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Effective-field renormalization-group study for the transverse Ising model in a quantum-spin system

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In this paper we suggest a method that combines the effective-field renormalization group with the discretized path-integral method to study the critical behavior of the transverse Ising model in a quantum-spin system. We find the results on a critical transverse field and critical exponent at zero temperature to be closely comparable to other results. This demonstrates the utility of this method in studying critical properties of quantum-spin systems.

I. INTRODUCTION

The transverse Ising model (TIM) in a quantum-spin system can be described by the Hamiltonian

$$H=-\sum_{i,j} J_{ij}\sigma_i^z\sigma_j^z-\Omega\sum_j \sigma_j^x , \qquad (1)$$

where the σ_j^x and σ_j^z are Pauli spin matrices,

$$\sigma^z=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},\quad \sigma^x=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \qquad (2)$$

Ω is the transverse field, and J_{ij} is the exchange interaction between spins in nearest-neighbor sites i and j.

TIM was originally introduced by de Gennes as a pseudospin model for hydrogen-bonded ferroelectrics such as KH_2PO_4,[1-3] in which the phase transition is associated to order-disorder phenomena with tunneling effects. Since then it has been used to study a variety of other systems, for example, magnetically ordered materials with strong uniaxial anisotropy in a transverse field, rare-earth compounds with a singlet crystal-field ground state, and cooperative Jahn-Teller systems like $DyVO_4$.[3,4] Recently TIM has also been used in meson-field theory and as a prototype system for lattice gauge theories.[5,6]

More recently, much interest has been focused on the quantum-spin system problem, such as in the anisotropic hierarchical lattice Heisenberg model,[7,8] tunneling-induced disorder at zero temperature,[9-11] and critical behavior.[12,13] There is, however, a difficulty in investigating critical features in such quantum systems. We must deal with the significant technical difficulty of solving a many-body problem involving noncommuting operators. In the TIM case, Suzuki[14] realized that a little-used relationship known as the Trotter-product formula[15] allows one to dispense with noncommutivity at the price of introducing another coordinate into the problem. By using the Suzuki-Trotter formula, the partition function of the quantum system in d dimensions can be rewritten as the corresponding partition function for a $(d+1)$-dimensional classical system (fully commuting). On the other hand, the discretized Feynman path-integral representation of a quantum-mechanical partition function was, in form, nothing more than a classical configurational integral.[16,17] Therefore, by means of the discretized path-integral representation (DPIR), the quantum Hamiltonian in TIM can be transformed into a classical one, and the resulting classical system can be treated by analytical methods. DPIR showed an easy way out of the difficulty.

There exist a variety of sophisticated techniques for studying the critical behavior of TIM in a classical spin system.[18-20] Recently, the mean-field renormalization-group (MFRG) method, combining mean-field results for a small cluster of spins with the renormalization-group idea, has been proposed to study the critical properties of the lattice-spin system.[21,22] By using MFRG with a diluted TIM, quite good results have been obtained using the simplest choice for the cluster.[23] According to the essential thoughts of MFRG theory, an effective-field renormalization-group (EFRG) method has been presented and applied to the Ising model system, with the results showing further improvement over MFRG.[24]

In this paper, we combine the EFRG with DPIR to deal with the TIM in quantum-spin systems, and results on the critical value of the transverse field and critical exponents are obtained.

II. PATH-INTEGRAL FORMULATION

For the quantum-spin system, the spin at each site is in a state corresponding to one of the two eigenfunctions of σ^z,

$$\begin{bmatrix}1\\0\end{bmatrix},\quad U_j=1,\quad\text{and}\quad \begin{bmatrix}0\\1\end{bmatrix},\quad U_j=-1 . \qquad (3)$$

The partition function of the lattice system can be written as

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_U \langle U | e^{-\beta H} | U \rangle \;, \tag{4}$$

where for an N-site lattice

$$\langle U | = \langle U_1, U_2, \ldots, U_N | = \langle U_1 | \langle U_2 | \cdots \langle U_N | \tag{5}$$

is a direct-product wave function for the whole system.

We will reformulate the quantal TIM Hamiltonian (1) in a DPIR,[11,16] thereby creating a classical problem out of the quantum-spin problem. The procedure for accomplishing this task has already been described by some authors;[10,11] so we will not belabor it here. We only give a brief interpretation of this idea, which is to convert the quantal two-state spin on each site into a p-component vector spin $\mathbf{U}$ ($U^{(1)}, U^{(2)}, \ldots, U^{(p)}$) and (eventually) to let p to infinite. Each component $U^{(t)}$ ($t=1,2,\ldots,p$) is taken to be a classical two-state variable, i.e., $U^{(t)} = \pm 1$. With this description and DPIR, the spin-spin interaction becomes an average over spin components

$$-J\sigma_i^z\sigma_j^z \to -(J/p)\mathbf{U}_i\cdot\mathbf{U}_j = -(J/p)\sum_{t=1}^{p} U_i^{(t)}U_j^{(t)} \;, \tag{6}$$

and the transverse field term

$$\beta\Omega\sigma_j^* \to \mathbf{U}_j\cdot\underline{a}\cdot\mathbf{U}_j + c = a\sum_{t=1}^{p} U_j^{(t)}U_j^{(t+1)} + c \;, \tag{7}$$

with

$$a = \tfrac{1}{2}\ln[\coth(\beta\Omega/p)] \;,$$
$$c = \tfrac{1}{2}\ln[\cosh(\beta\Omega/p)\sinh(\beta\Omega/p)] \;.$$

Combining the above considerations, the final form for the partition function in DPIR is obtained as

$$Z = \sum_{\mathbf{U}_1}\sum_{\mathbf{U}_2}\cdots\sum_{\mathbf{U}_N}\exp\left[(\beta J/p)\sum_{i,j}\mathbf{U}_i\cdot\mathbf{U}_j + \sum_j \mathbf{U}_j\cdot\underline{a}\cdot\mathbf{U}_j + c'\right] \;, \tag{8}$$

where

$$(\underline{a})_{t,t'} = a\,\delta_{t,t'-1},\ (\underline{a})_{p,1} = a, \text{ and } c' = Npc \;.$$

The starting point is that the new classical spin Hamiltonian can be broken up into a reference part, involving only the single-site terms

$$-\beta H_0 = \sum_j \mathbf{U}_j\cdot\underline{a}\cdot\mathbf{U}_j + c' \;, \tag{9}$$

and an interaction part

$$-\beta V = (\beta J/p)\sum_{i,j}\mathbf{U}_i\cdot\mathbf{U}_j \;. \tag{10}$$

The full Hamiltonian $H = H_0 + V$ would be suitable for perturbation theory. The free energy F of the full system can be expressed in terms of the reference system free energy F_0 and the cumulant expansion in the reference system

$$-\beta F = -\beta F_0 + \sum_{n=1}^{\infty}\left[\frac{1}{n!}\right](-\beta)^n C_n(V) \;, \tag{11}$$

with

$$-\beta F = \ln \mathrm{Tr}\, e^{-\beta H} \text{ and } -\beta F_0 = \ln \mathrm{Tr}\, e^{-\beta H_0} \;, \tag{12}$$

and the cumulant

$$C_1(V) = \langle V\rangle_0 \;,$$
$$C_2(V) = \langle V^2\rangle_0 - \langle V\rangle_0^2 \;, \tag{13}$$
$$C_3(V) = \langle V^3\rangle_0 - 3\langle V^2\rangle_0\langle V\rangle_0 + 2\langle V\rangle_0^3 \;,$$

where $\langle \cdots \rangle$ denotes an average in the reference system

$$\langle V\rangle_0 = \mathrm{Tr}(Ve^{-\beta H_0})/\mathrm{Tr}(e^{-\beta H_0}) \;. \tag{14}$$

Since Eq. (11) is ordered in powers of the inverse temperature $\beta = 1/k_BT$, it would appear that we were developing a high-temperature series. However, in path-integral applications, the cumulants themselves depend on β through the temperature dependence of the reference system Hamiltonian. In fact, this temperature dependence turns out to be just what is necessary to allow well-defined calculations at all temperatures, including ground state. It would therefore be better to regard Eq. (11) as an expansion in successively higher orders of fluctuations.

III. EFFECTIVE-FIELD RENORMALIZATION-GROUP (EFRG) METHOD

In order to study the critical behavior of the TIM in a quantum-spin system whose Hamiltonian is expressed by Eq. (1), we will combine the DPIR with the EFRG method. According to the EFRG procedure, we take the simple choice for the clusters, that is, $N'=1$ and $N=2$ spin clusters, respectively, and also restrict the structure to cubic.

For $N'=1$ single spin cluster, the Hamiltonian is written as

$$H_{N'} = -\sum_j J'_{ij}\sigma_j^z\sigma_1^z - \Omega'\sigma_1^x \;. \tag{15}$$

By use of the exact Callen identity[25] and the differential operator technique, within the framework of effective-field theory with correlation,[26,27] the longitudinal magnetization is given by

$$\langle\sigma_1^z\rangle_{N'} = \left\langle \exp\left[D_x\sum_j J'_{1j}\sigma_j^z\right]\right\rangle f(x)|_{x=0} \;, \tag{16}$$

where $\langle \cdots \rangle$ indicates the canonical thermal average, the differential operator $D_x = \partial/\partial x$, and $f(x)$ is defined by

$$f(x) = \frac{x}{(\Omega'^2 + x^2)^{1/2}}\tanh[\beta(\Omega'^2 + x^2)^{1/2}] \;. \tag{17}$$

Using the identity

$$e^{\lambda\sigma_j^z} = \cosh\lambda + \sigma_j^z\sinh\lambda$$

and (18)

$$e^{\alpha D_x}f(x) = f(x+\alpha) \;,$$

the expectation values $\langle \exp(D_x\sum_j J'_{ij}\sigma_j^z)\rangle$ reduced to

$$\left\langle \exp\left[D_x \sum_j J'_{ij}\sigma_j^z\right]\right\rangle = \left\langle \prod_j [\cosh(J'_{ij}D_x) + \sigma_j^z \sinh(J'_{ij}D_x)]\right\rangle . \quad (19)$$

As discussed in previous works,[26,27] we use the decoupling approximation[28] and take each boundary spin $\langle \sigma_j^z \rangle$ fixed to b'. We are interested in studying the critical behavior of the system, expanding the right-hand side of Eq. (16) with respect to $\langle \sigma_j^z \rangle$, and retaining only terms linear in $\langle \sigma_j^z \rangle$. We find

$$\langle \sigma_1^z \rangle_{N'} = G_1(\alpha', \kappa')b' , \quad (20)$$

$$G_1(\alpha', K') = 2d \cosh^{2d-1}(J'D_x)\sinh(J'D_x)f(x)|_{x=0} , \quad (21)$$

with $\alpha' \equiv \Omega'/J'$, $K' \equiv \beta' J'$, $\beta' = 1/k_B T'$, and d is the dimension of the system with cubic structure.

Similarly, the Hamiltonian for the two-spin cluster is given by

$$H_N = -J\sigma_1^z\sigma_2^z - \Omega(\sigma_1^x + \sigma_2^x) - \sum_{j\neq 2} J_{ij}\sigma_j^z\sigma_1^z - \sum_{j\neq 1} J_{2j}\sigma_j^z\sigma_2^z . \quad (22)$$

It is convenient to add a generating magnetic field $\mathbf{B}$ at each site along the z direction.[11] Equation (22) then becomes

$$H_N = -J\sigma_1^z\sigma_2^z - \Omega(\sigma_1^x + \sigma_2^x) - \lambda_1\sigma_1^z - \lambda_2\sigma_2^z , \quad (23)$$

where

$$\lambda_1 = \left[B + \sum_{j\neq 2} J_{1j}\sigma_j^z\right] , \quad \lambda_2 = \left[B + \sum_{j\neq 1} J_{2j}\sigma_j^z\right] . \quad (24)$$

As discussed in the above section, the Hamiltonian (23) can be rewritten in DPIR,

$$-\beta H_N = (\beta J/p)\mathbf{u}_1\cdot\mathbf{u}_2 + \sum_{j=1}^{2} (\mathbf{u}_j \cdot \underline{a} \cdot \mathbf{u}_j + \mathbf{h}_j\cdot\mathbf{u}_j + pc) , \quad (25)$$

where

$$\mathbf{h}_j = (\beta\lambda_j/p)(1,1,\ldots,1) . \quad (26)$$

The partition function of the reference system corresponding to Hamiltonian Eq. (25) is reduced to a product of the single-site partition function

$$Z_0 = \prod_{j=1}^{2} Z_0^{(j)} , \quad (27)$$

where

$$Z_0^{(j)} = \sum_{U_j^{(1)}=\pm 1}\sum_{U_j^{(2)}=\pm 1}\cdots\sum_{U_j^{(p)}=\pm 1} \exp\left[a\sum_{t=1}^{p} U_j^{(t)}U_j^{(t+1)} + \frac{\beta\lambda_j}{p}\sum_{t=1}^{p} U_j^{(t)} + c\right] . \quad (28)$$

This equation is nothing more than the partition function of a one-dimensional Ising model in a field with periodic boundary conditions and may be evaluated exactly[29]

$$Z_0^{(j)} = [Q_j^+]^p + [Q_j^-]^p , \quad (29)$$

$$Q_j^{\pm} = \cosh(\beta\lambda_j/p)\cosh(\beta\Omega/p) \pm [\cosh^2(\beta\lambda_j/p)\cosh^2(\beta\Omega/p) - 1]^{1/2} . \quad (30)$$

Taking the limit that $P \to \infty$, an exact quantum-mechanical result is obtained

$$Z_0^{(j)} = 2\cosh[\beta(\lambda_j^2 + \Omega^2)^{1/2}] . \quad (31)$$

The next step is to calculate the first cumulant

$$\langle V \rangle_0 = -(J/\beta^2)\left[\frac{\partial \ln Z_0^{(1)}}{\partial\lambda_1}\right]\left[\frac{\partial \ln Z_0^{(2)}}{\partial\lambda_2}\right] , \quad (32)$$

where we have taken

$$V = -(J/p)\mathbf{U}_1\cdot\mathbf{U}_2 = -(J/p)\sum_{t=1}^{p} U_1^{(t)}U_2^{(t)} . \quad (33)$$

Accordingly, the final free energy expression through $n = 1$ in Eq. (11) is

$$-\beta F = \sum_{j=1}^{2} \ln\{2\cosh[\beta(\lambda_j^2 + \Omega^2)^{1/2}]\} + BJ\prod_{j=1}^{2} \frac{\tanh[\beta(\lambda_j^2 + \Omega^2)^{1/2}]}{(\lambda_j^2 + \Omega^2)^{1/2}}\lambda_j . \quad (34)$$

The average magnetization $\langle \sigma_1^z + \sigma_2^z \rangle$ can be obtained by

$$\langle \sigma_1^z + \sigma_2^z \rangle_N = \left\langle -\frac{\partial F}{\partial B}\bigg|_{B=0}\right\rangle . \quad (35)$$

Similarly, introducing the differential operators $D_x = \partial/\partial x$ and $D_y = \partial/\partial y$, and using $\partial\lambda_j/\partial B = 1$ $(j = 1,2)$, then the above equation becomes

$$\langle \sigma_1^z + \sigma_2^z \rangle_N = \left\langle \exp\left[D_x \sum_{j\neq 2} \sigma_j^z + D_y \sum_{j\neq 1} \sigma_j^z\right]\right\rangle (f(x,y) + g(x,y)]|_{x=y=0} , \quad (36)$$

where the $f(x,y)$ and $g(x,y)$ are defined by

$$f(x,y)=\frac{\tanh[K(\alpha^2+x^2)^{1/2}}{(\alpha^2+x^2)^{1/2}}x\left[1+\frac{\tanh[K(\alpha^2+y^2)^{1/2}]}{(\alpha^2+y^2)^{1/2}}-\frac{\tanh[K(\alpha^2+y^2)^{1/2}]}{(\alpha^2+y^2)^{3/2}}y^2+\frac{K\,\mathrm{sech}^2[K(\alpha^2+y^2)^{1/2}]}{\alpha^2+y^2}y^2\right],$$

$$g(x,y)=\frac{\tanh[K(\alpha^2+y^2)^{1/2}]}{(\alpha^2+y^2)^{1/2}}y\left[1+\frac{\tanh[K(\alpha^2+x^2)^{1/2}]}{(\alpha^2+x^2)^{1/2}}-\frac{\tanh[K(\alpha^2+x^2)^{1/2}]}{(\alpha^2+x^2)^{3/2}}x^2+\frac{K\,\mathrm{sech}^2[K(\alpha^2+x^2)^{1/2}]}{\alpha^2+x^2}x^2\right]. \quad (37)$$

Let the boundary spin $\langle \sigma_j^z \rangle = b$ and, in the vicinity of the critical point, let us take only the linear term of $\langle \sigma_j^z \rangle$, then

$$\tfrac{1}{2}\langle \sigma_1^z+\sigma_2^z\rangle_N = G_2(\alpha,K)b\ , \quad (38)$$

where $\alpha \equiv \Omega/J$, $K=\beta J$, and

$$G_2(\alpha,K)=\frac{(2d-1)}{2}(\cosh^{2d-1}(D_x)\cosh^{2d-2}(D_y)\sinh(D_y)+\cosh^{2d-1}(D_y)\cosh^{2d-2}(D_x)\sinh(D_x)]$$
$$\times[f(x,y)+g(x,y)]|_{x=y=0}\ . \quad (39)$$

Combining Eq. (21) with Eq. (39) with a rescaling assumption, the fixed-point equation is obtained

$$G_1(\alpha,K_c)=G_2(\alpha,K_c) \quad (40)$$

where K_c is the critical coupling. The critical value of the transverse field at which T_c goes to zero can be obtained by letting $K_c \to \infty$ in Eq. (40), meanwhile, the critical exponent y_α can also be estimated from the recursion relation

$$\left[\frac{\partial \alpha'}{\partial \alpha}\right]_{\alpha=\alpha_c, K_c\to\infty} = l^{y_\alpha}\ , \quad (41)$$

where l is the rescaling factor and the derivative is taken at the fixed point of the particular set considered. We have known that MFRG gives poor estimates of the critical exponent. This can be traced to an unsatisfactory definition of the length scaling factor $l=(N/N')^{1/d}$, where d is the dimensionality, and N and N' are the number of spins in two clusters. A new definition that improves the estimates for the critical exponent has been proposed, wherein the length of the cluster is measured in terms of the number of interactions, including interactions with the surrounding mean field.[30,31] Here we also use the new definition to calculate the critical exponent y_α for TIM. In Tables I,[32] II, and III, results for α_c, l, and y_α are given and compared to predictions from other techniques.

We can find from Table III that the critical exponent value has been improved by means of the new definition of the length scaling factor. The reasons for taking the new definition are clear: Since the cluster considered is surrounded by an effective field, it stimulates a larger cluster than that defined by the old scaling definition. On the other hand, the new definition for anisotropic scaling is consistent with the standard procedure used in finite-size scaling. Actually, as some authors[33–35] have shown the new definition of the length scaling preserves the convexity of the free energy. This means that heat capacity, susceptibility, etc., will be positive. By use of other choices for the scaling factor, there is no guarantee that the free energy will be convex. Therefore, we can understand that the new rescaling factor including the anisotropy could give a good critical exponent y_α for TIM.

IV. DISCUSSION AND CONCLUSION

In this paper, we have used the EFRG to study the critical behavior of TIM in a quantum-spin system with DPIR in which the Hamiltonian in the quantum system is transformed into the classical Hamiltonian, thereby creating a classical spin problem from quantum problem. Our results compare well with other approximation methods.

TIM in a quantum-spin system proved difficult to use in solving a many-body problem involving noncommuting operators. With the EFRG perturbation expansion for the Hamiltonian of a two-spin cluster, the direct diagonalization cannot be carried out. However, EFRG leads to considerable improvement over other frequently used real-space renormalization-group and MFRG methods without involving much more computational work. It is

TABLE I. Critical transverse field α_c for TIM.

Lattice	Square	Simple cubic
Z	4	6
MFRG (Ref. 23)	3.334	5.348
EFA (Ref. 31)	2.752	4.704
Kirkwood (Ref. 11)	3.225	5.291
Present work	2.988	4.946
MFA	4	6
SE (Series expansion)	3.04	5.08

TABLE II. Rescaling factor l.

Lattice	Square	Simple cubic
Z	4	6
Old	$(2)^{1/2}$	$(2)^{1/3}$
New	$3(\frac{2}{13})^{1/2}$	$3(\frac{3}{22})^{1/2}$

TABLE III. Critical exponent y_α for TIM.

Lattice	Square	Simple cubic
Z	4	6
MFRG (Ref. 23)	0.700	0.707
Present work (old)	0.810	0.762
Present work (new)	1.726	1.719
SE (series expansion)	1.587	1.724

possible to obtain good results that combine the EFRG with DPIR. The discretized path integral, which is used here, is used to transform the quantal spin into a classical spin with "internal structure" (see Eqs. (5) and (6)]. In the transverse field case, we take advantage of the idea that internal structure can be thought of as a p-dimensional vector, that is, to convert the quantal two-state "spin" on each lattice site into a p-component vector $\mathbf{U}=(U^{(1)},U^{(2)},\ldots,U^{(p)})$ and eventually to let p go to infinity. Each component, $U^{(t)}$ is taken to be a classical two-state variable ($U^{(t)}=\pm1$); so the resulting partition function can be treated with the cumulant-expansion method, and the corresponding partition function of reference system is nothing more than the partition function of a one-dimensional Ising model in a field.

The purpose of this paper is to demonstrate the utility of the new approximation method in dealing with the critical properties of quantum-spin systems. We propose that a significant and quantitative improvement results from going to the next order in Eq. (11) on the addition of the first fluctuation correction, the $n=2$ term. We believe that this method can be extended to other more complicated quantum systems such as the Heisenberg model, the $S=1$ Ising model, and alloy and surface problems with transverse field.

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