Simulations of the low–dimensional Ising and Heisenberg models

G. Kamieniarz[1], G. Musiał[1], L. Dębski[1], M. Bieliński[1] and R. Dekeyser[2]

[1] Computational Physics Division, Institute of Physics, A.Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland
e-mail: gjk@pearl.amu.edu.pl

[2] Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium
e-mail: raf.dekeyser@fys.kuleuven.ac.be

Abstract

The critical coupling and spontaneous magnetization curve for the $2d$–Ising model are calculated using the effective–field method with correlations. An application of the method to the quantum $S=\frac{1}{2}$ $1d$–Heisenberg model is presented and reliable low–temperature estimates of the specific heat are evaluated.

We develop the effective–field method with correlations proposed in [1]. For a classical system with short range interactions the lattice can always be divided into a finite cluster Ω, its boundary $\partial\Omega$ and $\overline{\Omega}$, the complement of $\Omega \cup \partial\Omega$, in such a way that its Hamiltonian can be written as $-\beta\mathcal{H} = H_0(\Omega, \partial\Omega) + H_1(\partial\Omega, \overline{\Omega})$. The idea is to correct for the neglect of $\overline{\Omega}$ by some extra terms acting on the boundary $\partial\Omega$, so that in the classical case the thermal expectation value is:

$$\langle A \rangle \approx \frac{\sum_\tau \sum_\sigma A\, e^{H_0 + H'(\tau)}}{\sum_\tau \sum_\sigma e^{H_0 + H'(\tau)}} = \frac{\sum_\tau \sum_\sigma A\, e^{H_0}\, Q(\tau)}{\sum_\tau \sum_\sigma e^{H_0}\, Q(\tau)}, \tag{1}$$

where the degrees of freedom are denoted by the variables $\sigma \in \Omega$ and $\tau \in \partial\Omega$, while $H'(\tau)$ and $Q(\tau)$ are given by $Q(\tau) \equiv e^{H'(\tau)} = \sum_{\overline{\sigma}} e^{H_1}$.

The effective Hamiltonian $H'(\tau)$ [1, 2] can be expanded into the form

$$H'(\tau) = \sum_i a_i \tau_i + \sum_{i \neq j} b_{ij} \tau_i \tau_j + \ldots, \tag{2}$$

where the coefficients b_{ij} take into account the correlations between the spins of $\partial\Omega$. A sequence of systematically improvable approximations can be worked out by imposing self-consistent conditions on the coefficients in Eq. (2) for $H'(\tau)$, in analogy with the usual MFA.

First we consider here the Ising Ω clusters with L^2 sites on the square lattice and we calculate the critical coupling and magnetization per spin $\langle\sigma\rangle$ with zero external magnetic field. The computations require finding a *selfconsistent* solution to a set of nonlinear equations of the form $\langle\sigma\rangle = \langle\tau\rangle$ and similar ones for pair correlations. Moreover we have to trace over the spin σ and τ configurations to compute the summations in Eq. (1).

The estimates of critical coupling $K_c = J/k_B T_c$ are given in Table 1, where L denotes the size of the Ω cluster whereas n is the number of b coefficients taken into account in $H'(\tau)$. The exact result is $K_c = \frac{1}{2}\ln(\sqrt{2}+1) \approx 0.4407$. In the second column the MFA results are

L	MFA	$n=0$	$n=1$	$n=2$	$n=4$
1	0.250	0.346			
2	0.286	0.353	0.376	0.412	
3	0.308	0.368	0.392	0.414	0.417
4	0.323	0.378	0.400	0.416	0.420

Table 1: The estimates of the critical coupling K_c for the $2d$–Ising model.

displayed. The *selfconsistent* calculations with 0, 1, 2 and 3 parameters in Eq. (2) for the pair correlations of τ, gave K_c shown in the next columns of Table 1.

The magnetization as a function of $K^{-1} = k_B T/J$ is shown in Figure 1. The lower thick solid curve is the exact result of Yang [3] while the upper one represents the standard MFA. The sparse dotted curve is calculated for $L = 1$ where there is only one spin σ and no correlations are possible to include. The magnetization for $L = 2$ is represented by the dense dotted curves and for $L = 3$ by the thin solid curves. The upper curves for every L are calculated when no correlations are included in $H'(\tau)$, the middle ones when the nearest neighbor correlations are included in $H'(\tau)$ and the lower ones when the nearest and the next nearest neighbor correlations are included in $H'(\tau)$. Apart from the critical exponent β

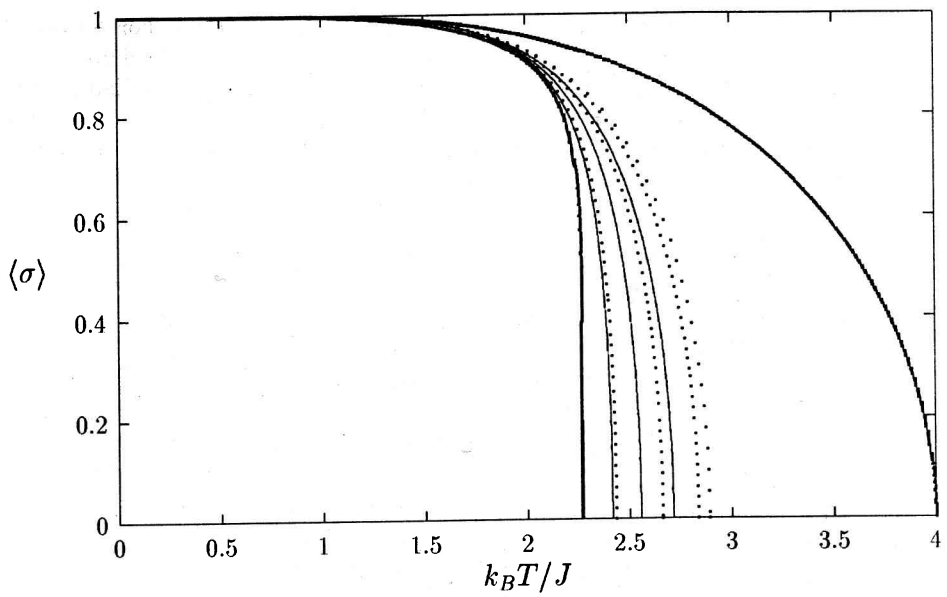

Figure 1: The magnetization as a function of k_BT/J for $2d$–Ising model.

(which retains its classical value), our curves approach the exact magnetization curve in the entire temperature region, even for small clusters. It can be noticed that one obtains a better improvement of the results by increasing the order of the approximation than by increasing the size of the cluster.

For quantum–mechanical models the factorization in Eq. (1) is not applicable and we

should allow the dependence of H' on the variables σ from the interior of the cluster Ω. We propose a method based on the assumption that the strongest contributions to H' appear at or around the boundary $\partial\Omega$.

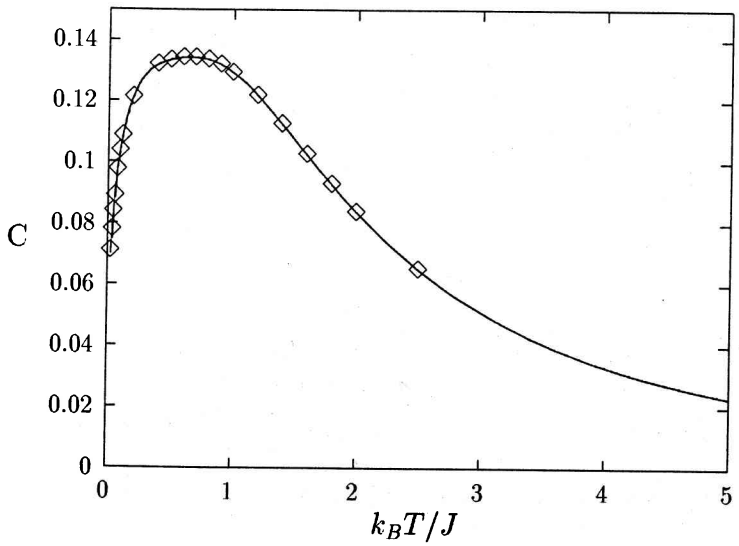

Figure 2: The zero-field specific heat per site for the $1d$–Heisenberg model. The present data are plotted by continuous curve and the $\diamond$ symbols represent numerical estimates of Blöte.

For the simple $1d$–Heisenberg Hamiltonian without external field no broken symmetry can be expected and we can argue that for symmetry reasons no external field can appear in H'. The first contributions which can be expected in H' are extra Heisenberg interactions between the spins at the ends of a finite segment.

The zero–field specific heat calculated for the isotropic Heisenberg model in the entire temperature region is plotted in Fig. 2 and compared with the numerical data of Blöte [4] represented by $\diamond$ symbols. We have performed direct diagonalization of the matrix representation with free boundary conditions. We have carried out the standard finite-segment calculations ($2 \leq N \leq 15$) as well as we have included up to 2 extra effective interactions. We have obtained good convergence of the finite–size data and consistent extrapolated values down to $k_BT/J = 0.05$.

Finally, we have performed large-scale quantum transfer–matrix calculations [5] for $k_BT/J \leq 0.1$, to obtain independent estimates of the specific heat in the region of quantum fluctuations. Our new findings for the system size $N \leq 360$ and the Trotter number $m \leq 13$ have confirmed our direct diagonalization data. The variation of the finite–size specific estimates (per site, in units of k_B) with respect to $1/N$ and $1/m^2$ for both methods at $k_BT/J = 0.1$ is plotted in Fig. 3.

We expect that our results will have an impact on simulations of some quasi–one–dimensional systems like $C_6H_{11}NH_3 \cdot CuBr_3$ [6] or Sr_2CuO_3 [7] as well as, after some further effort, will enable calculation of some quantum critical characteristics [8].

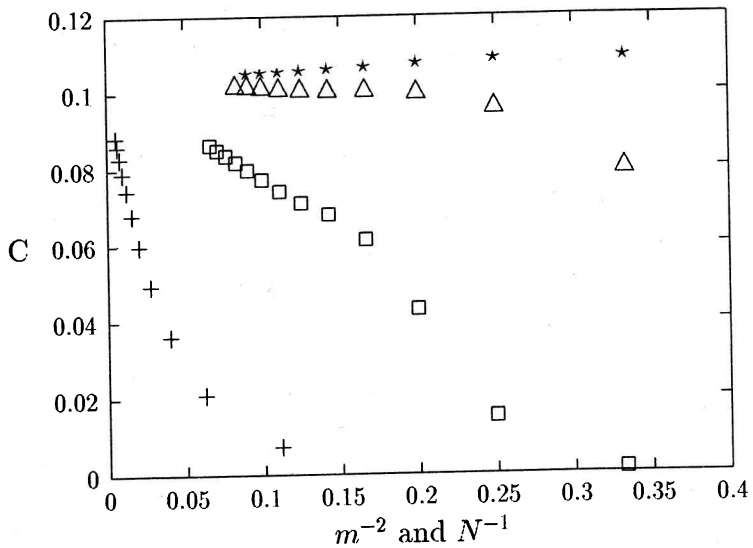

Figure 3: Variation of the zero-field specific heat per site at $k_BT/J = 0.1$ against $1/N$ for the finite-chain diagonalization data ($3 \leq N \leq 15$; the symbols $\Box$, $\triangle$, $\star$ represent the standard, 1- and 2-parameter approximation, respectively) and against $1/m^2$ for the transfer-matrix data (+ symbols, $3 \leq m \leq 13$).

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