terms. Generally speaking, approximations obtained from smaller clusters do not give good scaling properties, and these are not suitable for fitting. On the other hand, if we use only a few approximations obtained from larger clusters, the range of g_c is narrower and the error of fitting becomes larger. We start from the series which consists of all the approximations listed in table 1, and leave out the approximations obtained from the smallest pair of clusters in the series one by one. The estimates obtained from this procedure are not consistent with one another at the first stage, and come to be consistent after a few approximations are excluded. Here we have determined our estimates from the following two series of approximations: $(N_A, N_B) = (2,4), (3,4), \ldots, (8,9)$ and $(N_A, N_B) = (3,4), (3,5), \ldots, (8,9)$. The temporary estimates of the critical exponents and their corresponding critical points are given in table 2, where the values and errors are determined to include the ones obtained from these two series. Here 'errors' indicate the standard deviations in the estimates obtained by the fitting. Although there exist three free parameters (namely the critical point g_c^*, the exponent ψ and the constant $f^{(sc)}$) in the fitting, the errors are small. This fact shows that these series of approximations are highly canonical, and that the scaling form (2.15) is adequate (see figure 2).

Table 2. The estimates of the critical exponents (CE) and the corresponding values of the critical point of the one-dimensional $S = \frac{1}{2}$ transverse Ising model. The exponent $\alpha^{\rm I}$ ($\rm I \equiv A$ or B) denotes the estimate obtained from the cluster I. The notation $\gamma = 1.760(9)$ means $\gamma = 1.760 \pm 0.009$. The errors in γ, β and δ indicate the standard deviations in the estimates by the least-squares fitting, and those of $\alpha^{\rm A}$ and $\alpha^{\rm B}$ stand for the difference of the estimates obtained from the $\Delta N = 1, N_{\rm A} = 6$–8 approximations and the $\Delta N = 1, N_{\rm A} = 5$–7 approximations.

Exponents	γ	β	δ	$\alpha^{\rm A}$	$\alpha^{\rm B}$
Values of CE	1.760(9)	0.125(7)	15.1(6)	0(log)	0(log)
Values of $g_{\rm c}^*$	0.4999(6)	0.5011(8)	0.5005(1)	0.5013(7)	0.5038(13)

The logarithmic singularity of $C_+^{\rm I}$ cannot be expressed by the form (2.15). Instead, we have assumed the following form [23]

$$C_+^{\rm I}(g_{\rm c}) \sim a^{\rm I} \log(g_{\rm c} - g_{\rm c}^*) + b^{\rm I}. \tag{4.1}$$

The quantity $C_+^{\rm I}$ slowly converges to the form (4.1), and the previous procedure for fitting cannot be used in (4.1). The estimates of $g_{\rm c}^*$ given in table 2 are obtained from the following two series of approximations: $\Delta N = 1, N_{\rm A} = 6$–8 and $\Delta N = 1, N_{\rm A} = 5$–7. The values of $g_{\rm c}^*$s are given by the former one, and the errors of them indicate the difference of the estimates obtained from each one. The $\Delta N = 1$ or 2 series of approximations do not belong to the same canonical series in $C_+^{\rm I}$, because it is not the critical coefficient but the thermodynamic quantity itself, and the terms which do not show the coherent anomaly (for example, the first term of equation (3.13)) may be included in it. On the other hand, if we use the form (2.15), we have $g_{\rm c}^* = 0.391(78)$ ($\rm I \equiv A$) or $g_{\rm c}^* = 0.453(13)$ ($\rm I \equiv B$) from the same series of approximations. These values are not consistent with the estimates obtained from other critical coefficients at all. Thus, in the CAM framework we can conclude that $C_+^{\rm I}$ shows a logarithmic divergence at the critical point.

4.2. One-dimensional $S = \frac{1}{2}$ XZ model

In this model the ground states of *even*-spin clusters are singlet, and those of *odd*-spin clusters are two-fold degenerate. Thus, we have to treat *even*-spin clusters in order to know the behaviour of the infinite system, in which the ground state is singlet. In fact, the series of approximations obtained from *odd*-spin clusters do not show the coherent anomaly well. Here we consider the $\Delta N = 2$, $N_{\rm A} = 2$–10 and $\Delta N = 4$, $N_{\rm A} = 2$–8 approximations. The values of $g_{\rm c}$ and various critical coefficients are given in table 3.

We have made the least-squares fitting just as in the one-dimensional $S = \frac{1}{2}$ transverse Ising model. The temporary estimates of the critical exponents and their corresponding critical points are given in table 4. The estimates of γ, β and δ are obtained from the $(N_{\rm A}, N_{\rm B}) = (4,6), (4,8), \cdots, (10,12)$ series of approximations and the $(N_{\rm A}, N_{\rm B}) = (4,8), (6,8), \cdots, (10,12)$ one, and those of $\alpha^{\rm I}$ are obtained from the $\Delta N = 2$, $N_{\rm A} = 8, 10, 12$ one and the $\Delta N = 2$, $N_{\rm A} = 6, 8, 10$ one. Because of the restriction that $N_{\rm I}$ should be *even*, we have used the $\Delta N = 4$ series of approximations to increase the number of data for fitting. Although there is no such justification for the $\Delta N = 4$ series as for the $\Delta N = 2$ series, these results show that these series of approximations are also highly canonical (see figure 3).

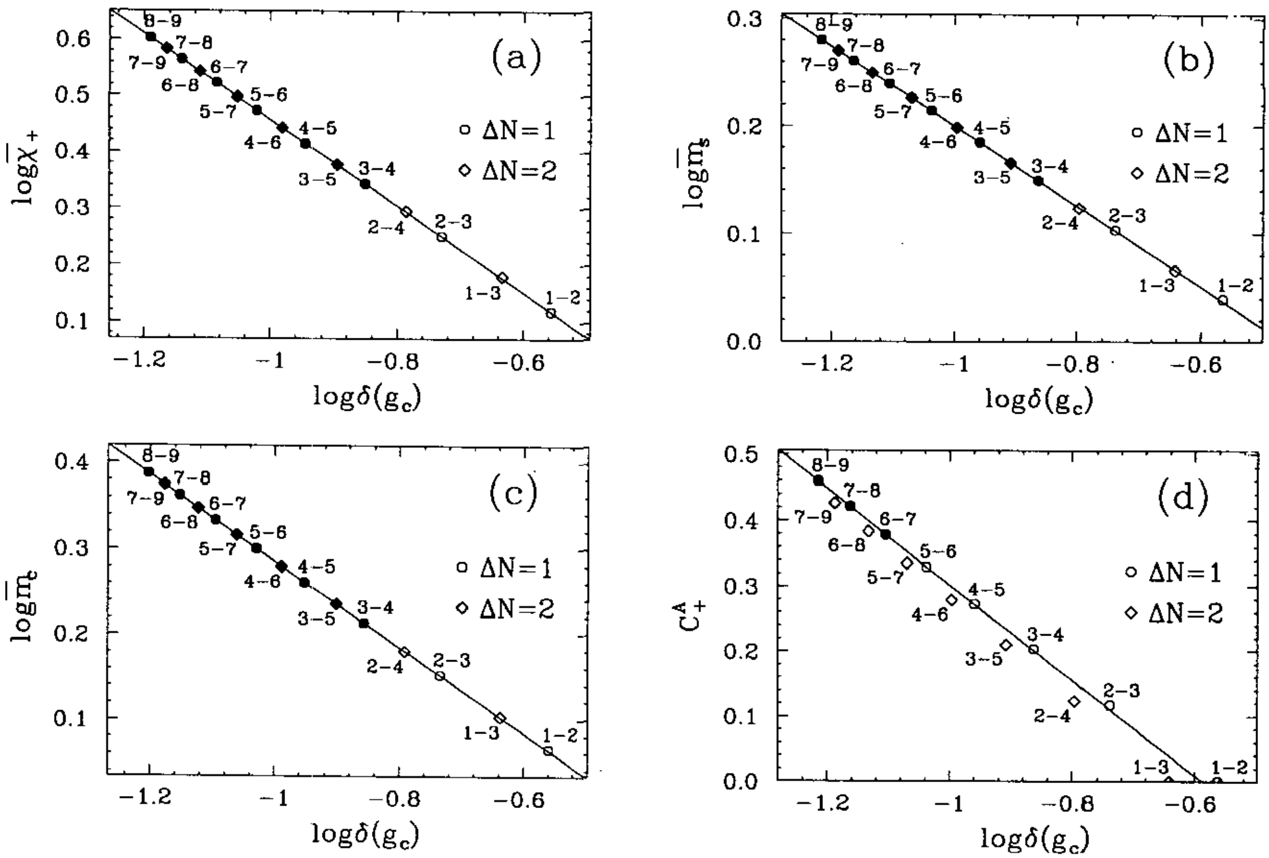

Figure 2. Coherent anomalies in the one-dimensional $S = \frac{1}{2}$ transverse Ising model: (*a*) $\log \bar{\chi}_+$, (*b*) $\log \bar{m}_s$, (*c*) $\log \bar{m}_c$ and (*d*) C_+^A are plotted against $\log \delta(g_c)$, respectively. Each pair of numbers denotes N_A and N_B. The straight line, the slope of which is equal to $-\psi$, is determined by the least-squares fitting using the data represented by the full symbols ● and ◆. The $\Delta N = 1$ and 2 series of approximations belong to the same canonical series in (*a*), (*b*) and (*c*), but not in (*d*).

Table 3. The mean-field critical point and critical coefficients of the one-dimensional $S=\frac{1}{2}$ XZ model.

N_A	N_B	g_c	$\bar{\chi}_+$	$\bar{m}_s$	$\bar{m}_c$	C_+^A	C_+^B
2	4	1.143440	2.0854	0.9407	1.2266	0.00000	0.03652
2	6	1.121763	2.2650	0.9761	1.2923	0.00000	0.05997
4	6	1.099750	2.5219	1.0256	1.3843	0.03875	0.06184
4	8	1.088179	2.6798	1.0553	1.4397	0.03938	0.07978
6	8	1.076511	2.8851	1.0929	1.5105	0.06390	0.08113
6	10	1.069325	3.0278	1.1186	1.5590	0.06456	0.09568
8	10	1.062095	3.2037	1.1495	1.6177	0.08285	0.09670
8	12	1.057198	3.3351	1.1723	1.6611	0.08344	0.10893
10	12	1.052275	3.4914	1.1987	1.7119	0.09811	0.10974

Table 4. The estimates of the critical exponents (CE) and the corresponding values of the critical point of the one-dimensional $S=\frac{1}{2}$ XZ model. The exponent α^I ($I \equiv A$ or B) denotes the estimate obtained from the cluster I. The notation $\gamma = 1.52(4)$ means $\gamma = 1.52 \pm 0.04$. The errors in γ, β and δ indicate the standard deviations in the estimates by the least-squares fitting, and those of α^A and α^B stand for the *difference of the estimates obtained* from the $\Delta N = 2, N_A = 8, 10, 12$ approximations and the $\Delta N = 2, N_A = 6, 8, 10$ approximations.

Exponents	γ	β	δ	α^A	α^B
Values of CE	1.52(4)	0.264(16)	6.8(1.1)	0(log)	0(log)
Values of g_c^*	0.998(6)	1.002(5)	0.999(4)	0.991(9)	1.005(3)

4.3. Discussion

The one-dimensional $S=\frac{1}{2}$ transverse Ising model was solved by S Katsura [7] and P Pfeuty [8], and the one-dimensional $S=\frac{1}{2}$ XZ model was solved by E Lieb, T Schultz and D Mattis [9] and B M McCoy [10]. These solutions are listed in table 5 together with our final estimates, in which the values and errors of the critical points are determined to include all the estimates obtained from the least-squares fitting of various critical coefficients except for C_+^I. Our estimates and the exact solutions are consistent with each other, which shows that our approach is powerful for the study of zero-temperature phase transitions of quantum spin systems.

Table 5. The estimates and the exact solutions of the critical points and critical exponents of (*a*) the one-dimensional $S=\frac{1}{2}$ transverse Ising model and (*b*) the one-dimensional $S=\frac{1}{2}$ XZ model. The 'exact' exponents γ and δ are obtained from other exact values and the scaling relations.

	Quantities	g_c^*	γ	β	δ	α
(*a*)	Our estimates	0.5005(14)	1.760(9)	0.125(7)	15.1(6)	0(log)
	Exact solutions [7, 8]	0.5	1.75	0.125	15	0(log)
(*b*)	Our estimates	1.000(8)	1.52(4)	0.264(16)	6.8(1.1)	0(log)
	Exact solutions [9, 10]	1	1.5	0.25	7	0(log)

The phenomenological derivation of the double-cluster approximation [26] is based on the finite-size scaling hypothesis, namely based on the assumptions that the size

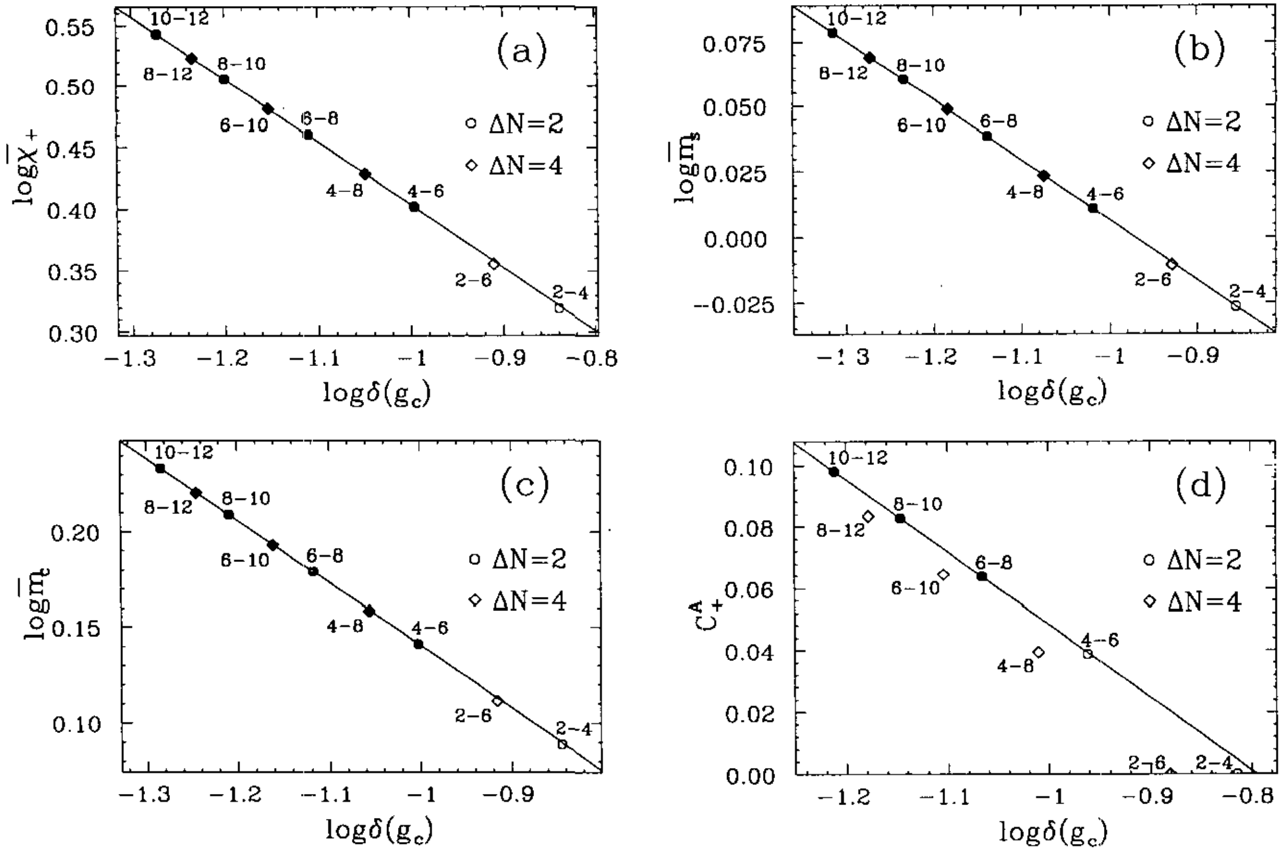

Figure 3. Coherent anomalies in the one-dimensional $S = \frac{1}{2}$ XZ model: (a) $\log \bar{\chi}_+$, (b) $\log \bar{m}_s$, (c) $\log \bar{m}_c$ and (d) C_+^A are plotted against $\log \delta(g_c)$, respectively. Each pair of numbers denotes N_A and N_B. The straight line, the slope of which is equal to $-\psi$, is determined by the least-squares fitting using the data represented by the full symbols ● and ◆. The $\Delta N = 2$ and 4 series of approximations belong to the same canonical series in (a), (b) and (c), but not in (d).

of each cluster is large enough and that the two clusters have the same shape and their sizes are close to each other. However, the results obtained in the present section show that the approximations using small clusters or large-ΔN pairs of clusters are also canonical. These facts suggest that in the double-cluster approximation the CAM scaling is satisfied beyond the range of validity of the finite-size scaling. This property is expected to be useful when we treat higher-spin or higher-dimensional systems, because many approximations can be obtained from several clusters.

In the present paper we have tried to estimate the critical exponents not only of the disordered phase (γ and α), but also of the ordered phase (β) and at the critical point (δ). For this purpose we have had to calculate all the excited states of the cluster Hamiltonian, and consequently we can only treat small clusters because of the limited memories of computers. However, if we only want to know the critical phenomena of the disordered phase, it is possible to calculate $\bar{\chi}^{\mathrm{I}}_{+}$ and C^{I}_{+} using only the ground state of the cluster Hamiltonian and numerical differentiation with respect to H, H_{eff} or g at most twice. On the other hand, in order to evaluate $\bar{m}^{\mathrm{I}}_{\mathrm{s}}$ and $\bar{m}^{\mathrm{I}}_{\mathrm{c}}$, we have to perform this numerical differentiation four times, which is practically difficult because of the limited accuracy of the numerical computations.

Thus, using the Lanczös algorithm we can treat rather large clusters, the sizes of which are comparable with those used in the finite-size scaling method [4]. Then our approach is expected to give better results than those obtained from the finite-size scaling method, because much more data are available for fitting in our scheme. Using this technique we are now studying two-dimensional quantum spin systems and $S = 1$ quantum spin systems.

5. Summary

In the present paper we have formulated the double-cluster approximation for quantum spin systems at $T = 0$, and we have estimated not only the critical points but also the critical exponents γ, β, δ and α of the one-dimensional $S = \frac{1}{2}$ transverse Ising model and the one-dimensional $S = \frac{1}{2}$ XZ model using the CAM. Our estimates are in good agreement with the exact solutions, which shows that the CAM works well in zero-temperature phase transitions of quantum spin systems. Studies by us are now in progress to apply the present method to higher-dimensional quantum spin systems and higher-spin quantum spin systems.

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Appendix

Here we briefly derive the explicit expression of the derivative $\mathrm{d}P^{\mathrm{I}}/\mathrm{d}g|_{g=g_c}$ ($\mathrm{I} \equiv$ A or B).

At first we differentiate the Schrödinger equation of the unperturbed Hamiltonian $\mathcal{H}^{(\mathrm{cl})}_{N_\mathrm{I}}$,

$$\mathcal{H}^{(\mathrm{cl})}_{N_\mathrm{I}}|n\rangle^{\mathrm{I}} = \left(-\sum_{i=1}^{N_\mathrm{I}-1} S_i^z S_{i+1}^z - g\sum_{i=1}^{N_\mathrm{I}} S_i^x\right)|n\rangle^{\mathrm{I}} = E_n^{\mathrm{I}}|n\rangle^{\mathrm{I}} \tag{A1}$$

with respect to g, and expand the derivative $\mathrm{d}|n\rangle^{\mathrm{I}}/\mathrm{d}g$ in terms of $\{|m\rangle^{\mathrm{I}}\}$, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}g}|n\rangle^{\mathrm{I}} = \sum_m a^{\mathrm{I}}_{n,m}|m\rangle^{\mathrm{I}}. \tag{A2}$$

After a short calculation we obtain

$$\frac{\mathrm{d}}{\mathrm{d}g}|n\rangle^{\mathrm{I}} = \sum_{\substack{m \\ E_m^{\mathrm{I}} \neq E_n^{\mathrm{I}}}} |m\rangle^{\mathrm{I}}\langle m|S_\mathrm{t}^x|n\rangle^{\mathrm{I}}\frac{1}{E_m^{\mathrm{I}} - E_n^{\mathrm{I}}} + \sum_{\substack{l \\ E_l^{\mathrm{I}} = E_n^{\mathrm{I}}}} a^{\mathrm{I}}_{n,l}|l\rangle^{\mathrm{I}}. \tag{A3}$$

In particular, when $|n\rangle^{\mathrm{I}} = |g\rangle^{\mathrm{I}}$, we have

$$\frac{\mathrm{d}}{\mathrm{d}g}|g\rangle^{\mathrm{I}} = \sum_{n\neq g} |n\rangle^{\mathrm{I}}\langle n|S_\mathrm{t}^x|g\rangle^{\mathrm{I}}\frac{1}{E_n^{\mathrm{I}} - E_g^{\mathrm{I}}} \tag{A4}$$

because $|g\rangle^{\mathrm{I}}$ is not degenerate.

Then after some straightforward calculation the derivative $\mathrm{d}P^{\mathrm{I}}/\mathrm{d}g|_{g=g_c}$ is given by

$$\begin{aligned}\left.\frac{\mathrm{d}}{\mathrm{d}g}P^{\mathrm{I}}\right|_{g=g_c} &= \frac{1}{N_\mathrm{I}}\sum_{n\neq g}\sum_{m\neq g}(\langle g|S_\mathrm{t}^z|n\rangle^{\mathrm{I}}\langle n|S_\mathrm{b}^z|m\rangle^{\mathrm{I}}\langle m|S_\mathrm{t}^x|g\rangle^{\mathrm{I}} \\ &\quad + \langle n|S_\mathrm{t}^z|m\rangle^{\mathrm{I}}\langle m|S_\mathrm{b}^z|g\rangle^{\mathrm{I}}\langle g|S_\mathrm{t}^x|n\rangle^{\mathrm{I}} \\ &\quad + \langle m|S_\mathrm{t}^z|g\rangle^{\mathrm{I}}\langle g|S_\mathrm{b}^z|n\rangle^{\mathrm{I}}\langle n|S_\mathrm{t}^x|m\rangle^{\mathrm{I}})\frac{2}{(E_n^{\mathrm{I}} - E_g^{\mathrm{I}})(E_m^{\mathrm{I}} - E_g^{\mathrm{I}})} \\ &\quad - \frac{1}{N_\mathrm{I}}\sum_{n\neq g}\langle g|S_\mathrm{t}^z|n\rangle^{\mathrm{I}}\langle n|S_\mathrm{b}^z|g\rangle^{\mathrm{I}}\langle g|S_\mathrm{t}^x|g\rangle^{\mathrm{I}}\frac{2}{(E_n^{\mathrm{I}} - E_g^{\mathrm{I}})^2}.\end{aligned} \tag{A5}$$

References

[1] Sneddon L and Stinchcombe R B 1979 *J. Phys. C: Solid State Phys.* **12** 3761

[2] Hamer C J and Barber M N 1980 *J. Phys. A: Math. Gen.* **13** L169

[3] For example, Hamer C J and Barber M N 1981 *J. Phys. A: Math. Gen.* **14** 241, 259, 2009

[4] For example, Hamer C J and Johnson C H J 1986 *J. Phys. A: Math. Gen.* **19** 423

[5] Suzuki M 1986 *J. Phys. Soc. Japan* **55** 4205

[6] Suzuki M, Katori M and Hu X 1987 *J. Phys. Soc. Japan* **56** 3092

[7] Katsura S 1962 *Phys. Rev.* **127** 1508

[8] Pfeuty P 1970 *Ann. Phys.* **57** 79; see also [9] and [10]

[9] Lieb E, Schultz T and Mattis D 1961 *Ann. Phys.* **16** 407; see also [7]

[10] McCoy B M 1968 *Phys. Rev.* **173** 531
Wu T T 1966 *Phys. Rev.* **149** 380
[11] Oguchi T and Ono I 1966 *J. Phys. Soc. Japan* **21** 2178
[12] Oguchi T and Kitatani H 1988 *J. Phys. Soc. Japan* **57** 3973
[13] Fujiki S, Katori M and Suzuki M 1990 *J. Phys. Soc. Japan* **59** 2681
[14] Lipowski A 1991 *J. Magn. Magn. Mater.* **96** 267
[15] Lipowski A 1991 *Physica* A **173** 293
[16] Hatano N and Suzuki M 1992 *J. Stat. Phys.* **66** in press
[17] Suzuki M 1991 *Evolutionary Trends in the Physical Sciences* ed M Suzuki and R Kubo (Berlin: Springer)
[18] Ito N and Suzuki M 1988 *Int. J. Mod. Phys.* B **2** 1
[19] Mano H 1990 *J. Magn. Magn. Mater.* **90–91** 281
[20] Suzuki M 1976 *Prog. Theor. Phys.* **56** 1454
[21] Fradkin E and Susskind L 1978 *Phys. Rev.* D **17** 2637
[22] Kogut J B 1979 *Rev. Mod. Phys.* **51** 659
[23] Hu X, Katori M and Suzuki M 1987 *J. Phys. Soc. Japan* **56** 3865
[24] Hu X and Suzuki M 1988 *J. Phys. Soc. Japan* **57** 791
[25] Hu X and Suzuki M 1990 *J. Phys. A: Math. Gen.* **23** 3051
[26] Suzuki M, Hatano N and Nonomura Y 1991 *J. Phys. Soc. Japan* **60**; see also [6]
Ito N and Suzuki M 1991 *Phys. Rev.* B **43** 3483