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EFFECTIVE FIELD METHODS FOR MAGNETIC SYSTEMS

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The self-consistency conditions inherent in the mean-field approximation are extended to take into account some pair correlations. It is shown that this extension is systematically improvable and applicable to the spin systems with short-range interactions in the entire temperature region. With two correlations included and the renormalization-group ideas implemented, the critical properties of the Ising model are satisfactorily revealed. Moreover, the improved estimates of the thermodynamical quantities for the quantum linear XY model from the finite-size calculations are found down to very low temperatures.

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1. Introduction

The molecular field approximation (MFA) has always been a valuable tool for obtaining a qualitative understanding of the phase diagram and for deriving quantitative estimates of nonsingular thermodynamic properties. The accuracy of such estimates has been improved by various correction schemes. We will briefly review some of these and show how they may be generalized so that also the correlations, completely neglected in the standard MFA, are taken into account.

We will also show how this improved method may be applied to the low--dimensional quantum-mechanical models of magnetism, combining our idea with exact finite-size calculations, to obtain accurate estimates of thermodynamical quantities. These exact calculations on small finite-size lattices are considered an important complement and a check on computer simulations on larger lattice systems. Although limited to substantially smaller sizes, they do not encounter possible sources of errors in simulation studies such as the Trotter approximation or metastability in Monte Carlo sampling. In this report we show that some implementation of our method for the quantum chains improves the finite-size estimates so that the accuracy accessible for the transfer-matrix technique can be reached [1].

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2. Generalized mean field approximations

We suppose that we want to study a classical system with short range interactions, which can be divided into a finite cluster Ω, its boundary $\partial\Omega$ and $\overline{\Omega}$, the complement of $\Omega \bigcup \partial\Omega$, in such a way that the Hamiltonian can be written as

$$-\beta\mathcal{H} = H_0(\Omega, \partial\Omega) + H_1(\partial\Omega, \overline{\Omega}). \tag{1}$$

Denoting the degrees of freedom by the variables $\sigma \in \Omega$, $\tau \in \partial\Omega$ and $\overline{\sigma} \in \overline{\Omega}$, we address here a problem of estimating the thermal expectation value $\langle A \rangle$ of an operator $A(\sigma, \tau)$.

The first category of approximations uses some probability distribution $P(\tau)$ for the boundary states. The expectation value $\langle A \rangle$ is then a weighted average [2] with the properly chosen expression for $P(\tau)$. In this scheme the standard MFA consists in fixing the boundary spins.

A second category of approximations introduces molecular fields into the Hamiltonian. The idea is to correct for the neglect of $\overline{\Omega}$ by these extra terms acting on the boundary $\partial\Omega$:

$$\langle A \rangle \approx \frac{\sum_\tau \sum_\sigma A\, \mathrm{e}^{H_0 + H'(\tau)}}{\sum_\tau \sum_\sigma \mathrm{e}^{H_0 + H'(\tau)}} = \frac{\sum_\tau \sum_\sigma A\, \mathrm{e}^{H_0}\, Q(\tau)}{\sum_\tau \sum_\sigma \mathrm{e}^{H_0}\, Q(\tau)}, \tag{2}$$

where $H'(\tau)$ and $Q(\tau)$ are given by

$$Q(\tau) \equiv \mathrm{e}^{H'(\tau)} = \sum_{\overline{\sigma}} \mathrm{e}^{H_1}. \tag{3}$$

The function $Q(\tau)$ (and also $P(\tau)$) can be expanded in a form

$$Q(\tau) = \prod_i (1 + a_i \tau_i) \prod_{i \neq j} (1 + b_{ij} \tau_i \tau_j) \ldots \tag{4}$$

where the coefficients b_{ij} take into account the correlations between the spins of $\partial\Omega$. Symmetry properties of the cluster will be reflected in symmetry properties between these coefficients. This implies that the effective Hamiltonian $H'(\tau)$, apart from the standard linear term in τ corresponding to MFA, may contain the higher order terms in τ, i.e. some correlations.

A sequence of systematically improvable approximations can be worked out by: (a) imposing self-consistent conditions on the coefficients in Eq. (4) for P or Q, in analogy with the usual mean field approximation; (b) applying standard series expansion on (3) to get approximate expressions for the correlations induced through H_1; (c) implementation of the renormalization-group ideas — in analogy with the mean-field renormalization group method (MFRG)[3] — which leads to non-classical critical exponents.

3. Applications to the Ising model

We consider here clusters with L^2 sites on the square lattice and we apply both the Q and P-schemes. The critical couplings $K_c = J/k_B T_c$ are given in Table I. The exact result is $K_c = \frac{1}{2}\ln(\sqrt{2}+1) \approx 0.4407$. In the second column the cluster mean-field approximation results are displayed. In the third column, the original MFRG predictions [3] are reported for comparison.

Performing the *self-consistent* calculations with two parameters in (4), we find the results for K_c given in the 4th and 5th columns of Table I for the P and Q-schemes, respectively. In the 6th column of Table I (denoted Q^{nsc}) we report our estimates of K_c for the *non-self-consistent* calculations, with Q expanded up to the 6th order in $x = \tanh K$ and expressed by the Padé approximants.

So far our self-consistent calculations have been combined with the MFRG only for the P-scheme with *no correlations*. The corresponding data for K_c are denoted by P_1^{rg} in Table I. Applying a renormalization group procedure in two steps [3], we find the estimates denoted by P_2^{rg}. Finally, renormalizing the clusters $L = 1$ and $L = 2$ within our Q^{nsc} scheme, we get the data Q^{rg}. It can be noticed that one obtains a much slower convergence by increasing the cluster size than by increasing the order of the approximation.

The corresponding critical exponents y_T and y_H for the thermal and ordering fields are given in Table II. The notation follows that introduced in Table I. The exact values are $y_T = 1$ and $y_H = 15/8$.

TABLE I

The critical coupling K_c of the classical $2d$-Ising model.

L	MFA	MFR	P^{sc}	Q^{sc}	Q^{nsc}	P_1^{rg}	P_2^{rg}	Q^{rg}
1	0.250							
2	0.286	0.361	0.361	0.387	0.407	0.371		0.428
3	0.308	0.381	0.379	0.397	0.415	0.385	0.404	
4	0.323	0.393				0.395	0.418	
5	0.335	0.401						

TABLE II

The critical exponents for the $2d$-Ising model.

L	MFR	P_1^{rg}	P_2^{rg}	Q^{rg}	MFR	P_1^{rg}	P_2^{rg}	Q^{rg}
	y_T				y_H			
1								
2	0.69	0.822		0.801	1.50	1.490		1.715
3	0.78	0.930	0.942		1.57	1.585	1.609	
4	0.82	0.979	0.996		1.60	1.636	1.676	
5	0.84				1.62			

4. Application to the quantum XY model

In general, Eq. (3) is not applicable for quantum mechanical models, because the factor $\exp(H_1)$ cannot be extracted from the Boltzmann factor. Instead, we should define

$$e^{H_0+H'} = \sum_{\overline{\sigma}} e^{H_0(\Omega,\partial\Omega)+H_1(\partial\Omega,\overline{\Omega})}, \tag{5}$$

where H' may also depend on the variables σ from the interior of the cluster Ω.

We propose the method based on Eq. (5) under the assumption that the strongest contributions to H' appear at or around the boundary $\partial\Omega$. We test the efficiency of the method by applying it to the quantum XY-chain which is exactly solvable [4].

For the simple XY-Hamiltonian without external field, we can argue that for symmetry reasons no external field can appear in H'. The first contribution that can be expected in H' is an extra XY-interaction between the first and the second spin in a finite segment, and equally between the last and next last

$$H_0 + H' = -\frac{1}{2}\sum_{i=0}^{N} K_i(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y), \tag{6}$$

where $K_0 = K_N = K + D$ and $K_i = K$ for all other i.

We solved this model by direct diagonalization with the free boundary conditions. We determined D by imposing $\langle\sigma_0^x\sigma_1^x\rangle = \overline{\langle\sigma_i^x\sigma_{i+1}^x\rangle}$, where $\overline{F_i}$ means the average of F_i over all $1 \leq i < N$. Our predictions for the internal energy are illustrated in Fig. 1.

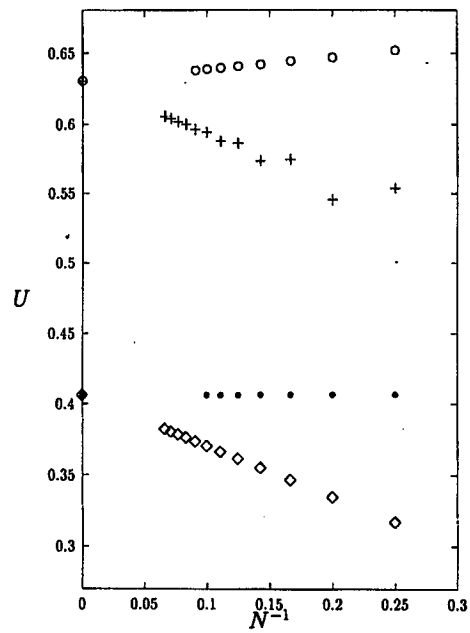

Fig. 1. The finite-size results for the internal energy of the XY model. The symbols ◇, • report the standard and improved data at $K = 1.0$, whereas +, o — the corresponding data at $K^{-1} = 0.15$. Double symbols show the exact predictions for the infinite chain.

Our results are very promising for future applications to more complicated systems, like CHAB ($C_6H_{11}NH_3 \cdot CuBr_3$) or $CsNiF_3$ [1, 2]. They also justify further efforts with higher order approximations, e.g., by using more parameters to be determined simultaneously from self-consistency conditions.

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