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Renormalization Transformations for Quantum Spin Systems*

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An operator renormalization transformation is proposed for quantum spin systems which is manifestly basis independent and preserves the fundamental symmetries of the spin Hamiltonian. We develop a cumulant expansion suitable for noncommuting operators and illustrate the general techniques with several sample calculations.

During the past few years the renormalization-group approach has been applied with considerable success to the study of the critical behavior of generalized Ising models[1] and related classical spin models. It is of considerable interest to generalize this approach to quantum spin models like the spin-s Heisenberg and X-Y models, and the Ising model in a transverse magnetic field, where the spin components satisfy the angular momentum commutation relations. Recently several workers[2-5] have suggested interesting generalizations for these quantum spin models of the renormalization transformation introduced by Niemeijer and van Leeuwen.[1] However, these transformations require a specific choice of basis and it is not clear whether the physical results derived thereby are basis independent. Furthermore, since symmetries of the Hamiltonian are used to motivate the choice of basis, one cannot study crossover effects from one symmetry to another. For example, the transformation of Rogiers and Dekeyser[2] and of Betts and Plischke[3] for the X-Y Hamiltonian, which generates Ising-like couplings, does not preserve the limit of Heisenberg symmetry. Therefore, the Heisenberg model has to be treated separately by a special procedure.[2]

In this Letter, we propose an operator formulation of renormalization transformations for quantum spin systems which preserves manifestly their fundamental symmetries. The problem in constructing a quantum renormalization transformation is to generalize, for spin operators, Kadanoff's idea that in the neighborhood of a phase transition blocks or cells of spins act like single spins. We propose to determine the relation between the site-spin operators $\vec{\sigma}_{im}$ of the ith Kadanoff cell of L spins (with $m=1,2,\ldots,L$) where m labels the cell sites, and the renormalized spin operator of the cell[6] $\vec{\tau}_i$, by an operator $t(\vec{\tau}_i,\vec{\sigma}_{im})$ which acts on the joint Hilbert space of the site and cell spins. The choice of $t(\vec{\tau}_i,\vec{\sigma}_{im})$ is restricted by symmetry considerations and other requirements to be discussed below.

Given $\mathcal{H}_N(\vec{\sigma})$, the Hamiltonian for a system of N spins on a lattice, the renormalized Hamiltonian $\mathcal{H}_{N/L}'(\vec{\tau})$ is determined by the operator equation

$$\exp[\mathcal{H}_{N/L}'(\vec{\tau})+Ng_N]=\mathrm{Tr}_\sigma[\exp(\mathcal{H}_N)T(\vec{\tau},\vec{\sigma})], \quad (1)$$

where Tr_σ denotes the trace with respect to the spins $\vec{\sigma}_{im}$, g_N is a c number corresponding to the self-energy per spin of the Kadanoff cells, and by translation invariance

$$T(\vec{\tau},\vec{\sigma})=\prod_i^{N/L} t(\vec{\tau}_i,\vec{\sigma}_{im}).$$

We impose on the partition functions the usual requirement of invariance under this transformation which implies the condition $\mathrm{Tr}_{\tau_i} t(\vec{\tau}_i,\vec{\sigma}_{im})=1$.

The renormalization transformation $T(\vec{\tau},\vec{\sigma})$ should preserve the symmetries of Hamiltonians

$\mathcal{H}_N$ within a universality class. For example, if $\mathcal{H}_N$ is invariant under rotations, then $T(\vec{\tau},\vec{\sigma})$ should also be chosen to be rotationally invariant in the combined $(\vec{\tau},\vec{\sigma})$ space. Actually, it may often be desirable that $T(\vec{\tau},\vec{\sigma})$ have a higher degree of symmetry than $\mathcal{H}_N$, so that the transformation can be used globally to connect Hamiltonians with different symmetries; e.g., a rotationally invariant $T(\vec{\tau},\vec{\sigma})$ can also be applied to Hamiltonians which are invariant only under rotations about a single axis like the Ising and X-Y models [see Eq. (15)]. Therefore, assuming rotational invariance and permutational symmetries on the individual spins $\vec{\sigma}_{im}$ in a block (with $m=1,\ldots,L$), the most general transformation for spin-$\frac{1}{2}$ objects is

$$t(\vec{\tau}_i,\vec{\sigma}_i)=\tfrac{1}{2}+\vec{\tau}_i\cdot\vec{\sigma}_i Q(\vec{\sigma}_i^{\,2}), \tag{2}$$

where

$$\vec{\sigma}_i=\sum_{m=1}^{L}\vec{\sigma}_{im}$$

is the total block-spin operator, and $\vec{\sigma}_{im}$ and $\vec{\tau}_i$ are the 2×2 Pauli matrices. Since $\vec{\sigma}_i^{\,2}$ has only a finite set of eigenvalues $\sigma_i(\sigma_i+2)$, with $\sigma_i=L,L-2,\ldots$, a general form for Q is a finite polynomial,

$$Q(\vec{\sigma}_i^{\,2})=\sum_{m=0}^{M}q_m(\vec{\sigma}_i^{\,2})^m,$$

of order $M=\frac{1}{2}L$ or $\frac{1}{2}(L-1)$ for L even or odd, respectively. Next, we must consider how best to constrain the coefficients q_m to impose the physical requirement that t strongly favors configurations with $\vec{\tau}_i$ and $\vec{\sigma}_i$ aligned.

We suggest that $t(\vec{\tau}_i,\vec{\sigma}_i)$ be chosen so that its eigenvalues be unity when the spins $\vec{\sigma}_i$ and $\vec{\tau}_i$ are added in "parallel" to form the maximum total angular momentum for $\vec{\sigma}_i+\vec{\tau}_i$ for each value of $\vec{\sigma}_i^{\,2}$. This gives a closed expression for any block size L,

$$t(\vec{\tau}_i,\vec{\sigma}_i)=\tfrac{1}{2}+\tfrac{1}{2}\vec{\tau}_i\cdot\vec{\sigma}_i[(1+\vec{\sigma}_i^{\,2})^{1/2}-1]^{-1} \tag{3}$$

or $Q(\vec{\sigma}_i^{\,2})=1/2\sigma_i$ on the eigenstates of $\vec{\sigma}_i^{\,2}$. For instance, with $L=3$ this is equivalent to $q_0+15q_1=\frac{1}{6}$ and $q_0+3q_1=\frac{1}{2}$.

Our transformation (3) seems to be the most natural quantum version of the majority-rule transformation of Niemeijer and van Leeuwen. In both cases, the transformations are undefined for zero-total-spin configurations of blocks with an even number of spins L, and we supplement our definition (3) by setting $t=\frac{1}{2}$ for $\sigma_i=0$.

For any choice of the coefficients, it is easily seen that if $\mathcal{H}_N$ is in the class of Ising Hamiltonians, we recover the well-known renormalization equations for the Ising model. Hence another possible choice of the coefficients q_m reproduces exactly the majority rule of Niemeijer and van Leeuwen for Ising models. For example, with $L=3$, this gives slightly different coefficients: $q_0+15q_1=\frac{1}{6}$ and $q_0+3q_1=\frac{2}{3}$. However, our transformation (3) gives nearly as good results for the cumulant expansion of the Ising model.

It is interesting to note that the transformation (3) has negative eigenvalues $-1/\sigma_i$ for anti-aligned states. Instead we could have chosen these eigenvalues to be zero and obtained

$$Q(\vec{\sigma}_i^{\,2})=\tfrac{1}{2}[(\vec{\sigma}_i^{\,2}+1)^{1/2}+1]^{-1}. \tag{4}$$

This choice [Eq. (4)] corresponds to a generalization of Kadanoff's transformation for the Ising model

$$t(\vec{\tau}_i,\vec{\sigma}_i)=\lim_{p\to\infty}[\exp(p\vec{\sigma}_i\cdot\vec{\tau}_i)/\mathrm{Tr}_{\tau_i}\exp(p\vec{\sigma}_i\cdot\vec{\tau}_i)]. \tag{5}$$

Although this is an appealing way[7] to force the alignment of $\vec{\tau}$ and $\vec{\sigma}$, for the Heisenberg (or Ising) model it fails at zero temperature to map the ground states of $\mathcal{H}_N$ into those of $\mathcal{H}_{N/L}{}'$.

In order to map[8,9] the d_0-fold degenerate ground states $|n\rangle$ of $\mathcal{H}_N$ into the d_0'-fold degenerate ground states $|n'\rangle$ of $\mathcal{H}_{N/L}{}'$, the zero-temperature limit of Eq. (1) should become

$$\frac{1}{d_0'}\sum_{n'=1}^{d_0'}|n'\rangle\langle n'|=\frac{1}{d_0}\sum_{n=1}^{d_0}\langle n|T(\vec{\tau},\vec{\sigma})|n\rangle, \tag{6}$$

which gives an expression for the projection operator onto the ground states of $\mathcal{H}_{N/L}{}'$. For the isotropic ferromagnetic Heisenberg model the degeneracies are $d_0=N+1$ and $d_0'=N/L+1$, and we can prove Eq. (6), provided that

$$\langle n|Q(\vec{\sigma}_i^{\,2})|n\rangle=1/2L \tag{7}$$

[which is satisfied by our transformation (3)], by showing that as the temperature goes to zero any two spins $\vec{\tau}_i$ and $\vec{\tau}_j$ become totally aligned:

$$\langle\vec{\tau}_i\cdot\vec{\tau}_j\rangle=\frac{\mathrm{Tr}_\tau\exp(\mathcal{H}_{N/L}{}')\vec{\tau}_i\cdot\vec{\tau}_j}{\mathrm{Tr}_\tau\exp(\mathcal{H}_{N/L}{}')}\to1. \tag{8}$$

However, for the Heisenberg model some difficulties may arise in describing the ordered phase. We know that in order to have spontaneous symmetry breaking[10] at zero temperature, a magnetic eigenvalue $\lambda_H=L$ is required. In the limit $N/L\to\infty$ we can demonstrate that there is an eigenvalue $\lambda_H=L$ by studying the zero-temperature condi-

tion,

$$\sum_{n'}\langle n'|\tau_i^z\sum_l h_l'O_l'|n'\rangle = \frac{1}{L}\frac{(N/L+1)}{(N+1)}\sum_n\langle n|\sigma_i^z\sum_l h_lO_l|n\rangle, \quad (9)$$

for the odd-spin interactions O_l and O_l' with their infinitesimal couplings h_l and h_l'. The argument is almost identical to that for the Ising model, with the important exception that it breaks down for finite N. Indeed, we found for the two-cell cluster ($N/L=2$) that $\lambda_H=\frac{1}{2}(L+1)<L$, so that in order to do finite-lattice calculations for the order parameter, new techniques may have to be developed. Also, note that for other systems like the Ising model in a transverse field, we have not demonstrated that Eq. (6) holds. Perhaps less symmetric forms for T will have to be chosen in some cases.

In the cumulant expansion, the Hamiltonian $\mathcal{H}$ is separated in the form

$$\mathcal{H}=\mathcal{H}_0+V, \quad (10)$$

where $\mathcal{H}_0$ is the sum of the corresponding Hamiltonians for each cell, and V contains all the interaction terms among cells. Then the interaction V is treated as a perturbation by expanding the right-hand side of Eq. (1) in powers of V. To take into account that $\mathcal{H}_0$ and V do not commute for quantum spin systems, we apply the identity

$$\exp(\mathcal{H}_0+V)=\exp(\mathcal{H}_0)\mathcal{T}\exp[\int_0^1 d\lambda\, V(\lambda)], \quad (11)$$

where

$$V(\lambda)=\exp(-\lambda\mathcal{H}_0)V\exp(\lambda\mathcal{H}_0) \quad (12)$$

and $\mathcal{T}$ is the time-ordering operator with respect to the variable λ. Substituting Eq. (11) in Eq. (1), and taking the logarithm of the operators on both sides of the resulting equation, we obtain[11]

$$\mathcal{H}_{N/L}'+Ng_N=\ln \mathrm{Tr}_\sigma \exp(\mathcal{H}_0)T+\ln[\sum_{n=0}^{\infty}\int_0^1 d\lambda_1\int_0^{\lambda_1}d\lambda_2\cdots\int_0^{\lambda_{n-1}}d\lambda_n\langle V(\lambda_1)V(\lambda_2)\cdots V(\lambda_n)T\rangle], \quad (13)$$

where the angular brackets denote a generalized thermal average for an operator A with respect to the cell Hamiltonian $\mathcal{H}_0$:

$$\langle AT\rangle=\mathrm{Tr}_\sigma[\exp(\mathcal{H}_0)AT]/\mathrm{Tr}_\sigma[\exp(\mathcal{H}_0)T]. \quad (14)$$

Equation (13) is a linked cluster expansion in the interaction V, i.e., only cells which are connected by spin interactions contribute to the sum, and the classification of these contributions in a given order is the same as for the Ising model. The calculations can be readily carried out in the basis which diagonalizes each cell Hamiltonian.

We are presently engaged in calculations on several quantum spin systems, and some of our results are summarized below. Consider the anisotropic Heisenberg model

$$\mathcal{H}=\sum_{\langle ij\rangle}K_\perp(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)+K_\parallel\sigma_i^z\sigma_j^z \quad (15)$$

with nearest-neighbor interactions in the region $\eta\equiv K_\perp/K_\parallel\leq 1$. We have evaluated the cumulant expansion to first and second orders on a triangular lattice. In Fig. 1, the specific heat is plotted for $\eta=0$ and $\eta=0.7$. On the Ising axis ($\eta=0$) we reproduce the results of Niemeijer and van Leeuwen.[1] For every value of $\eta<1$, there is a critical value $K_\parallel^c(\eta)$ of $K_\parallel$ that maps into the Ising fixed point (see Fig. 1, inset), at which the specific heat and the susceptibility diverge. The steep rise of the critical line away from the Ising axis is in accordance with the high-temperature series for a square lattice.[12] For $K_\parallel>K_\parallel^c(\eta)$ and $\eta<1$, there will be spontaneous magnetization in accordance with a recent existence theorem.[13]

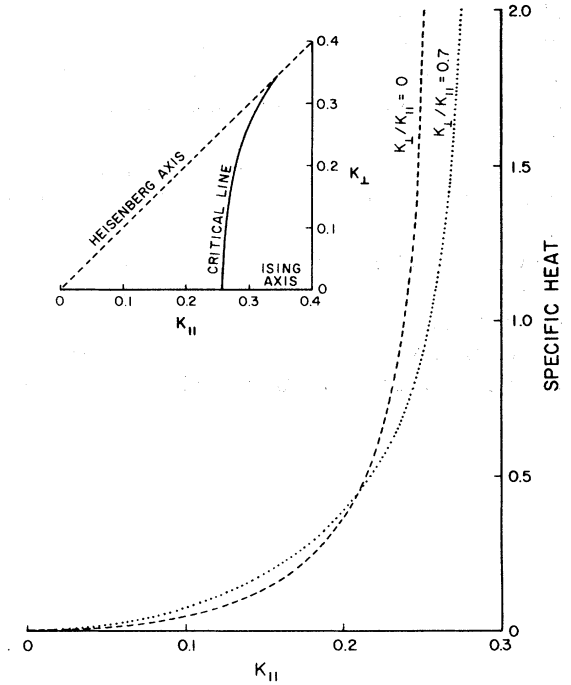

FIG. 1. Specific heat of the anisotropic Heisenberg model Eq. (15) as a function of $K_\parallel$ in second-order cumulant expansion. The critical line is shown in inset.

TABLE I. Free energy of the Heisenberg model.

K	Renormalization	High-temp. series[a]
0	0.693	0.693
0.1	0.720	0.721
0.2	0.796	0.794
0.3	0.915	0.901
0.4	1.066	1.032
0.5	1.237	1.182

[a]Free energy generated by M. Plischke (private communication) by Padé approximants from the series of Rushbrooke, Baker, and Wood (Ref. 14).

In second order a fixed point in the isotropic Heisenberg subspace appears and correspondingly a critical point along the Heisenberg axis. By contrast, in first order there is no Heisenberg fixed point and the critical line turns away towards infinity as the Heisenberg axis is approached Also, calculations with a cluster of two cells on a square lattice with four spins each do not give the Heisenberg fixed point either, which therefore may be a spurious effect of the second-order cumulant expansion. The results for the free energy of the Heisenberg Hamiltonian in the above-mentioned cluster calculation are given in column 1 of Table I to be compared with the high-temperature-expansion results[14] in column 2.

These calculations give an intriguing glimpse of the new domains in which the quantum renormalization transformation can be applied.[15] Particularly interesting is the possibility of giving a global description, relating models with different symmetries as in the example of the anisotropic Heisenberg model. Detailed calculations are being pursued and will be presented in a subsequent article.

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[1]For a recent review, see Th. Niemeijer and J. M. J. van Leeuwen, *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (to be published), Vol. 6; S. K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, Reading, Mass., 1976).

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[6]The cell-spin operators $\vec{\tau}_i$ belong to the same representation of the rotation group as the site-spin operators.

[7]However, we note that in the limit $L=1$ of one spin per cell the choice of Eq. (3) leads to the identity transformation whereas the choice of Eq. (4) does not.

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[11]We assume in Eq. (13) and (14) that $\mathrm{Tr}_\sigma \exp(H_0)T$ is a multiple of the unit operator. Otherwise modifications are needed as in the presence of a magnetic field.

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[15]Of course, we are also aware of the potentially interesting applications to quark confinement in lattice gauge theories.