Improved chain mean-field theory for quasi-one-dimensional quantum magnets

Synge Todo[1,2,*] and Akira Shibasaki[1,†]
[1]*Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan*
[2]*CREST, Japan Science and Technology Agency, Kawaguchi 332-0012, Japan*
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A mean-field approximation for quasi-one-dimensional (Q1D) quantum magnets is formulated. Our mean-field approach is based on the Bethe-type effective-field theory, where thermal and quantum fluctuations between the nearest-neighbor chains as well as those in each chain are taken into account exactly. The self-consistent equation for the critical temperature contains the boundary-field magnetic susceptibilities of a multichain cluster, which can be evaluated accurately by some analytic or numerical methods, such as the powerful quantum Monte Carlo method. We show that the accuracy of the critical temperature of Q1D magnets as a function of the strength of interchain coupling is significantly improved compared with the conventional chain mean-field theory. It is also demonstrated that our approximation can predict nontrivial dependence of critical temperature on the sign (i.e., ferromagnetic or antiferromagnetic) of interchain coupling as well as on the impurity concentration in randomly diluted Q1D Heisenberg antiferromagnets.

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I. INTRODUCTION

Space dimensionality plays an essential role in phase transitions and critical phenomena of quantum magnets. As the dimension is lowered, effects of thermal and quantum fluctuations generally become stronger. As a result, the quantum antiferromagnetic Heisenberg model in two dimensions, for example, does not exhibit long-range order any more except at the ground state,[1] though a finite-temperature phase transition occurs in its three-dimensional (3D) counterpart. Furthermore, there is no long-range order even at zero temperature in one dimension.[2] Such one-dimensional magnets arose great interests as many phenomena characteristic of systems with strong quantum fluctuations, e.g., Tomonaga-Luttinger liquid state or Haldane gap state, have been observed theoretically as well as in the experiments.[3]

Real materials, however, cannot be purely one dimensional but three dimensional, i.e., there always exist interactions between one-dimensional chains (*interchain* interactions) albeit it is much weaker, often by orders of magnitude, than the dominant interactions along the chains (*intrachain* interactions). Three-dimensional materials with strong spatial anisotropy are often referred to as quasi-one-dimensional (Q1D) systems. Indeed, in many Q1D materials a long-range order emerges at low temperatures, which is a direct consequence of three dimensionality of the system. In order to explain low-energy behavior of such Q1D materials correctly, a theory which properly incorporates the effect of interchain interaction is essential.

So far, effects of weak interchain interactions in Q1D quantum magnets have been studied mainly by means of the chain mean-field approximation, where interchain spin fluctuations are ignored completely.[4,5] Within the framework of the chain mean-field approximation, a Q1D magnet is reduced to a single chain in an effective external field. For the latter system, fortunately there exist a couple of exact solutions; otherwise one can still use powerful analytic methods, such as bosonization, as well as numerical simulations, such as exact diagonalization or density-matrix renormalization-group method, which are effective especially in one dimension.

Naively, one may expect that the chain mean-field approximation becomes more and more accurate not only qualitatively but also quantitatively, as the interchain interactions become weak enough compared to those along the chains. The recent theoretical study[6] as well as the sensitive Monte Carlo simulations[7,8] on Q1D spin models, however, have revealed that this is not the case; there remains systematic error of the chain mean-field theory even in the weak interchain coupling limit. Instead, the critical temperature as a function of the interchain coupling is well described by a chain mean-field formula with a renormalized effective coordination number (or effective interchain coupling[9]). Especially, in the Q1D classical Ising models, it is proved that the renormalization factor is exactly given by the critical transverse field of the quantum phase transition of a two-dimensional quantum Ising model.[8] This analytic result demonstrates clearly that the weak interchain coupling limit of the Q1D magnet is *not* the weak-coupling limit but is still the strongly correlated regime.

The renormalization of effective interplane coupling is also observed in weakly coupled two-dimensional planes.[7] For this quasi-two-dimensional system, a scaling theory was developed,[10] in which it is expected different scaling behavior depending on whether the purely two-dimensional system is in a quantum critical regime or in a renormalized classical regime. This prediction has been verified by a recent quantum Monte Carlo (QMC) simulation.[11]

Thus it has become evident by the recent theoretical and numerical studies that we need a theory beyond the conventional chain mean-field approximation to describe the critical temperature of the Q1D magnets in the weak interchain coupling regime more accurately. Even worse, when the chain mean-field theory is applied to a system with quenched disorder, the random average in each chain is taken before the thermal average on the whole lattice. The adverse impact of interchanging the average operations is further nontrivial. It is naturally expected that some of these drawbacks of the chain mean-field theory might be remedied by considering

multiple chains, instead of a single chain, and taking the interactions between those chains into account in a proper way. Along this line, Sandvik[12] proposed a multichain mean-field theory and applied it successfully to the problem of ground-state staggered magnetization in a two-dimensional Heisenberg antiferromagnet.

In the present paper, we propose a different type of chain mean-field theory, i.e., the chain Bethe approximation. Actually, it is well known that there are two different formulations in traditional mean-field theories for classical spin models; that is, the Weiss[13] approximation and the Bethe approximation.[14,15] In the former, the effective field is identified explicitly with the order parameter. In the latter, on the other hand, the effective field is determined implicitly so that the local order parameter at the central spin and that of spins on the cluster boundary coincide with each other. In the Bethe mean-field theory, therefore, spin fluctuations between nearest-neighboring sites are taken into account even in the lowest-order approximation. Furthermore, as the cluster size increases, the critical temperature by the Bethe-type approximation converges to the exact value more rapidly being free from logarithmic corrections which is observed in the Weiss-type theory.[16] By applying the idea of the Bethe-type effective-field theory, we introduce a different chain mean-field theory for Q1D quantum magnets.

The present paper is organized as follows. In Sec. II, after a brief review of the conventional chain mean-field approximation, we formulate our Bethe-type chain mean-field theory: the chain Bethe approximation. In Sec. III, the chain Bethe approximation is applied to the Q1D Heisenberg antiferromagnets, where we show that by using our approximation, the accuracy of the critical temperature is significantly improved compared with the conventional chain mean-field theory. In addition, we demonstrate that the present theory can predict a *lower* critical temperature for the ferromagnetic interchain coupling than in the antiferromagnetic case, which is also confirmed by the QMC simulation. In Sec. IV, we apply the chain Bethe theory to a random quantum magnet, the site-diluted Q1D Heisenberg antiferromagnet, where the existence of a finite critical impurity concentration, above which the long-range order does not emerge even in the zero-temperature limit, is predicted by using the chain Bethe approximation. Section V is for a summary and discussion.

II. CHAIN BETHE MEAN-FIELD THEORY

A. Conventional chain mean-field approximation

The Hamiltonian of spin-1/2 Heisenberg model on a Q1D simple-cubic lattice is defined by

$$\mathcal{H} = J\sum_{i,j,k} \boldsymbol{S}_{i,j,k}\cdot\boldsymbol{S}_{i,j,k+1} + J'\sum_{i,j,k} \boldsymbol{S}_{i,j,k}\cdot\boldsymbol{S}_{i+1,j,k} + J'\sum_{i,j,k} \boldsymbol{S}_{i,j,k}\cdot\boldsymbol{S}_{i,j+1,k} - h\sum_{i,j,k} \phi^{i+j}(-1)^k S^z_{i,j,k}, \quad (1)$$

where $\boldsymbol{S}_{i,j,k}=(S^x_{i,j,k},S^y_{i,j,k},S^z_{i,j,k})$ is an $S=1/2$ quantum spin operator at site (i,j,k). We take the lattice z axis as the chain direction. The first term in Eq. (1) represents the intrachain interactions (with coupling constant J), while the second and third terms denote the interchain interactions (J'). In the present paper we consider only the case where the intrachain coupling J is antiferromagnetic ($J>0$), whereas the interchain coupling J' is either antiferromagnetic ($J'>0$) or ferromagnetic ($J'<0$). Generalization to the case with ferromagnetic intrachain coupling is also straightforward. The last term in Eq. (1) represents an external magnetic field conjugate to the order parameter, where the phase factor ϕ is defined as $\phi=-\mathrm{sgn}(J')$.

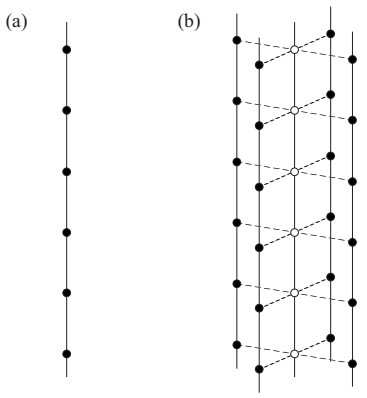

FIG. 1. Clusters for (a) chain Weiss and (b) chain Bethe approximations. The solid and dashed lines denote the intrachain (J) and interchain (J') interactions, respectively. In the chain Weiss approximation, an alternating effective field with the same amplitude applies on all spins. In the chain Bethe approximation, on the other hand, a staggered effective field applies only on the spins on the side chains (filled symbols).

In the conventional chain mean-field approximation referred to as the *chain Weiss theory* hereafter, spin fluctuations between the chains are ignored and replaced by an effective field, i.e.,

$$J'\boldsymbol{S}_{i,j,k}\cdot\boldsymbol{S}_{i',j',k} \simeq J'\boldsymbol{S}_{i,j,k}\cdot\langle\boldsymbol{S}_{i',j',k}\rangle + J'\langle\boldsymbol{S}_{i,j,k}\rangle\cdot\boldsymbol{S}_{i',j',k} + \mathrm{const}, \quad (2)$$

where $(i',j')=(i\pm1,j)$ or $(i,j\pm1)$. As a result, the original Hamiltonian (1) is decoupled into a set of independent chains [Fig. 1(a)]. The effective chain Hamiltonian for $(i,j)=(0,0)$ is written as

$$\mathcal{H}_c = J\sum_k \boldsymbol{S}_k\cdot\boldsymbol{S}_{k+1} + J'\sum_k \boldsymbol{S}_k\cdot\boldsymbol{M}_k - h\sum_k (-1)^k S^z_k, \quad (3)$$

with $\boldsymbol{S}_k\equiv\boldsymbol{S}_{0,0,k}$ and

$$\boldsymbol{M}_k \equiv \langle\boldsymbol{S}_{1,0,k}\rangle + \langle\boldsymbol{S}_{-1,0,k}\rangle + \langle\boldsymbol{S}_{0,1,k}\rangle + \langle\boldsymbol{S}_{0,-1,k}\rangle. \quad (4)$$

In the low-temperature-ordered phase, a finite magnetization appears spontaneously even at $h=0$. We assume that the magnetization is along the z direction in the spin space, i.e., $\langle\boldsymbol{S}_{i,j,k}\rangle=[0,0,\phi^{i+j}(-1)^k m(T)]$. Chain Hamiltonian (3) with $h=0$ is then reduced to

$$\mathcal{H}_c = J\sum_k \boldsymbol{S}_k\cdot\boldsymbol{S}_{k+1} - 4|J'|m(T)\sum_k (-1)^k S^z_k. \quad (5)$$

Since the magnitude of the spontaneous magnetization does not depend on the position of the spin, the self-consistent condition

$$m(T) = m_c[T, 4|J'|m(T)] \tag{6}$$

must be fulfilled, where

$$m_c(T,h) \equiv \frac{1}{L}\sum_k (-1)^k \langle S_k^z \rangle_c \tag{7}$$

is the staggered magnetization density of genuinely one-dimensional antiferromagnetic chain of length L. The average $\langle \cdots \rangle_c$ in Eq. (7) means the expectation value of the one-dimensional chain [i.e., Eq. (3) with $J'=0$], while $\langle \cdots \rangle$ [e.g., in Eqs. (1) and (4)] denotes the average with respect to the original (full-3D) Hamiltonian (1).

At high temperatures, on the other hand, no spontaneous magnetization appears. Under the presence of small external magnetic field, however, a finite magnetization $\langle \boldsymbol{S}_{i,j,k} \rangle = [0, 0, \phi^{i+j}(-1)^k m(T,h)]$ is induced. In this case, the effective chain Hamiltonian (5) is modified as

$$\mathcal{H}_c = J\sum_k \boldsymbol{S}_k \cdot \boldsymbol{S}_{k+1} - [h + 4|J'|m(T,h)]\sum_k (-1)^k S_i^z. \tag{8}$$

Since $m(T,h) \ll 1$ for $h \ll 1$ in the disordered phase, one can consider only the lowest order in h,

$$m(T,h) \simeq [h + 4|J'|m(T,h)]\chi_c(T), \tag{9}$$

where $\chi_c(T)$ is the zero-field staggered susceptibility of one-dimensional antiferromagnetic chain. Noticing that $m(T,h)$ in the both sides can also be written as $h\chi(T)$ for $h \ll 1$, we obtain the following mean-field expression for the susceptibility:

$$\chi(T) = \frac{\chi_c(T)}{1 - 4|J'|\chi_c(T)}. \tag{10}$$

In terms of the chain Weiss theory, the critical temperature is thus given by the pole of the right-hand side of Eq. (10). For generic Q1D lattices the self-consistent equation is written as follows:

$$1 - z|J'|\chi_c(T_c) = 0, \tag{11}$$

where z is the coordination number of the lattice, i.e., the number of nearest-neighbor chains. Note that the self-consistent equation depends not on the sign of J' but only on its absolute magnitude. In other words, the conventional chain Weiss theory does not distinguish between the antiferromagnetic and ferromagnetic interchain interactions. This is one of the major drawbacks of the conventional chain mean-field theory. Another problem is that most of physical quantities, such as the energy, specific heat, correlation functions, etc., are the same as those of the genuine one-dimensional chain at temperatures higher than T_c, since the effective field is proportional to the order parameter, which is zero at $T > T_c$. We will see below that these disadvantages of the chain Weiss approximation are solved in the chain Bethe mean-field theory.

B. Bethe-type mean-field theory

In the chain Weiss approximation, the effect of interchain interaction was replaced by an effective field. The effective interchain interaction is directly related with the order parameter and interchain spin fluctuations are thus ignored completely. The approximation can be improved by taking interchain spin fluctuations into account systematically. In the chain Bethe approximation introduced in this section, the interaction between the nearest-neighbor chains is taken into account exactly and those around the multichain cluster are treated as effective fields. In the Bethe approximation,[14,15] the effective field is determined so that the magnetization of the central spin and that on the cluster boundary coincide with each other. Contrary to the Weiss theory, the order parameter is not given explicitly by the effective field but is its implicit function.

Let us consider the chain Bethe approximation for the simple-cubic lattice. In this case we prepare a cluster of five chains [Fig. 1(b)], where an effective field is applied only to the spins on the side chains (black circles). The effective Hamiltonian is written as

$$\mathcal{H}_\Omega = J\sum_{\alpha=0}^{4}\sum_k \boldsymbol{S}_{\alpha,k} \cdot \boldsymbol{S}_{\alpha,k+1} + J'\sum_{\alpha=1}^{4}\sum_k \boldsymbol{S}_{0,k} \cdot \boldsymbol{S}_{\alpha,k} - h\sum_k (-1)^k S_{0,k}^z - (h + h_{\mathrm{eff}})\sum_{\alpha=1}^{4}\sum_k \phi(-1)^k S_{\alpha,k}^z, \tag{12}$$

where $\alpha=0$ denotes the central chain $[(i,j)=(0,0)]$ and $\alpha = 1, \ldots, 4$ denotes the side chains $[(i,j)=(\pm 1, 0)$ or $(0, \pm 1)]$.

In the chain Bethe approximation, we impose the condition that the absolute value of the local magnetization does not depend on its position,

$$(-1)^k \langle \boldsymbol{S}_{0,k} \rangle_\Omega = \phi(-1)^{k'} \langle \boldsymbol{S}_{\alpha,k'} \rangle_\Omega \tag{13}$$

for any k, k', and $\alpha = 1, \ldots, 4$, or equivalently

$$m_{\Omega,0}(T,h,h_{\mathrm{eff}}) = \frac{\phi}{4}\sum_{\alpha=1}^{4} m_{\Omega,\alpha}(T,h,h_{\mathrm{eff}}), \tag{14}$$

where $m_{\Omega,\alpha}(T,h,h_{\mathrm{eff}})$ is the staggered magnetization density of the αth chain,

$$m_{\Omega,\alpha}(T,h,h_{\mathrm{eff}}) = \frac{1}{L}\sum_k (-1)^k \langle \boldsymbol{S}_{\alpha,k} \rangle_\Omega. \tag{15}$$

Here $\langle \cdots \rangle_\Omega$ denotes the expectation value of the chain Bethe cluster and L denotes the number of spins in the chain direction.

In Fig. 2, the h_{eff} dependence of both sides in Eq. (14) is demonstrated for $J'=0.1J$ and $h=0$, where the magnetization is calculated by means of the QMC method for a $L=64$ chain Bethe cluster (see Sec. III A for simulation details). It is clearly seen that Eq. (14) has only one trivial solution, $h_{\mathrm{eff}}=0$, at high temperatures. On the other hand, at low temperatures two more nontrivial solutions ($h_{\mathrm{eff}} \neq 0$) appear, which correspond to the the symmetry-broken phase.

The critical temperature in the framework of the chain Bethe approximation is defined as the point where the three solutions at low temperatures get degenerated with each other (Fig. 2). In practice, we set $h=0$ in Eq. (14) and expand

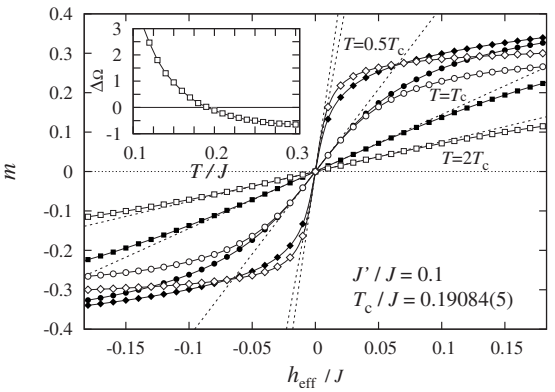

FIG. 2. h_{eff} dependence of the local magnetization of the center spins (open symbols) and the boundary spins (filled symbols) of $L=64$ chain Bethe cluster with $J'/J=0.1$. At temperatures higher than the critical temperature (squares) two curves intersect only at $h_{\mathrm{eff}}=0$, while at lower temperature (diamonds) nontrivial solutions corresponding to the symmetry-broken phases appear. The dashed lines denote the tangent of each curve at $h_{\mathrm{eff}}=0$. In the inset, temperature dependence of Δ_Ω [Eq. (16)] is also presented.

both sides in terms of h_{eff}. The self-consistent equation for the critical temperature is then written as

$$\Delta_\Omega(T_c) \equiv J\left[\chi_{\Omega,0}(T_c) - \frac{\phi}{4}\sum_{\alpha=1}^{4}\chi_{\Omega,\alpha}(T_c)\right] = 0 \tag{16}$$

with the boundary-field susceptibilities

$$\chi_{\Omega,\alpha}(T) = \left.\frac{\partial m_{\Omega,\alpha}(T,h,h_{\mathrm{eff}})}{\partial h_{\mathrm{eff}}}\right|_{h=0,h_{\mathrm{eff}}=0}$$

$$= \frac{\beta}{L}\sum_{\alpha'=1}^{4}\sum_{k,k'}\langle S^z_{\alpha,k};S^z_{\alpha',k'}\rangle_\Omega, \tag{17}$$

where $\langle A;B\rangle_\Omega$ denotes the canonical correlation,

$$\langle A;B\rangle_\Omega = \frac{1}{\beta}\frac{\mathrm{Tr}\int_0^\beta Ae^{-\tau\mathcal{H}_\Omega}Be^{-(\beta-\tau)\mathcal{H}_\Omega}d\tau}{\mathrm{Tr}\,e^{-\beta\mathcal{H}_\Omega}} \tag{18}$$

of two operators A and B. In the inset of Fig. 2, we show the temperature dependence of $\Delta_\Omega(T)$. As the temperature increases, $\Delta_\Omega(T)$ decreases monotonically. The critical temperature, in terms of the chain Bethe approximation, is given as the zero of $\Delta_\Omega(T)$. For $J'/J=0.1$, we obtained $T_c/J=0.19084(5)$.

III. CRITICAL TEMPERATURE OF Q1D QUANTUM HEISENBERG MODELS

A. Numerical method

In this section, we discuss the interchain coupling dependence of the critical temperature for the $S=1/2$ Heisenberg model on a Q1D simple-cubic lattice [Eq. (1)] in terms of the chain Bethe approximation. Since the boundary-field susceptibility of the chain Bethe cluster [Eq. (17)] cannot be evaluated analytically, one needs to introduce some reasonable approximation or some numerical method. In the present paper, we adopt the continuous-time loop cluster QMC algorithm, which is one of the most effective methods for simulating unfrustrated quantum spin systems.[17,18] It is a variant of the world-line QMC method based on the Suzuki-Trotter path-integral expansion. The continuous-time loop algorithm, however, works directly in the imaginary-time continuum, and thus it is completely free from the time discretization error. Furthermore, the correlation between successive spin configurations on the Markov chain is greatly reduced often by several orders of magnitude. This is manifested by the fact that clusters of spins called loops, whose linear size corresponds directly to the length scale of relevant spin fluctuations, are flipped at once in the loop algorithm.

The boundary-field susceptibilities in Eq. (17) are calculated by means of the improved estimator.[17] The largest system size in the chain direction is $L=64$ for $|J'|/J\geq 0.05$. For smaller $|J'|$'s, longer systems (e.g., $L=512$ for $|J'|/J=0.01$) are needed to obtain the susceptibilities in the thermodynamic limit $L\to\infty$, since the critical temperature decreases as $|J'|$ does. Periodic boundary conditions are imposed along the chains. We interpolate the QMC results at various temperatures by a polynomial and estimate the zero of $\Delta_\Omega(T)$, which gives the critical temperature. (See, e.g., the inset of Fig. 2.)

B. Comparison of chain Bethe theory with other methods

The accuracy of the present chain Bethe approximation is checked by comparing with the results of QMC simulations of full-3D systems, i.e., simple-cubic lattice of $L_x\times L_y\times L_z$ sites with periodic boundary conditions along all the lattice axes. For the antiferromagnetic interchain interactions $J'/J>0$, we take the full-3D QMC results from Ref. 7. For $J'/J<0$, the critical temperature is estimated from the crossing point of the Binder cumulant,

$$Q = \frac{\langle m^2\rangle^2}{\langle m^4\rangle} \tag{19}$$

of the generalized magnetization density

$$m = \frac{1}{L_xL_yL_z}\sum_{i,j,k}(-1)^k S^z_{i,j,k} \tag{20}$$

for different system sizes. The largest system size we simulate is $(L_x,L_y,L_z)=(40,40,40)$ and $(12,12,264)$ for $|J'|/J=1$ and 0.01, respectively. The results of finite-size scaling are summarized in Table I.

In Fig. 3, we show the J' dependence of the critical temperature calculated in terms of the chain Bethe approximation both for antiferromagnetic $(J'>0)$ and ferromagnetic $(J'<0)$ interchain interactions together with the full-3D QMC results. The intrachain interaction is antiferromagnetic $(J>0)$ in either case. In Fig. 3, we also present the results of the chain Weiss approximation and the Green's function method with Tyablikov decoupling.[19,20] As for the chain Weiss theory, we use the susceptibility of genuinely one-dimensional antiferromagnetic chain calculated by the QMC

TABLE I. J' dependence of the critical temperature for antiferromagnetic ($J'>0$) and ferromagnetic ($J'<0$) interchain interactions obtained by the full-3D QMC calculation. The results for $J'>0$ are from the previous QMC study (Ref. 7). The figure in the parenthesis denotes the error in the last digit.

	T_c/J	
$\lvert J'\rvert/J$	$J'>0$	$J'<0$
1	0.94416(9)	0.87330(2)
0.5	0.59248(6)	0.55419(3)
0.3	0.4151(2)	
0.2	0.30202(5)	0.28685(2)
0.1	0.16917(2)	0.16295(2)
0.05	0.09129(4)	0.08900(3)
0.02	0.039432(7)	0.03899(2)
0.01	0.020763(8)	0.02080(2)

method for the antiferromagnetic chain of 256 spins.

In both of antiferromagnetic and ferromagnetic interchain coupling cases, the critical temperature decreases monotonically as $|J'|/J$ does. For $|J'|\approx J$, it is observed that the chain Weiss theory overestimates the critical temperature greatly. This is is because this approximation ignores the interchain spin fluctuations completely. On the other hand, for $|J'|\ll J$ the Tyablikov approximation gets worse. Indeed, it predicts the critical temperature proportional to the square root of $|J'|/J$, which does not agree with the correct asymptotic behavior $T_c\sim|J'|/J$ (with some logarithmic corrections).[4,5] It should be noted that the chain Weiss theory and the Tyablikov approximation both give the identical critical temperature dependence regardless of the sign of the interchain coupling.

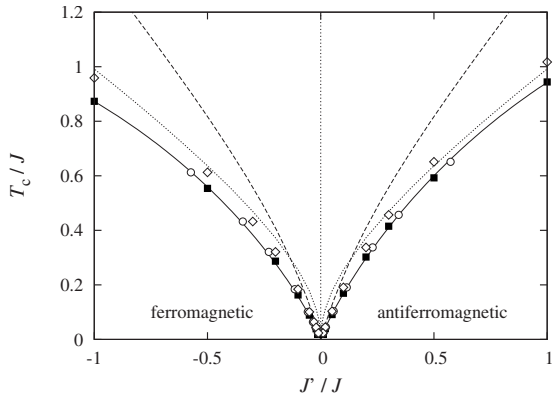

FIG. 3. J' dependence of the critical temperature calculated by chain Bethe theory (diamonds), chain Weiss theory (dashed lines), Tyablikov approximation (dotted lines), and full-3D QMC (filled squares), for antiferromagnetic (right) and ferromagnetic (left) interchain couplings. The QMC results for the antiferromagnetic interchain coupling are taken from Ref. 7. The chain Weiss and Tyablikov approximations both produce the identical results for the antiferromagnetic and ferromagnetic cases. The solid lines are guides for the eyes. The error bar of each data is much smaller than the symbol size. The results of modified chain Bethe approximation with $J'_{\rm eff}=0.872J'$ (see the text) are also presented as open circles.

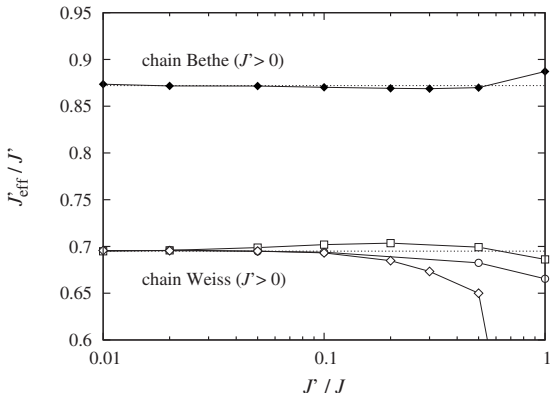

FIG. 4. J' dependence of the renormalization factor $J'_{\rm eff}/J'$ for chain Bethe (filled diamonds) and chain Weiss ($S=1/2$ open diamonds, $S=3/2$ circles, and $S=\infty$ squares) approximations. The horizontal dashed lines denote their limiting values (0.872 and 0.695, respectively) for $J'/J\to 0$.

The results of the chain Bethe approximation are fairy well in the whole region (Fig. 3). The relative errors from the full-3D QMC values are about 7–10% at $|J'|/J=1$, which should be compared with the conventional chain Weiss results (48–60 %). Surprisingly, the present chain Bethe approximation predicts a *lower* critical temperature for the ferromagnetic interchain coupling than the antiferromagnetic case, e.g., $T_c/J=1.017$ and 0.958 for $J'/J=1$ and -1, respectively. This result is seemingly counterintuitive, since quantum fluctuations, which is expected to suppress the classical ordering, are generally much stronger in the antiferromagnetic cases. However, it is not an artifact by our approximation. Indeed, a lower critical temperature for the ferromagnetic interchain coupling is also confirmed by our full-3D QMC calculation (Table I). Thus, the chain Bethe approximation predicts not only quantitatively more accurate critical temperatures, but also its nontrivial dependence on the sign of the interchain coupling.

C. Effective interchain interaction

In order to evaluate the accuracy of the present theory for small $|J'|/J$ in a more systematic way, next we discuss the effective interchain coupling $J'_{\rm eff}(J')$. This quantity first introduced in Ref. 7 is defined as the coupling constant which predicts the true critical temperature if it is used in the self-consistent equation instead of the original J'. For the chain Weiss approximation, $J'_{\rm eff}$ is explicitly obtained from Eq. (11) as

$$J'_{\rm eff}(J')=\frac{\mathrm{sgn}(J')}{z\chi_c[T_c(J')]}, \tag{21}$$

where we use the full-3D QMC results for $T_c(J')$ (Table I), which is considered to be exact within the error bar. On the other hand, for the chain Bethe approximation, we obtained $J'_{\rm eff}$ by solving Eq. (16) numerically. In Fig. 4, we plot the J' dependence of the effective interchain coupling for chain Bethe approximation ($J'>0$ and $S=1/2$) together with those of the chain Weiss approximation ($J'>0$ and $S=1/2$, 3/2, and

∞).[7] In both cases, $J'_{\rm eff}/J'$ converges to a finite value for $J'/J \ll 1$. The limiting values are 0.872 and 0.695 for the chain Bethe and Weiss approximations, respectively. The larger (or closer to unity) value of $J'_{\rm eff}/J'$ in the former supports that it is indeed a better approximation compared with the latter. Interestingly, the chain Bethe approximation has the largest $J'_{\rm eff}/J'$ at $J'/J=1$; in other words, one may say that it becomes the most accurate in the isotropic limit from the viewpoint of the renormalized factor of interchain coupling.

One should note that in the chain Bethe approximation, not only the renormalization factor $J'_{\rm eff}/J'$ is improved very much but also it converges to its limiting value quite rapidly (already converged at $J'/J=0.5$). This result suggests that the critical temperature might be well described for any values of J'/J by the chain Bethe approximation using the renormalized interchain coupling constant $0.872J'$ instead of the bare interchain coupling J' (modified chain Bethe approximation). In Fig. 3, we also plot the result of the modified chain Bethe theory by open circles, which satisfactorily agrees with the true critical temperature in the whole range of $|J'|/J$. Note that in this plot we use the same renormalization factor 0.872 for both the antiferromagnetic and ferromagnetic interchain coupling cases.

IV. SITE-DILUTED Q1D HEISENBERG ANTIFERROMAGNET

In Sec. III C, we see that the critical temperature of Q1D system is quantitatively improved greatly by the chain Bethe approximation. In this section, we discuss a more nontrivial example, the site-diluted Q1D Heisenberg antiferromagnet, where the chain Weiss approximation fails even qualitatively.

The Hamiltonian of the site-diluted Heisenberg antiferromagnet is defined as follows:

$$\mathcal{H} = J\sum_{i,j,k} \epsilon_{i,j,k}\epsilon_{i,j,k+1}\boldsymbol{S}_{i,j,k}\cdot\boldsymbol{S}_{i,j,k+1} + J'\sum_{i,j,k} \epsilon_{i,j,k}\epsilon_{i+1,j,k}\boldsymbol{S}_{i,j,k}\cdot\boldsymbol{S}_{i+1,j,k} + J'\sum_{i,j,k} \epsilon_{i,j,k}\epsilon_{i,j+1,k}\boldsymbol{S}_{i,j,k}\cdot\boldsymbol{S}_{i,j+1,k}, \tag{22}$$

where $\{\epsilon_{i,j,k}\}$ are the quenched dilution factors. They take either 1 (occupied) or 0 (vacant) independently with probability $(1-x)$ and x, respectively, with x $(0\le x\le 1)$ being the concentration of vacancies or nonmagnetic impurities.

The ground state of the classical site-diluted spin model is equivalent to the site-percolation problem.[21] The system undergoes a second-order phase transition at the percolation threshold x_p, above which there exist no infinite-size clusters. For the simple-cubic lattice, the percolation threshold is determined as

$$x_p = 0.688\ 392\ 3(4) \tag{23}$$

by the most recent simulation.[22] In the quantum spin cases, whether a long-range order exists or not near the percolation threshold is a nontrivial problem due to the presence of quantum fluctuations. However, it has been established by the extensive QMC simulation that the staggered magnetization persists up to the percolation threshold on the two-dimensional square lattice.[23] We expect that this is also the case for the present anisotropic simple-cubic lattice.

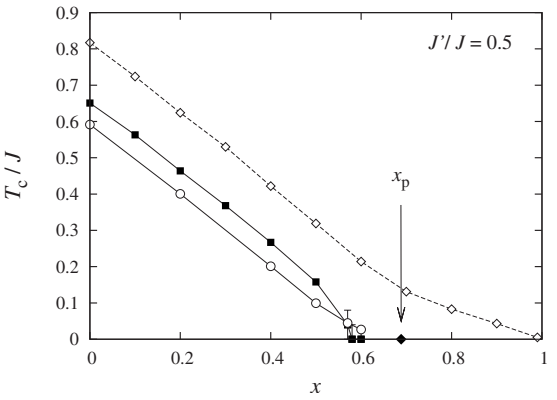

FIG. 5. x dependence of the Néel temperature of the $S=1/2$ diluted Heisenberg antiferromagnet with $J'/J=0.5$ obtained by the full-3D QMC calculation (open circles), the chain Weiss approximation (open diamonds), and the chain Bethe approximation (solid squares). The percolation threshold of the simple-cubic lattice $x_p \simeq 0.688$ is indicated by the arrow.

In Fig. 5, we show the x dependence of the critical temperature for $J'/J=0.5$ (antiferromagnetic interchain interaction) obtained by the chain Weiss and chain Bethe approximations together with the results of the full-3D QMC simulation. The largest system size used in the full-3D QMC simulation is $(L_x,L_y,L_z)=(16,16,64)$. The Néel temperature is estimated from the crossing point of Binder cumulant (19) of the staggered magnetization for different system sizes. From the full-3D QMC calculations, we thus confirm that the Néel temperature remains finite at least up to $x=0.6$. For larger impurity concentration, it is not very easy to estimate the critical temperature with satisfactory accuracy in the present scale of simulation. The staggered susceptibility of one-dimensional chain used in the chain Weiss approximation is also evaluated by means of the QMC method. We simulate chains with spins $L=128$ and 256 for various impurity concentrations and confirm that there is no significant systematic difference in the results for those two system sizes. The Néel temperature is then estimated by solving the self-consistent Eq. (11) numerically. Since the staggered susceptibility of one-dimensional chain diverges monotonically as the temperature decreases irrespective of impurity concentration, the self-consistent equation always has a solution (see the discussion below).

For the chain Bethe approximation, we evaluate $\Delta_\Omega(T)$ [Eq. (16)] by calculating the boundary-field susceptibilities of five-chain clusters with $L=32$ and 64 by means of the QMC method. We observe any significant differences between the $L=32$ and 64 results for $0\le x\le 0.6$ in the temperature range we simulate $(T/J\ge 0.01)$. We find that the function $\Delta_\Omega(T)$ tends to positively or negatively diverge depending on the impurity concentration. To see the tendency at low temperatures more clearly, we plot $T\Delta_\Omega(T)/J$, instead of $\Delta_\Omega(T)$ itself, as a function of temperature in Fig. 6. At low enough temperatures the quantity tends to converge

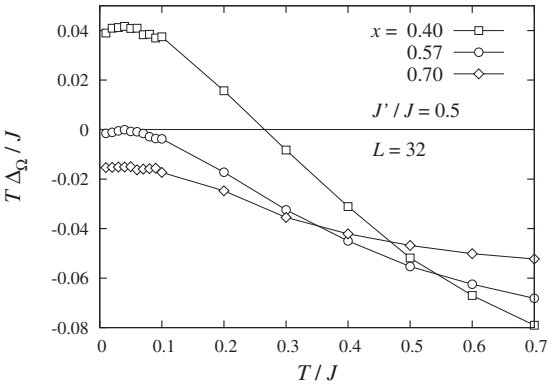

FIG. 6. Temperature dependence of $T\Delta_\Omega/J$ [Eq. (16)] of the $S=1/2$ diluted Heisenberg antiferromagnet with $J'/J=0.5$ at $x=0.40$ (squares), 0.57 (circles), and 0.70 (diamonds) obtained by the QMC method for the five-chain cluster of length $L=32$. The error bars are smaller than the symbol size.

to a finite value, which gives the coefficient of Curie-type behavior of $\Delta_\Omega(T)$. It is clearly seen that for $x<0.57$, the coefficient is positive, and thus the self-consistent Eq. (16) has a solution, while the coefficient is negative and $\Delta_\Omega(T)$ has no zero for $x>0.57$.

In all the cases, the Néel temperature decreases monotonically as x increases, as shown in Fig. 5. However, we emphasize that the result of the chain Weiss approximation is qualitatively different from the others for large x; it predicts nonvanishing Néel temperature for any $x<1$, though the others has a finite critical concentration of impurities ($x_c \simeq x_p$ and $x_c \simeq 0.57$ for QMC and the chain Bethe approximation, respectively). Since no long-range order can persist for $x>x_p$, the result of the chain Weiss theory in this regime is unphysical at all.

Indeed, the asymptotic behavior of T_c near $x=1$ can be discussed more precisely as follows. In the chain Weiss theory, the staggered susceptibility of the purely one-dimensional chain appears in the self-consistent Eq. (11). The percolation threshold of a single chain is unity, i.e., the chain is decoupled into a set of finite-length segments immediately by an infinitesimal impurity density. Thus the staggered susceptibility can be expressed as a weighted average of contributions from finite-length segments,

$$\chi_c(T) = \sum_{\ell=1} p_\ell \chi_\ell(T), \tag{24}$$

where $\chi_\ell(T)$ is the staggered susceptibility of a finite segment of length ℓ and $p_\ell \equiv (1-x)^\ell x^2$ is the average number of segment of length ℓ per site. For $(1-x) \ll 1$, only single-site clusters ($\ell=1$) contribute to the susceptibility,

$$\chi_c(T) = (1-x)\frac{1}{4T} + \mathcal{O}[(1-x)^2]. \tag{25}$$

By solving the self-consistent Eq. (11), the critical temperature is then obtained as

$$T_c = (1-x)\frac{zJ'}{4} + \mathcal{O}[(1-x)^2]. \tag{26}$$

This expression gives the exact asymptotic behavior of T_c of the chain Weiss theory in the vicinity of $x=1$. For $J'/J=0.5$ and $x=0.9$, Eq. (26) gives $T_c/J=0.05$, which agrees fairly well with the result of the chain Weiss approximation $T_c/J=0.043$.

A similar discussion applies also to the chain Bethe approximation. For $x \approx 1$, only single-site clusters contribute to the susceptibility. Since in the chain Bethe approximation the effective field is applied only on the side chains, a single-site cluster on the central chain does not feel the effective field, and thus the boundary-field susceptibility vanishes in the lowest order,

$$\chi_{\Omega,0} = \mathcal{O}[(1-x)^2]. \tag{27}$$

On the other hand, the susceptibility of boundary spins is given by the same expression as in the chain Weiss approximation,

$$\chi_{\Omega,\alpha} = (1-x)\frac{1}{4T} + \mathcal{O}[(1-x)^2] \quad \text{for} \quad \alpha = 1, \ldots, 4. \tag{28}$$

If these two expressions are substituted into the self-consistent Eq. (16), one immediately finds that it has no solution for $0 \le x \le 1$. If one further considers contribution from dimers (i.e., clusters consist of two sites) the boundary-field susceptibilities are calculated as

$$\chi_{\Omega,0} = (1-x)^2\frac{1}{2J'} + \mathcal{O}[(1-x)^3] \tag{29}$$

$$\chi_{\Omega,\alpha} = (1-x)\frac{1}{4T} + (1-x)^2\frac{1}{2J'} + 2(1-x)^2\frac{1}{J} + \mathcal{O}[(1-x)^3] \quad \text{for} \quad \alpha = 1, \ldots, 4. \tag{30}$$

Again the self-consistent equation has no solution for $J'/J \ge 3/4$. On the other hand, for a smaller J' ($J'/J < 3/4$), there exists a solution

$$T_c \approx \frac{1}{2(1-x)\left(\frac{3}{4} - \frac{J'}{J}\right)}. \tag{31}$$

However, this solution is unphysical, since it diverges as $x \to 1$. We infer that even how one takes higher-order contribution from large clusters into account, there exists no physical solution of the self-consistent equation. This implies that the chain Bethe approximation has a finite critical threshold $x_c < 1$, above which no long-range order appears at finite temperatures.

Before closing this section, we briefly mention the initial reduction rate in the critical temperature

$$R = -\left.\frac{d \log T_c(x)}{dx}\right|_{x=0}. \tag{32}$$

From the present QMC results, this quantity is estimated as $R=1.61$ for $J'/J=0.5$, which is significantly larger than that

of the isotropic cubic lattice ($R=1.22$ and 1.36 from renormalization-group[24] and series[25] studies, respectively). Accordingly, the critical temperature is a convex function of the impurity concentration, which is in a sharp contrast to the linear behavior observed in the isotropic cubic lattice.[24] Such a large initial reduction rate is also observed experimentally in quasi-two-dimensional Heisenberg antiferromagnet.[26] The enhancement in the initial reduction rate and the convexity might be attributed to the spatial anisotropy of the lattice.

V. SUMMARY

In this paper, we proposed a chain Bethe theory for Q1D quantum magnets. In the present approximation, the self-consistent equation is written in terms of the boundary-field magnetic susceptibilities of a multichain cluster instead of a single chain. Not only the correlations along the chains but also those between the nearest-neighboring chains are taken into account exactly. As a result, the accuracy of the critical temperature of the Q1D Heisenberg models is improved greatly compared with the conventional chain Weiss theory. It is also demonstrated that our approximation can predict nontrivial dependence of critical temperature on the sign of interchain coupling as well as on the impurity concentration in randomly diluted Q1D Heisenberg magnets. The conventional chain Weiss approximation takes the random average in each chain before the thermal average on the whole lattice; whereas the present theory can take fluctuations due to the randomness between the neighboring chains effectively. This difference in the order of thermal and random averaging has a great impact especially in the system with strong quenched disorder.

In the present study, we restricted ourselves to the nearest-neighbor spin models on the simple-cubic lattice. This is because unbiased high-precision full-3D data, by which the accuracy of the theory has been checked quantitatively, are available only for such unfrustrated models. It should be emphasized that however with the help of other numerical methods specialized to one-dimensional systems, such as the exact diagonalization and the density-matrix renormalization-group method, the present chain Bethe theory itself can be applied straightforwardly to spin models with strong frustration or even to fermionic models. In such models, effects of correlations between neighboring chains are much more important, and thus the improved chain mean-field approach formulated in the present paper could be an essential tool to investigate exotic phase transitions as well as anomalous low-energy properties.

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*wistaria@ap.t.u-tokyo.ac.jp
†Present address: Canon Inc., Tokyo 146-8501, Japan.

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