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Approximate Mapping of Two-Dimensional Quantum-Spin Models on Staggered Eight-Vertex Models

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Analytic results have been obtained for the thermodynamics of the two-dimensional $S=\frac{1}{2}$ X-Y model using the simplest form of the generalized Trotter formula for the partition function. The model exhibits a phase transition of unconventional nature. It is claimed that this is one of the best descriptions given so far of the critical thermodynamics of the $S=\frac{1}{2}$ two-dimensional X-Y model. Central in the present approach is the mapping of a family of two-dimensional $S=\frac{1}{2}$ models on staggered eight-vertex models having unconventional weights.

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The critical behavior of two-dimensional (2D) spin models has been the subject of a number of recent investigations. Of much current interest is the planar rotor model, also referred to as the classical X-Y model, which shows fascinating critical properties.[1,2] Many of the theoretical tools being used for these classical models like renormalization-group approaches and high-temperature expansions are much harder to apply to quantum models. Several rather crude real-space renormalization-group studies on the 2D $S=\frac{1}{2}$ X-Y model have not led to a clear picture.[3,4] These methods do not agree with each other, and do not agree with the high-T expansions concerning the very existence of a phase transition. A more promising approach in the understanding of quantum thermodynamics is the use of path summations because in these methods quantum models are mapped on classical models.[5,6] Monte Carlo experiments on 1D quantum models of reasonable size have already been reported.[7,8] The inherent complexity of this line of attack makes it very difficult to apply this technique to the critical behavior of 2D and higher-dimensional quantum models. In this Letter we want to demonstrate that the simplest possible approximant for the partition function of the 2D $S=\frac{1}{2}$ X-Y model using the path-summation method can be solved analytically.

The basis of the path-summation method is the Trotter formula,

$$e^{A+B}=\lim_{m\to\infty}(e^{A/m}e^{B/m})^m, \tag{1}$$

holding for bounded operators.[6] Formula (1) can easily be generalized to more than two operators. The link with thermodynamics is that one is interested in $e^{-\beta\mathcal{H}}$, in which $\beta=1/k_BT$, and in which $\mathcal{H}$ is a sum of operators. In this work we will write the Hamiltonian $\mathcal{H}$ for the $S=\frac{1}{2}$ 2D quantum model in its real-space decomposition,

$$\mathcal{H}=\sum_I \mathcal{H}_I, \tag{2}$$

in which I runs over all nearest-neighbor pairs of spins, and in which $\mathcal{H}_I$ is the pair interaction. Single-site interactions are partitioned equally over the pair interactions. The simple model we want to discuss in this Letter is the $m=1$ approximant to the partition function, $Z\equiv \mathrm{Tr}\exp(-\beta\times\sum_I\mathcal{H}_I)$,

$$Z_1=\mathrm{Tr}\prod_I \exp(-\beta\mathcal{H}_I). \tag{3}$$

We will introduce the approximation $Z=Z_1$, and we will refer to it as the independent-pair approximation (IPA). The IPA conserves all symmetries, rotational and translational, which is very important for the description of phase transitions. In the 1D case the IPA does not introduce spurious phase transitions (compare with the mean-field approximation). The IPA becomes exact for high temperatures, and its results remain physical down to 0 K. The critical behavior of the IPA at 0 K cannot be trusted but in contrast to 1D systems the interesting temperature range for the critical behavior of many 2D models is not close to 0 K. In any case the IPA description of the 2D $S=\frac{1}{2}$ X-Y model is superior to the already mentioned renormalization-group approaches and high-temperature expansions in the tem-

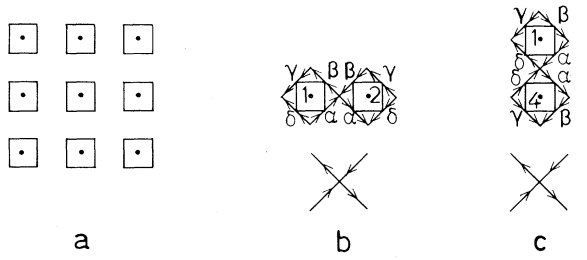

FIG. 1. (a) A small part of a square lattice, in which the dots represent quantum spins and where the square around each dot symbolizes the four Ising spins associated with each quantum spin. (b) A possible configuration for the four Ising spins at site 1 and site 2, and the vertex representing the horizontal coupling. (c) The same as (b) but for the vertical coupling between sites 1 and 4.

perature range of interest. We will demonstrate that the IPA for the 2D $S=\frac{1}{2}$ X-Y model can be solved rigorously.

We will now outline the mapping of Z_1 on the partition function of a staggered eight-vertex model. Inserting complete sets in the product (3) we find

$$Z_1=\sum_{\{\Phi_I\}}\prod_{I=1}^{M}\langle\Phi_I|\exp(-\beta\mathcal{H}_I)\Phi_{I+1}\rangle\,, \tag{4}$$

$$\Phi_{M+1}=\Phi_1,$$

in which M is the number of nearest-neighbor pairs: $M=zN/2$, in which z is the coordination number of the lattice, and N is the number of spins. In Eq. (4) each Φ_I is an N-spin wave function. However, $\mathcal{H}_I$ contains only operators of two sites, and for that reason Φ_I and Φ_{I+1} can only differ in two of the N-spin wave functions. A specific site only occurs in z pair interactions. Consequently for a specific site only z different wave functions will occur in Eq. (4). From now on we will limit ourselves to a square ($z=4$) lattice. For this lattice any spin site will have four spin wave functions associated with it in Eq. (4). Another way of saying this is that with each quantum $S=\frac{1}{2}$ spin, four Ising spins are associated. In Fig. 1 we have symbolically depicted the lattice. The corner points of the square surrounding a lattice point symbolize the Ising spins. So a certain $\{\Phi_I\}$ can be characterized by 4^N Ising spins. To indicate whether a certain Ising spin is up or down we will draw a line (bond) through the corner point in question parallel to the other diagonal of the square, and having the same length as the diagonal. Arrows on that line indicate whether the Ising spin is up or down. The rules are the following[9]: If a spin at a corner is pointing up (down), the arrow on the bond through that corner runs northeast (southeast) or northwest (southwest). In Fig. 1(b) we have given an example of an eight Ising-spin configuration for two neighboring sites: site 1 and site 2. The vertex between site 1 and site 2, which is reproduced separately in the same figure, can be used to represent the matrix element

$$\langle\Sigma_\alpha(1)\Sigma_\alpha(2)|\exp(-\beta\mathcal{H}_{\langle12\rangle})\Sigma_\beta(1)\Sigma_\beta(2)\rangle\,,$$

in which $\Sigma_\alpha(1)$ refers to the αth Ising spin on site 1. All the possible matrix elements, or weights, associated with the interaction between neighboring sites can be represented by vertices. If we limit ourselves to interactions with an even number of up and down Ising spins, only eight different vertices with weights ω_{1H}–ω_{8H} come into play, and they are depicted in Fig. 2. The subscript H refers to horizontal coupling. If we use a vertical coupling as in Fig. 1(c) the weights are ω_{1V}–ω_{8V}. The matrix element being presented by the vertex in Fig. 1(c) is

$$\langle\Sigma_\alpha(1)\Sigma_\alpha(4)|\exp(-\beta\mathcal{H}_{\langle14\rangle})\Sigma_\delta(1)\Sigma_\delta(4)\rangle,$$

and it is clear that for the special example of Fig. 1 the horizontal and vertical weights are different: $\omega_{5H}\neq\omega_{5V}$. In general the weights for the vertical coupling are a permutation of the weights for the horizontal coupling:

$$\begin{pmatrix}1\,2\,3\,4\,5\,6\,7\,8:\mathrm{H}\\ 1\,2\,3\,4\,8\,7\,6\,5:\mathrm{V}\end{pmatrix}.$$

We now want to prove that a path through the lattice, that is any set $\{\Phi_I\}$ contributing to Z_1, can be presented by a set of horizontal and vertical couplings, and that any set of vertices corresponds to a set $\{\Phi_I\}$. The latter is trivial, since

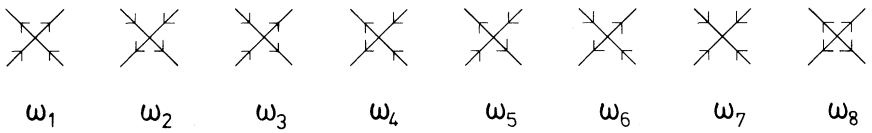

FIG. 2. The eight vertices with their weights.

this is true by construction, but the former is nontrivial. To construct a path through the lattice we have to start at a certain lattice site, say 1, and consider its coupling to one of its neighbors, say 2, thus generating

$$\langle \Sigma_\alpha(1)\Sigma_\alpha(2)\,|\exp(-\beta\mathcal{H}_{\langle 12\rangle})\Sigma_\beta(1)\Sigma_\beta(2)\rangle\,.$$

The next time we consider site 1 the first Ising spin in the matrix element should be $\Sigma_\beta(1)$. That is to say, once a site has been used for the first time for an interaction there is no freedom anymore as to what Ising spin to use for the next three times when this site is being considered. So after having gone partly through the lattice, and after having taken into account some pair interactions, one will encounter situations in which there is no freedom any more for a certain pair interaction because both neighbors involved in this interaction have been considered before in other pair interactions. If the two Ising spins of these neighboring sites which have to be treated first are not nearest neighbors, one could not insert a vertex between them. This is a nontrivial topological problem on first sight. But an actual construction of a finite lattice shows that it is very simple to fulfill the constraints. We will indicate a sequence for a 4×4 lattice with periodic boundary conditions: The first row contains sites 1,2,3,4, and the second row 5,6,7,8, etc. A possible sequence of pair interactions is (1,2), (1,13), (1,4), (1,5), (2,14), (2,3), (2,6), (3,7), (4,8), (3,4), (3,15), (4,16), (5,6), (7,8), (5,9), (6,10), (7,11), (6,7), (8,12), (5,8), (9,12), (10,11), (13,16), (14,15), (9,13), (10,14), (9,10), (13,14), (11,15), (12,16), (11,12), (15,16).

So we have shown that the $m=1$ 2D $S=\frac{1}{2}$ model can be represented by a sixteen-vertex model having different weights for horizontal and vertical couplings. This corresponds to a staggered sixteen-vertex model. Many possible sequences of pair interactions give the same result but we cannot prove that this holds for all sequences. On the other hand we cannot exclude this possibility. This possible ambiguity is well known in functional integration techniques and has been discussed by Hubbard.[10] He suggests the inclusion of the symmetry aspect of possible sequences, and this is what is effectively done in our approach. The models we will consider in the following are staggered eight-vertex models because eight weights vanish by symmetry.

The Hamiltonian we want to discuss is described by the pair interaction

$$\mathcal{H}_{\langle ij\rangle} = -J_\perp(\sigma_i{}^x\sigma_j{}^x+\sigma_i{}^y\sigma_j{}^y) - J_\parallel(\sigma_i{}^z\sigma_j{}^z) - \tfrac{1}{4}H(\sigma_i{}^z+\sigma_j{}^z), \qquad (5)$$

if i and j are nearest neighbors. In Eq. (5) $\vec{\sigma}_i$ is a Pauli spin operator for the spin at site i, and H is a magnetic field perpendicular to the plane of the 2D system. Hamiltonian (5) contains the 2D Heisenberg model and 2D X-Y model with a perpendicular field. The weights for the corresponding staggered eight-vertex model are given in Table I. For simplicity we have excluded anisotropic X-Y couplings although they could be incorporated without problems. The general staggered eight-vertex model has not been solved yet, but the X-Y version (that is $J_\parallel=0$) can be solved exactly because in that case the vertex weights satisfy the free-fermion condition.[11] The result for the $m=1$ X-Y model is that the free energy has a diverging second derivative at the temperature T_c defined by $\sinh(2\beta_c J_\perp)=1$. The second derivative of the free energy behaves as $C+\ln|T-T_c|$ in the neighborhood of the phase transition. At the phase transition we have an Onsager type of singularity in the specific heat. The magnetization in the z direction and the corresponding susceptibility can be calculated exactly. There is no spontaneous z magnetization and the susceptibility remains continuous. Unfortunately the X-Y model with a field in the x direction cannot be mapped on a model satisfying the free-fermion condition. Comparison with the high-T expansion of the quantum X-Y model shows that the IPA is very good.[3] Our free energy differs by 1% from the free energy in the high-T expansion at the point where the high-T results start to fail: $\beta J_\perp=0.4$ [there is a difference of a factor of 2 in definition of the coupling constant between Ref. 3 and us]. The phase transition occurs at $\beta J_\perp=0.44$, a region where the IPA is still very reliable.

The staggered eight-vertex models we have

TABLE I. The eight horizontal vertex weights for Hamiltonian (5).[a]

$\omega_{1H}=e^{y}\exp K_\parallel$
$\omega_{2H}=e^{-y}\exp K_\parallel$
$\omega_{3H}=\omega_{4H}=\exp(-K_\parallel)\sinh K_\perp$
$\omega_{5H}=\omega_{6H}=\exp(-K_\parallel)\cosh K_\perp$
$\omega_{7H}=\omega_{8H}=0$

[a] $y=\frac{1}{2}\beta H$, $K_\parallel\equiv\beta J_\parallel$, $K_\perp\equiv 2\beta J_\perp$.

introduced form an interesting class of models. The "quantum" character of these classical models lies in their weights. Almost all vertex models studied so far have weights of the form $\omega_i = \exp(-\beta\epsilon_i)$, in which ϵ_i is an energy. Our weights are of a different nature: They are hyperbolic functions of the interaction energies. This has far-reaching consequences as can be seen by considering the uniform eight-vertex models with weights $\omega_{1H}-\omega_{8H}$. These models do not have the unphysical retention of correlations at infinite temperature as some of the conventional models with weights of the form $\exp(-\beta\omega_i)$ have.

We have shown that there exists an approximate mapping of the $S=\frac{1}{2}$ 2D XYZ model, which includes the Heisenberg and X-Y model, on a staggered eight-vertex model. This mapping results as the first approximation in the path-summation method of Suzuki, Miyashita, and Kuroda.[6] The X-Y version shows a phase transition without long-range order in the z magnetization, and without a divergence in the z susceptibility. This method introduces vertex weights of a different character from the classical ones. The study of these models is very interesting in itself.

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Irrational Decimations and Path Integrals for External Noise

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Irrational decimation schemes are constructed for functional integrals with the very interesting feature of preserving several distinct site Hamiltonians into the fixed-point limit. This method is applied to the quasiperiodicity transition to turbulence in order to compute the effects of external noise.

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In an important paper, Shraiman, Wayne, and Martin[1] determined the effect of noise on the period-doubling behavior of maps on an interval. In this paper we shall extend their methodology to determine the role of noise on the recently developed theory for the transition to chaos from quasiperiodic motion.[2,3] In order to perform our calculation, however, rather than using only existing renormalization ideas, we have constructed new decimation schemes that might prove useful in other contexts. Specifically, we construct *irrational* decimation schemes which at each level of renormalization produce *several* distinct Hamiltonians deployed along the lattice, approaching distinct fixed points. This is in contradistinction to the usual technique which produces the same Hamiltonian at each site, so that our technique accommodates dynamics whose critical behavior maintains multiple clusterings.

Let us recall Shraiman's adaption of decimation to the context of iterated maps. To a one-dimensional causal system we add external noise and so consider the stochastic process $x_{n+1} = f(x_n) + \xi_n$, where ξ_n is a noise sample drawn from a distribution with density ρ. Accordingly, $P_1(x_{n+1}|x_n) = \rho(x_{n+1}$