Renormalization-group calculation for the two-dimensional square Ising model in a transverse magnetic field

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We apply a recently proposed real-space renormalization-group method to the two-dimensional square Ising model in a transverse magnetic field at zero temperature. We do the calculation to first and second order in the intercell coupling; in both cases we find a nontrivial fixed point. We compare the obtained critical exponents with accepted values for the three-dimensional Ising model from high-temperature series expansions. In first order the agreement is poor, in second order we obtain good agreement with the expected values.

In a recent paper[1], we proposed a real-space renormalization-group (RG) method for quantum spin systems on a lattice at zero temperature. Our method is a systematic perturbation expansion which reduces, to lowest order, to a truncation method discussed by several authors.[2-4] In that method, one divides the lattice into cells, diagonalizes exactly the intracell Hamiltonian and takes a truncated basis consisting of the lowest-lying states in each cell. The renormalized Hamiltonian is then the part of the original Hamiltonian spanned by these low-lying states. We show in Ref. 1 that this procedure can be viewed as a first-order calculation in the intercell coupling, and show how to systematically carry it out to arbitrary order. In Ref. 1 we applied the method to the one-dimensional Ising model in a transverse field to second order and to the two-dimensional triangular Ising model in a transverse field to first order. In the triangular lattice, complications arise if one tries to do a second-order calculation because, due to geometric reasons, one generates a renormalized Hamiltonian that does not have the same threefold symmetry as the original one. In this paper, we apply our method to the two-dimensional square lattice, which is simpler from a geometrical point of view. It is known[5] that the critical behavior of a d-dimensional Ising model at zero temperature as a function of a transverse field is the same as that of $(d+1)$-dimensional Ising system in zero transverse field as a function of temperature; therefore, we obtain from our calculation the critical exponents for the three-dimensional Ising model. We compare our results with high-temperature expansion results for the critical exponents of a three-dimensional Ising model.

We consider the Hamiltonian

$$H_\sigma = \epsilon \sum_i \sigma_z^i - \Delta \sum_{\langle i,j \rangle} \sigma_x^i \sigma_x^j , \tag{1}$$

where i and j run over nearest neighbors in a square lattice. We divide the system into square cells of four sites each, as shown in Fig. 1, and diagonalize exactly the intracell Hamiltonian. The cell Hilbert space of 16 states splits into two sets of eight states each, corresponding to states with even and odd number of spins up (or down). The eigenstates and eigenvalues for those two sets can be found analytically and are listed in Tables I and II. Note that the ground state for both limiting cases $\Delta/\epsilon \to 0$ and $\epsilon/\Delta \to 0$ can be formed from the lowest even and odd cell states, $|0\rangle$ and $|1\rangle$; for $\Delta/\epsilon \to 0$ the ground state is simply

$$|\Psi\rangle = \prod_p |0\rangle_p , \quad E_\Psi = -N\epsilon , \tag{2a}$$

(with p labeling the cells), while for $\epsilon/\Delta \to 0$ the de-

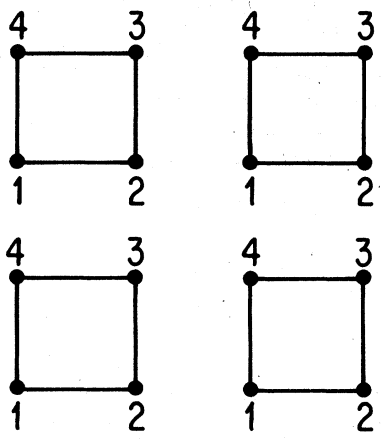

FIG. 1. Construction of four-site square cells.

TABLE I. Eigenstates and eigenvalues of the cell Hamiltonian for the even subspace.

State	Energy
$\|0\rangle = C_1(0)\|++++\rangle + C_2(0)\|----\rangle + C_3(0)\frac{\|++--\rangle+\|--++\rangle+\|-++-\rangle+\|+--+\rangle}{2} + C_4(0)\frac{\|+-+-\rangle+\|-+-+\rangle}{2^{1/2}}$	$E_0 = -\{8[\epsilon^2+\Delta^2+(\epsilon^4+\Delta^4)^{1/2}]\}^{1/2}$
$\|2\rangle = C_1(2)\|++++\rangle + C_2(2)\|----\rangle + C_3(2)\frac{\|++--\rangle+\|--++\rangle+\|-++-\rangle+\|+--+\rangle}{2} + C_4(2)\frac{\|+-+-\rangle+\|-+-+\rangle}{2^{1/2}}$	$E_2 = -\{8[\epsilon^2+\Delta^2-(\epsilon^4+\Delta^4)^{1/2}]\}^{1/2}$
$\|4\rangle = \frac{1}{2}(\|++--\rangle+\|--++\rangle-\|-++-\rangle-\|+--+\rangle)$	$E_4 = 0$
$\|6\rangle = \frac{1}{2}(\|++--\rangle-\|--++\rangle-\|-++-\rangle-\|+--+\rangle)$	$E_6 = 0$
$\|8\rangle = \frac{1}{2}(\|++--\rangle-\|--++\rangle-\|-++-\rangle+\|+--+\rangle)$	$E_8 = 0$
$\|10\rangle = \frac{1}{2^{1/2}}(\|+-+-\rangle-\|-+-+\rangle)$	$E_{10} = 0$
$\|12\rangle = C_1(12)\|++++\rangle + C_2(12)\|----\rangle + C_3(12)\frac{\|++--\rangle+\|--++\rangle+\|-++-\rangle+\|+--+\rangle}{2} + C_4(12)\frac{\|+-+-\rangle+\|-+-+\rangle}{2^{1/2}}$	$E_{12} = \{8[\epsilon^2+\Delta^2-(\epsilon^4+\Delta^4)^{1/2}]\}^{1/2}$
$\|14\rangle = C_1(14)\|++++\rangle + C_2(14)\|----\rangle + C_3(14)\frac{\|++--\rangle+\|--++\rangle+\|-++-\rangle+\|+--+\rangle}{2} + C_4(14)\frac{\|+-+-\rangle+\|-+-+\rangle}{2^{1/2}}$	$E_{14} = \{8[\epsilon^2+\Delta^2+(\epsilon^4+\Delta^4)^{1/2}]\}^{1/2}$

$$C_1(j) = \frac{E_j+4\epsilon}{A_j},\quad C_2(j) = \frac{E_j-4\epsilon}{A_j},\quad C_3(j) = \frac{16\epsilon^2-E_j^2}{2\Delta A_j},\quad C_4(j) = 2^{1/2}\frac{E_j^2-16\epsilon^2}{E_j A_j}$$

$$A_j = [8(\epsilon^4+\Delta^4)^{1/2}|E_j^2-16\epsilon^2|]^{1/2}/\Delta$$

generate ground state is

$$|\Psi\rangle = \prod_p \frac{1}{\sqrt{2}}(|0\rangle_p \pm |1\rangle_p)\ ,\quad E_\Psi = -N\Delta\ , \tag{2b}$$

where one has to take the same sign for all cells. When Δ increases from zero (the "disordered phase"), the gap between the ground state and the first excited state narrows, till at a critical value $y_c = (\epsilon/\Delta)_c$ they become degenerate; beyond that point we have the "ordered phase," with $\langle\sigma_x\rangle \neq 0$.

Following the formalism described in Ref. 1, we calculated the renormalized Hamiltonian to first and second order in the intercell coupling. In first order, we simply truncate H_σ by keeping only its matrix elements with products of cell states $|0\rangle_p$ and $|1\rangle_p$. In second order, we take into account transitions that start from a state composed of cell states $|0\rangle_p$ and $|1\rangle_p$, go through an intermediate state where at least one cell state is higher than those, and return to a state of only $|0\rangle$ and $|1\rangle$'s. The general expression for the renormalized Hamiltonian to second order in the intercell coupling V is

$$H^{(2)} = \sum_{i,j}|i\rangle\left[E_i\delta_{ij} + V_{ij} + \frac{1}{2}\sum_\alpha V_{i\alpha}V_{\alpha j}\left(\frac{1}{E_i-E_\alpha}+\frac{1}{E_j-E_\alpha}\right)\right]\langle j|\ , \tag{3}$$

where the states $|i\rangle, |j\rangle$ are products of cell states $|0\rangle_p$ and $|1\rangle_p$ only, and the states $|\alpha\rangle$ have a higher excited state in at least one cell. E_i is the unperturbed energy of state $|i\rangle$. Finally, we rename the cell states $|0\rangle_p$ and $|1\rangle_p$ as $|-\rangle_p$ and $|+\rangle_p$, the eigenstates of a new cell-spin operator μ_z^p.

To first order, the resulting Hamiltonian has exactly the same form as the original one (except for an additive constant)

$$H_\mu = d'\sum_p 1 + \epsilon'\sum_p \mu_z^p - \Delta'\sum_{\langle p,p'\rangle}\mu_x^p\mu_x^{p'}\ , \tag{4}$$

where p and p' run over the cells of the original sys-

TABLE II. Eigenstates and eigenvalues of the cell Hamiltonian for the odd subspace.

State	Energy
$\|1\rangle = \frac{1}{(1+a^2)^{1/2}}\left(a\frac{\|+++-\rangle+\|-++\rangle+\|+-+\rangle+\|++-+\rangle}{2} + \frac{\|---+\rangle+\|+--\rangle+\|-+-\rangle+\|--+-\rangle}{2}\right)$	$E_1=-2[(\epsilon^2+\Delta^2)^{1/2}+\Delta]$
$\|3\rangle = \frac{1}{2^{1/2}}(\|-+-\rangle-\|--+\rangle)$	$E_3=-2\epsilon$
$\|5\rangle = \frac{1}{2^{1/2}}(\|--+-\rangle-\|+--\rangle)$	$E_5=-2\epsilon$
$\|7\rangle = \frac{1}{(1+a^2)^{1/2}}\left(-a\frac{\|+++-\rangle+\|-++\rangle-\|+-+\rangle-\|++-+\rangle}{2} + \frac{\|--+-\rangle+\|+--\rangle-\|-+-\rangle-\|---+\rangle}{2}\right)$	$E_7=-2[(\epsilon^2+\Delta^2)^{1/2}-\Delta]$
$\|9\rangle = \frac{1}{(1+a^2)^{1/2}}\left(\frac{\|+++-\rangle+\|-++\rangle+\|+-+\rangle+\|++-+\rangle}{2} - a\frac{\|---+\rangle+\|+--\rangle+\|-+-\rangle+\|--+-\rangle}{2}\right)$	$E_9=2[(\epsilon^2+\Delta^2)^{1/2}-\Delta]$
$\|11\rangle = \frac{1}{2^{1/2}}(\|++-+\rangle-\|-++\rangle)$	$E_{11}=2\epsilon$
$\|13\rangle = \frac{1}{2^{1/2}}(\|+-++\rangle-\|+++-\rangle)$	$E_{13}=2\epsilon$
$\|15\rangle = \frac{1}{(1+a^2)^{1/2}}\left(\frac{\|++-+\rangle+\|-++\rangle-\|+-+\rangle-\|+++-\rangle}{2} + a\frac{\|--+-\rangle+\|+--\rangle-\|-+-\rangle-\|---+\rangle}{2}\right)$	$E_{15}=2[(\epsilon^2+\Delta^2)^{1/2}+\Delta]$

$$a=\frac{(\epsilon^2+\Delta^2)^{1/2}-\epsilon}{\Delta}$$

tem, and

$$\epsilon'=\tfrac{1}{2}(\{8[\epsilon^2+\Delta^2+(\epsilon^4+\Delta^4)^{1/2}]\}^{1/2} - 2[(\epsilon^2+\Delta^2)^{1/2}+\Delta]) , \quad (5)$$

$$\Delta'=2|\langle 0|\sigma_x|1\rangle|^2\Delta .$$

We iterate this procedure and look for a fixed point for the recursion relation for $y=\epsilon/\Delta$. Besides the trivial fixed points $y=\infty$ and $y=0$ (corresponding to the two limiting cases described previously) we find a nontrivial fixed point at

$$y_c=3.2801 , \quad (6)$$

which corresponds to the critical point described previously. Linearizing the recursion relation around the fixed point, we find for the "thermal exponent"

$$\nu=1.197 \quad (7)$$

to be compared with the result from high-temperature series expansion for the three-dimensional Ising model[6] $\nu=0.625$.

In second order, we generate new terms in the Hamiltonian, which we treat as second-order quantities. The Hamiltonian one gets after n iterations has the form

$$H_\mu^n = d_n\sum_i 1+\epsilon_n\sum_i \mu_z^i-\Delta_n\sum_{\langle i,j\rangle}\mu_x^i\mu_x^j-\mu_n\sum_{i,j}\mu_x^i\mu_x^j-\delta_n\sum_{i,j}\mu_x^i\mu_x^j-\alpha_n\sum_{i,k,j}\mu_x^i\mu_z^k\mu_x^j-\lambda_n\sum_{i,k,j}\mu_x^i\mu_z^k\mu_x^j-\beta_n\sum_{i,j}\mu_z^i\mu_z^j , \quad (8)$$

where the couplings are shown schematically in Fig. 2. The recursion relations are shown in the Appendix. We find a nontrivial fixed point at

$$\epsilon/\Delta = 2.7266\ , \quad \mu/\Delta = 0.885\,59\ ,$$
$$\lambda/\Delta = 0.167\,93\ , \quad \delta/\Delta = 0.468\,45\ , \tag{9}$$
$$\alpha/\Delta = 0.415\,55\ , \quad \beta/\Delta = 0.229\,00\ .$$

The intersection of the critical surface with the Ising axis gives

$$y_c = 3.556\ . \tag{10}$$

Linearizing the recursion relations around the fixed point and diagonalizing the resulting matrix we find six eigenvalues; two of them are complex but small (absolute value less than 0.3) and we attribute them to the approximation used; from the real ones, only one is relevant (i.e., greater than 1)

$$\lambda_T = 2.892\ . \tag{11}$$

From it, we find for the thermal exponent

$$\nu = 0.653 \tag{12}$$

in good agreement with the expected value.

We now introduce a magnetic perturbation

$$V_h \equiv h \sum_i \sigma_x^i\ . \tag{13}$$

To lowest order, the corresponding term in the renormalized Hamiltonian has the same form, with

$$h' = 4\langle 0|\sigma_x|1\rangle h\ . \tag{14}$$

At the first-order fixed point this gives for the magnetic eigenvalue

$$\lambda_h = 2.363 \tag{15}$$

and from the relation

$$\beta = \nu(2 - \log\lambda_h/\log 2) \tag{16}$$

we get for the magnetic exponent

$$\beta = 0.909\ , \tag{17}$$

to be compared with $\beta = 0.3125$ from high-temperature series expansions.[6] In the next order, we generate a contribution to the Hamiltonian

$$V_h^n = h_n \sum_i \mu_x^i + L_n \sum_{\langle i,j\rangle} (\mu_x^i \mu_z^j + \mu_z^i \mu_x^j)\ . \tag{18}$$

The recursion relations for h_n and L_n are shown in the Appendix. Diagonalizing the linearized recursion relations at the first-order fixed point we find the two eigenvalues

$$\lambda_1 = 2.956\ , \quad \lambda_2 = 1.648\ . \tag{19}$$

The fact that λ_2 is larger than 1 is unphysical, due to the approximation used. Taking the largest eigenvalue as our magnetic eigenvalue we find for the magnetic exponent

$$\beta = 0.285\ , \tag{20}$$

again a marked improvement over the first-order result.

As discussed in Ref. 1, the renormalization at the fixed point leaves the Hamiltonian invariant only up to a multiplicative constant

$$c(s) = \frac{\Delta_{n+1}}{\Delta_n} = \frac{\epsilon_{n+1}}{\epsilon_n} = \cdots\ .$$

As a further check on the method, we calculated $c(s)$, which can be shown from general arguments to be $1/s$, where s is the length scale change.[7,8] We find to first order

$$c(s) = 0.698\ , \tag{21}$$

to second order

$$c(s) = 0.597\ , \tag{22}$$

which appears to be approaching the correct value $c(s) = \frac{1}{2}$.

In Table III, we summarize our results for the critical exponents and compare them with other perturbative RG calculations. Reference 8 is a calculation

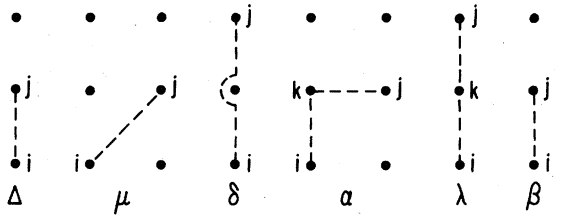

FIG. 2. Couplings in the second-order calculation.

TABLE III. Comparison of our results with high-temperature expansion and previous RG results.

Approximation	ν	β
High-temperature series	0.625	0.3125
This calculation, first order	1.197	0.909
This calculation, second order	0.653	0.285
Triangular[a]	0.924	0.512
$2\times2\times2$ cell[b]	0.827	0.332
$3\times3\times3$ cell[b]	0.844	0.460

[a]Reference 8. [b]Reference 10.

with Friedman's method[9] for the triangular Ising model in a transverse field to second order. Reference 10 is a calculation on the three-dimensional Ising model using the Niemeijer–Van Leeuwen cumulant expansion to second order. Our results to second order show somewhat better agreement with the expected values than the other approximate calculations.

In conclusion, we have applied a zero-temperature quantum renormalization-group method to the square Ising model in a transverse field to first and second order. In both cases, we find nontrivial fixed points, corresponding to the transition from a ground state with broken symmetry to a nondegenerate ground state. We find some unphysical eigenvalues due to the approximation used. The values of the exponents compared with accepted values from high-temperature series expansions for the three-dimensional Ising model are rather poor at first order and show a marked improvement in the second-order calculation.

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APPENDIX

We label the sites in the cell as shown in Fig. 1. The recursion relations for the even part of the Hamiltonian to second order are

$$
\begin{aligned}
&\epsilon_{n+1}=\tfrac{1}{2}(E_1^n-E_0^n)+\Delta_n^2(C_1-C_3)+2\beta_n(|\langle 1|\sigma_z|1\rangle|^2-|\langle 0|\sigma_z|0\rangle|^2)\\
&\quad -2\alpha_n(\langle 1|\sigma_x^1\sigma_z^2\sigma_x^3|1\rangle-\langle 0|\sigma_x^1\sigma_z^2\sigma_x^3|0\rangle)-\mu_n(\langle 1|\sigma_x^1\sigma_x^3|1\rangle-\langle 0|\sigma_x^1\sigma_x^3|0\rangle)-2\beta_n\langle 0|\sigma_z^1\sigma_z^2|0\rangle\ ,\\
&\Delta_{n+1}=2|\langle 0|\sigma_x|1\rangle|^2(\Delta_n+\mu_n+2\delta_n)+4\langle 0|\sigma_x|1\rangle\langle 0|\sigma_x^1\sigma_z^2|1\rangle(\alpha_n+\lambda_n)\ ,\\
&\mu_{n+1}=|\langle 0|\sigma_x|1\rangle|^2[\mu_n+\alpha_n(\langle 1|\sigma_z|1\rangle+\langle 0|\sigma_z|0\rangle)-\Delta_n^2(B_1+B_2)]\ ,\\
&\delta_{n+1}=-\tfrac{1}{2}[\Delta_n^2|\langle 0|\sigma_x|1\rangle|^2(A_1+A_2)]\ ,\quad \lambda_{n+1}=-\tfrac{1}{2}[\Delta_n^2|\langle 0|\sigma_x|1\rangle|^2(A_1-A_2)]\ ,\\
&\alpha_{n+1}=|\langle 0|\sigma_x|1\rangle|^2\tfrac{1}{2}\{[\alpha_n(\langle 1|\sigma_z|1\rangle-\langle 0|\sigma_z|0\rangle)-\Delta_n^2(B_1-B_2)]\}\ ,\\
&\beta_{n+1}=\tfrac{1}{2}\beta_n(\langle 1|\sigma_z|1\rangle-\langle 0|\sigma_z|0\rangle)^2+\tfrac{1}{4}(\Delta_n^2)(C_1-2C_2+C_3)\ ,
\end{aligned}
\tag{A1}
$$

with

$$
\begin{aligned}
A_1&=\sum_{n\neq 0}\langle 1|\sigma_x^1+\sigma_x^2|n\rangle\langle n|\sigma_x^3+\sigma_x^4|1\rangle\left(\frac{1}{E_0-E_n}+\frac{1}{2E_1-E_0-E_n}\right),\\
A_2&=\sum_{n\neq 1}\langle 0|\sigma_x^1+\sigma_x^2|n\rangle\langle n|\sigma_x^3+\sigma_x^4|0\rangle\left(\frac{1}{E_1-E_n}+\frac{1}{2E_0-E_1-E_n}\right),\\
B_1&=\sum_{n\neq 0}\langle 1|\sigma_x^1+\sigma_x^2|n\rangle\langle n|\sigma_x^2+\sigma_x^4|1\rangle\left(\frac{1}{E_0-E_n}+\frac{1}{2E_1-E_0-E_n}\right),\\
B_2&=\sum_{n\neq 1}\langle 0|\sigma_x^1+\sigma_x^2|n\rangle\langle n|\sigma_x^2+\sigma_x^4|0\rangle\left(\frac{1}{E_0-E_n}+\frac{1}{2E_1-E_0-E_n}\right),\\
C_1&=\sum_{(n,n')\neq(0,0)}|\langle 1|\sigma_x^1|n\rangle\langle 1|\sigma_x^4|n'\rangle+\langle 1|\sigma_x^2|n\rangle\langle 1|\sigma_x^3|n'\rangle|^2\frac{1}{2E_1-E_n-E_{n'}}\ ,\\
C_2&=\sum_{(n,n')\neq(0,1)}|\langle 0|\sigma_x^1|n\rangle\langle 1|\sigma_x^4|n'\rangle+\langle 0|\sigma_x^2|n\rangle\langle 1|\sigma_x^3|n'\rangle|^2\frac{1}{E_0+E_1-E_n-E_{n'}}\ ,\\
C_3&=\sum_{(n,n')\neq(1,1)}|\langle 0|\sigma_x^1|n\rangle\langle 0|\sigma_x^4|n'\rangle+\langle 0|\sigma_x^2|n\rangle\langle 0|\sigma_x^3|n'\rangle|^2\frac{1}{2E_0-E_n-E_{n'}}\ .
\end{aligned}
\tag{A2}
$$

When we include the magnetic perturbation, we obtain the additional recursion relations

$$h_{n+1} = 2\langle 0|\sigma_x|1\rangle[2-\Delta_n(S_1+S_2)]h_n + 4[\langle 0|\sigma_x|1\rangle(\langle 1|\sigma_z|1\rangle + \langle 0|\sigma_z|0\rangle) + 2\langle 0|\sigma_x^1\sigma_z^2|1\rangle]L_n ,$$
$$L_{n+1} = \Delta_n \tfrac{1}{2}(S_1-S_2)\langle 0|\sigma_x|1\rangle h_n + \langle 0|\sigma_x|1\rangle(\langle 1|\sigma_z|1\rangle - \langle 0|\sigma_z|0\rangle)L_n , \tag{A3}$$

with

$$S_1 = \tfrac{1}{2}\sum_{n\neq 1}\langle 0|\sigma_x^1+\sigma_x^2|n\rangle\langle n|\sigma_x^1+\sigma_x^2+\sigma_x^3+\sigma_x^4|0\rangle\left(\frac{1}{2E_0-E_1-E_n}+\frac{2}{E_0-E_n}+\frac{1}{E_1-E_n}\right),$$
$$S_2 = \tfrac{1}{2}\sum_{n\neq 0}\langle 1|\sigma_x^1+\sigma_x^2|n\rangle\langle n|\sigma_x^1+\sigma_x^2+\sigma_x^3+\sigma_x^4|1\rangle\left(\frac{1}{2E_1-E_0-E_n}+\frac{2}{E_1-E_n}+\frac{1}{-E_0-E_n}\right). \tag{A4}$$

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