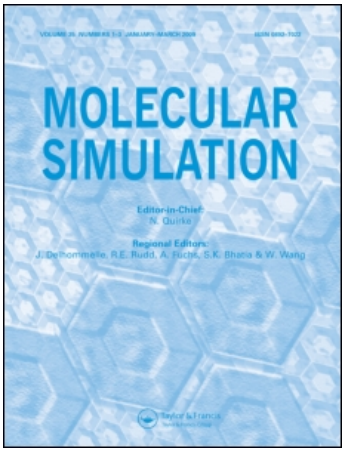

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HANDSCOMB MONTE-CARLO METHOD FOR $S = 1/2$ TRANSVERSE ISING MODEL

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A new stochastic simulation procedure for $S = 1/2$ Transverse Ising Model (TIM) is presented. The procedure is developed in different variants for certain types of exchange interaction, including ferromagnetic, antiferromagnetic and of arbitrary sign. The numerical results obtained by means of the new procedure for several types of one-dimensional TIM are presented, data being in good correspondence with the results of other approaches. Temperature dependence of transverse susceptibility of one-dimensional TIM with inverse-square interaction was found to have certain peculiarities apart from the Curie point.

KEY WORDS: Quantum spin lattice models, Handscomb Monte-Carlo, Transverse Ising model, phase transitions.

1 INTRODUCTION

Recently considerable attention has been paid to the development of stochastic simulation methods for quantum spin lattices [1, 2]. The Transverse Ising model (TIM), being applicable to certain physical phenomena, such as phase transitions in KDP-type ferroelectrics and rare-earth magnetics [3, 4], is of theoretical interest itself, because it is one of the simplest quatum spin lattice models. A number of methods has been applied to the theoretical study of the model e.g. the cluster approach [5], the mean field approximation (MFA) [3], and rigorous results [6, 7]. Among these methods we should also mention a stochastic simulation procedure based on a very fruitful idea of equivalence between d-dimensional quantum model and its $d + 1$-dimensional classical analogue – Ising model with some special temperature dependent pseudoexchange [2]. This method, however, is not accurate even for finite lattices because of the finite lattice size along the additional, $d + 1$-th dimension. Another way of Monte-Carlo procedure construction for quantum spin lattices is the Handscomb approach [9, 10]. It is accurate for finite lattices, but it appears to be a separate problem to "retune" it from the isotropic Heisenberg model (to which it had been originally applied), to the other quantum models. The main problem here remains a problem of simulation of the antiferromagnetic lattices and the lattices with concurrent exchange (see e.g. [1, 2]). In this paper we present variants of Handscomb method for TIM. We discuss the stochastic procedures for TIM with long-range ferromagnetic interactions and TIM with short-range arbitrary-sign interactions.

†Deceased.

2 THE HANDSCOMB METHOD FOR TIM WITH LONG-RANGE FERROMAGNETIC INTERACTIONS

We start with TIM Hamiltonian in the following form:

$$H = H_0 + H_{IS} + H_\omega + H_\Omega; \qquad H_\Omega = -\Omega \sum_{i=1}^{N} S_x^i;$$

$$H_{IS} = -(1/2) \sum_{i \neq j}^{N}{}' J_{ij} S_z^i S_z^j; \qquad H_\omega = -\omega \sum_{i=1}^{N} S_z^i;$$

$$H_0 = \text{const}, \tag{1}$$

where N is the total number of spins in the lattice under consideration, ω, Ω are the longitudinal and transverse magnetic fields respectively, J_{ij} is the exchange matrix. We require also here that

$$\forall i, j, \; i \neq j, \qquad J_{ij} > 0, \tag{2}$$

ferromagnetic long-range interaction.

In terms of S^+ and S^- operators we can rewrite (1) as follows:

$$-\beta H = \left[\sum_{t=1}^{N} (\lambda_- S_t^- S_t^+ + \lambda_+ S_t^+ S_t) + W \sum_{t=1}^{N} (S_t^- + S_t^+) \right.$$

$$\left. + (1/2) \sum_{t \neq t'}^{N} \kappa_{tt'} (S_t^+ S_{t'} + S_t^- S_{t'}^+ + S_t^- S_{t'}^- + S_t^+ S_{t'}^+) \right] + \beta(\Omega + \alpha)N, \tag{3}$$

where

$$K = \beta J(0); \qquad J(0) = \sum_{t \neq t'}^{N} J_{tt'};$$

$$W = \omega/J(0); \qquad \kappa_{tt'} = J_{tt'}/J(0);$$

$$\lambda_+ = \alpha/J(0); \qquad \lambda_- = (2\Omega + \alpha)/J(0);$$

$$\beta = \frac{1}{k_B T}, \qquad S_k^\pm = S_x^k \pm i S_y^k \tag{4}$$

α being an arbitrary constant, here taken as

$$\alpha = 1 + 1/N. \tag{5}$$

Within the Handscomb approach [9] for a system with Hamiltonian

$$H = H_0 + \sum_{i=1}^{N_0} H_i$$

each of H_i commuting with H_0, the canonic average $\langle \hat{Q} \rangle$ of any physical value operator $\hat{Q}$ can be written in the form:

$$\langle \hat{Q} \rangle = (Sp[\hat{Q} \exp\{-\beta H\}])/(Sp[\exp\{-\beta H\}]) = (\langle Q(C_r) x_\pi(C_r) \rangle_p / (\langle x_\pi(C_r) \rangle)_p, \tag{6}$$

where

$$C_r = \{i_1, \ldots, i_r\};$$

$$\pi(C_r) = \frac{(-\beta)^r}{r!} Sp[H_{i_1} \ldots H_{i_r} \exp\{-\beta H_0\}];$$

$$P(C_r) = |\pi(C_r)| \Big/ \sum_{r=0}^{\infty} \sum_{C_r} |\pi(C_r)|,$$

$$P(C_r) > 0, \sum_{r=0}^{\infty} \sum_{C_r} P(C_r) = 1; \qquad x_\pi(C_r) = \text{sign } \pi(C_r);$$

$$Q(C_r) = \frac{(-\beta)^r}{r!} Sp[\hat{Q} H_{i_1} \ldots H_{i_r} \exp\{-\beta H_0\}]/|\pi(C_r)|, \tag{7}$$

$P(C_r)$ being the probability distribution in the sampling space of ordered sets of indices C_r, $\langle \ \rangle_P$ means an average with the distribution $P(C_r)$. It is obvious that for the model with Hamiltonian (3) the ordered operator sets

$$H_{i_1} \ldots H_{i_r} \tag{8}$$

consist of following "units"

$$S_i^+ S_j^-, \ S_i^+ S_j^+, \ S_i^- S_j^+ \ - \text{ diades},$$

$$S_i^+ S_i^- \ (\text{or } S_i^- S_i^+) \ - \ (+) \ (\text{or } (-))\text{-pairs},$$

$$S_i^+ S_{N+1}^-, \ S_i^+ S_{N+1}^+, \ S_i^- S_{N+1}^-, \ S_i^- S_{N+1}^+ \ - \ W\text{-diades}, \tag{9}$$

if we treat the term of (1) which corresponds to interactions with the longitudinal magnetic field as an interaction with an additional, artificially included $N + 1$-th spin. Each "unit" (9) must be multiplied by a certain weight, which appears to be $\kappa_{ij}/2$ for diades, $\lambda_+((\lambda_-)$ for $(+)$ $((-))$-pairs, W – for W-diades.

Operator sets (8) consisting of the elements (9) can be represented as a product of two factors – a scalar factor (a product of weights) and an operator (sequence of S^+ and S^- operators). Moreover, with the conditions (2) and (5) fulfilled, the scalar contribution is strictly positive for any sequence of S^+ and S^- operators with any indices and can be definitely determined from this sequence.

The operator factor, also called "chain", is non trivial only if the following conditions are fulfilled [11]:

(i) quantities of S_k^+ and S_k^- operators in the chain should be equal for each lattice site, k;
(ii) the chain must be ordered in such a way that between every two S_k^- operators one S_k^+ operator is situated and vice versa. (10)

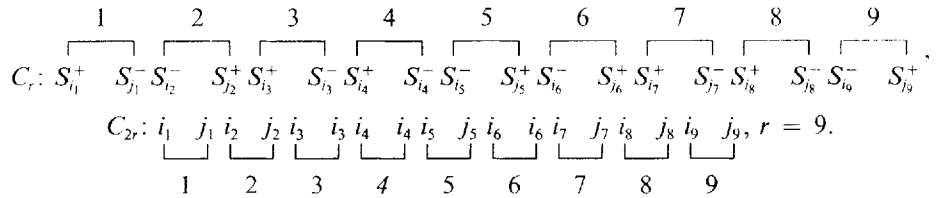
We call "essential" the chains with these conditions fulfilled. Only the contributions of essential chains are non zero and should be considered in the sums (6). In the terms

of essential chains we can write (see [12]):

$$\pi(C_r) = \frac{K^r}{r!}\left[\prod_j^{D(C_r)} \frac{\kappa_{i_j i_j}}{2}\right]\left[\prod_t^{\Pi(C_r)} \lambda_+^{n_t^+} \lambda^{n_t}\right], \tag{11}$$

where $D(C_r)$, a set of all the diades of C_r, $\Pi(C_r)$, a set of all the lattice sites, $(\pm)$, pairs of which are represented in C_r, $n_t^+ (n_t^-)$ – the total quantity of $(+)((-))$-pairs of index t in C_r, K being defined by (4).

Provided that a chain remains essential, if we replace all S^+ operators by S^- and vice versa for certain site, i, we can (as shown in [12]) make a partial summation, transforming (6) to a representations of chains C_{2r}, consisting of indices (numbers of lattice sites). The structure of C_{2r} chain in comparison with that of C_r chain may be illustrated by following example:



Here C_r and C_{2r} chains are given without their scalar weights that are equal in both cases. In C_{2r} the elements of $i_k j_k$ type are called diades (or w-diades, if one of the indices is equal to $N + 1$). Elements of $i_k i_k$ type are called pairs. We call $(+)$-pair of index i in C_{2r} a pair, before which in C_{2r} (starting from the front edge) there is even number of diades, containing index i. This number being odd, the pair is called $(-)$-pair. Essential in this representation are the chains in which each index appears even number of times. Within these notations (formally similar to the same notations for C_r), the contribution of an essential C_{2r} chain can be written as follows:

$$\pi(C_{2r}) = \frac{K^r}{r!}\left[\prod_j^{D(C_{2r})} \frac{\kappa_{i_j i_j}}{2}\right]\left[\prod_t^{\Pi(C_{2r})} (\lambda_+^{n_t^+} \lambda_-^{n_t^-} + \lambda_+^{n_t^-} \lambda_-^{n_t^+})\right],$$

$$P(C_{2r}) = |\pi(C_{2r})| \Big/ \sum_{r=0}^{\infty} \sum_{C_{2r}} |\pi(C_{2r})|, \tag{12}$$

Taking as the sampling space a space of all sets of indices, each varying from 1 to $N + 1$ and included even number of times in the set, we can easily organize the Markov chain with the limit distribution $P(C_{2r})$. A stochastic procedure should contain the steps that keep the number of certain index inclusions even. Such steps can look like an injection of a pair of equal indices into an index set or an annihilation of a pair of equal indices. A variant of this stochastic procedure (see Appendix) had been realized in [12]. It was tested on a model with

$$J_{ij} = J/N, \forall i, j \tag{13}$$

exchange. This model is known to be accurately described by MFA in the limit $N \to \infty$. The results of numerical simulation in comparison with MFA data and the standard Monte-Carlo method in the zero transverse field case are presented in Figure 1. Studied was a system of 30 spins, additional tests were made for $N = 100$ spins. The results show good correspondence of all the above mentioned methods.

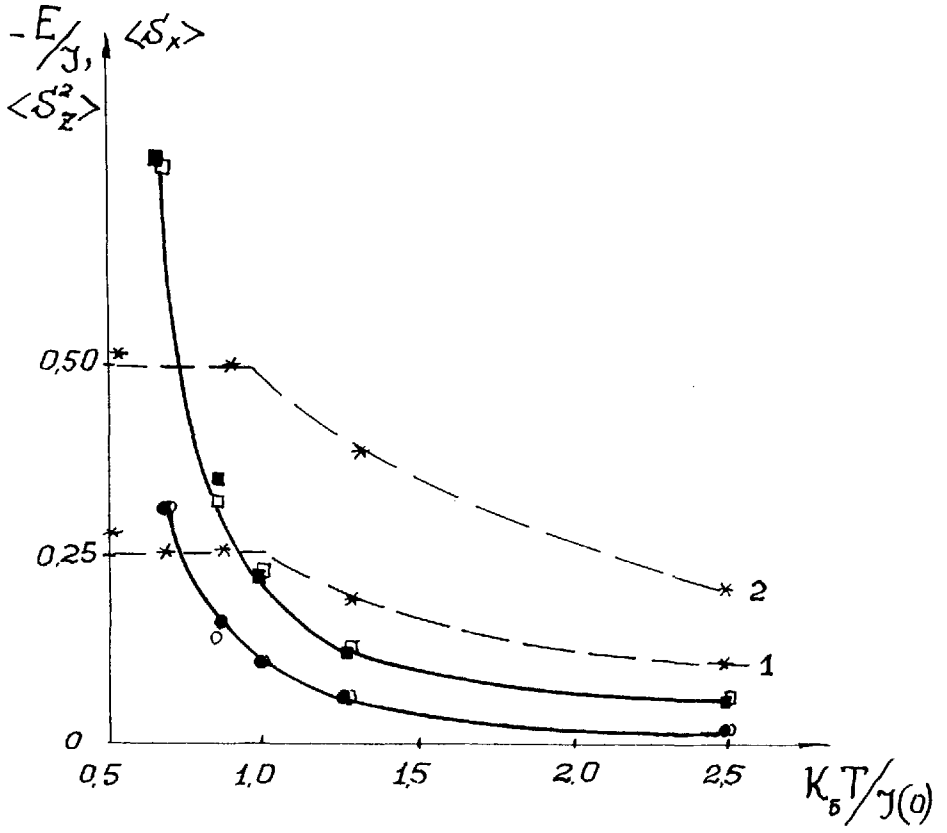


Figure 1 The results of a Monte-Carlo study (MCH) of the J/N model in comparison with the MFA ($\Omega \neq 0$) and standard Monte-Carlo ($\Omega = 0$) (MSt). 1, $\Omega/J = 0.1$; 2, $\Omega/J = 0.2$; ●, $(-E/J)$, MCH, $\Omega/J = 0$; ○, $(-E/J)$, MSt, $\Omega/J = 0$; ■, $\langle S_z^2 \rangle$, MCH, $\Omega/J = 0$; □, $\langle S_z^2 \rangle$, MSt, $\Omega/J = 0$; *, $\langle S_x \rangle$, MCH; —·—, $\langle S_x \rangle$, MFA.

The convergence of a new procedure appeared to be of the same order as that of the standard method.

Another system studied by the suggested method was a linear transverse Ising chain with inverse-square interactions. Such long-range interactions can occur in linear systems as a result of the renormalization of initial exchange with respect to spin-phonon interactions. The Ising chain without transverse field with inverse-square interactions studied by means of stochastic simulation methods (see e.g. reference [13]), displayed some peculiarities near the Curie point. First of all, the presence of a phase transition itself in the one-dimensional system is not trivial. Second, it was found that a temperature at which the longitudinal susceptibility becomes infinite does not correspond to the point where the heat capacity is maximal. Our numerical experiments were made with chains of 30, 60 and 90 spins. The Markov chain length was as large as 1000 mcs/spin. The results are given in Figure 2 in comparison with MFA data. The curves show that there is an additional peculiar temperature point in this system, where the transverse susceptibility has a pronounced peak. In 2- and

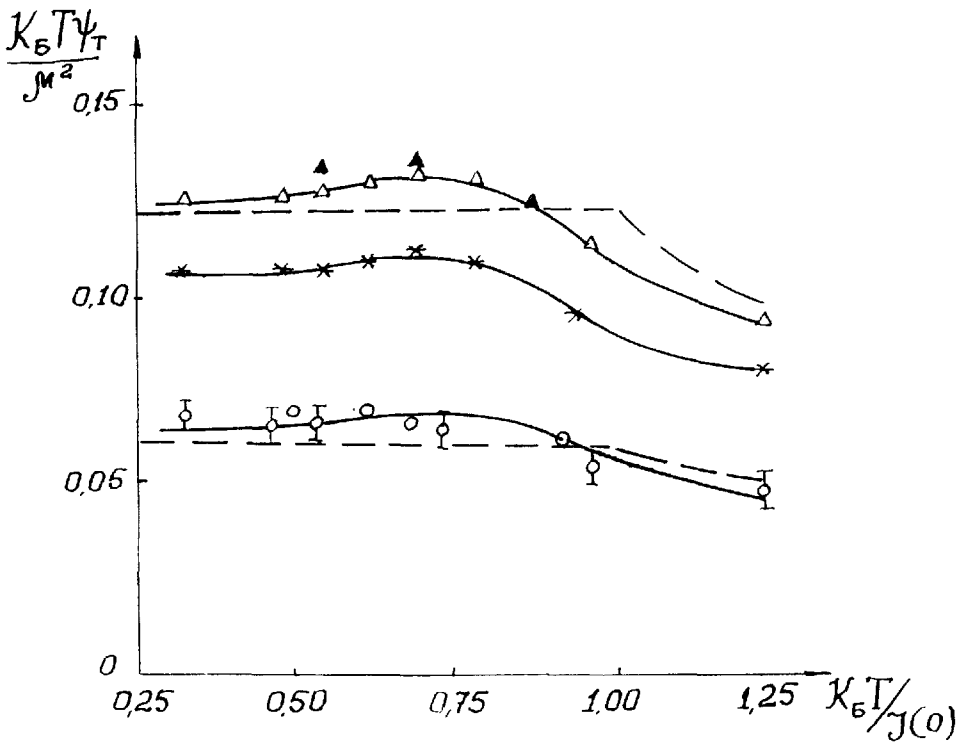


Figure 2 Transverse magnetization and transverse susceptibility $\chi_T|_{\Omega=0}$ for 1-dimensional TIM with inverse-square interaction. ○, $\Omega/J(0) = 0.061$, $N = 30$, MCH; △, $\Omega/J(0) = 0.122$, $N = 30$, MCH; △, $\Omega/J(0) = 0.122$, $N = 90$, MCH; *, $\chi_T|_{\Omega=0}$, $N = 30$, MCH; — —, MFA.

3-dimensional systems peaks of such shape correspond to T_c [14], while in the system in question its position appears to be much higher (at $k_BT/J(0) = 0.75$, with $k_BT_c/J(0) = 0.49$). This fact is additional evidence of the very complicated character of the phase transition in this system.

3 SHORT RANGE INTERACTION AND A PROBLEM OF NEGATIVE SIGNS IN INTERACTION

The above discussed procedure becomes ineffective for the systems with short-range and truncated exchange. The reason of this is the fact that conditions (10) provide only for nontriviality of operator part of a set (8) contribution. When the interaction is truncated, a number of chains (8) have zero contributions because condition (2) is not fulfilled. Organizing Markov chain in this case we must take this fact into account. Either we admit some states to have zero weights (the shorter is the truncation range, the larger is their number), or we should invent some cumbersome steps to avoid these states (see also [1, 8]). Both ways lead to procedures, successful only for special classes of exchange matrices J_{ij}.

There is one more way to solve this problem – to build an appropriate representation of Hamiltonian (1) especially for short-range exchange case. Here we present one of possible representations of such kind:

$$H = H_\omega + H_\Omega + H_{IS}^+ + H_{Is}^- + H_0;$$

$$-\beta H_\omega = K\left\{W \sum_{i=1}^{N} [2A_i^-(\alpha) + A_i^+(\alpha)]\right\};$$

$$-\beta H_\Omega = K\left\{\Gamma \sum_{i=1}^{N} [S_i^+ + S_i^-]\right\};$$

$$-\beta H_{IS}^+ = K\left\{(1/4) \sum_{\substack{i\neq j,\\ \kappa_{ij}>0}}^{N} \kappa_{ij}[A_i^+(\alpha)A_j^+(\alpha) + A_i^-(\alpha)A_i^-(\alpha)A_j^-(\alpha)]\right\};$$

$$-\beta H_{IS}^+ = K\left\{(1/4) \sum_{\substack{i\neq j,\\ \kappa_{ij}<0}}^{N} |\kappa_{ij}|[A_i^+(\alpha)A_j^-(\alpha) + A_i^-(\alpha)A_i^+(\alpha)A_j^-(\alpha)]\right\};$$

$$J(0) = \sum_{i,i\neq j}^{N} |J_{ij}|; \qquad \Gamma = \Omega/J(0); \qquad A_i^\pm(\alpha) = \lambda_\pm S_i^+ S_j^- + \lambda_\mp S_i^- S_j^+;$$

$$\lambda_\pm = 1 \pm \alpha, \forall\alpha, \quad -\beta H_0 = K\left(3\alpha W + \frac{\alpha^2}{2}\right)N. \tag{13}$$

Representation (14) produces in operator factor of (8) units of following types:

$$A_i^-(\alpha),\ A_i^+(\alpha),\ A_i^+(\alpha)A_j^-(\alpha),\ A_i^+(\alpha)A_j^+(\alpha),\ A_i^-(\alpha)A_j^-(\alpha),$$
$$A_i^-(\alpha)A_j^+(\alpha),\ S_i^+ \text{ and } S_i^-. \tag{14}$$

It can be shown that operator chains consisting of such elements will be essential if conditions (10) are fulfilled. Chains consisting only of $A_i^\pm(\alpha)$ operators are always essential. Moreover, Hamiltonian (14) does not contain members of negative sign. This fact, providing for all the $x_\pi(C_r)$ values being positive, gives us an opportunity to solve the well-known problem of different signs in Handscomb expansion (4) and to study the thermodynamics of TIM with antiferromagnetic and concurrent interactions.

Generally in this case stochastic procedure must contain following types of steps:

(1) Addition or exclusion of the units $A_i^-(\alpha)$, $A_i^+(\alpha)$, $A_i^+(\alpha)A_j^-(\alpha)$, $A_i^+(\alpha)A_j^+(\alpha)$, $A_i^-(\alpha)A_j^-(\alpha)$, $A_i^-(\alpha)A_j^+(\alpha)$ to (from) C_r (together with the corresponding weights);
(2) Addition or exclusion of a pair of S_k^+ and S_k^- operators into C_r with respect to conditions (10).

The method under consideration had been applied to one-dimensional TIM with the ferromagnetic and antiferromagnetic nearest-neighbour interactions. In the Table 1 we present different thermodynamic parameters of ferromagnetic model, calculated by means of our procedure compared with the results of accurate solution in the limit

Table 1 Results of Monte-Carlo simulation of linear transverse Ising chain with nearest-neighbour interaction. System size – 100 spins. Index MCH denotes numerical results, ACC – the rigorous results ($N \to \infty$), obtained using expressions from [7].

k_BT/J	Ω/J	$-E/J$, *MCH*	$-E/J$, *ACC*	$\langle S_x \rangle$, *MCH*	$\langle S_x \rangle$, *ACC*
0.2	0.0	0.2	0.197	0.0	0.0
0.2	0.2	0.205	0.205	0.1	0.096
0.2	0.5	0.25	0.246	0.1	0.097
0.6	0.2	0.57	0.55	0.11	0.096
0.6	0.5	0.64	0.63	0.26	0.237
0.6	1.0	0.93	0.91	0.48	0.46
1.0	0.0	0.76	0.76	0.0	0.0
1.0	0.2	0.77	0.775	0.12	0.118
1.0	1.0	1.12	1.12	0.57	0.559

$N \to \infty$ [7]. The results are in good correspondence, the convergence of a new method, as above, being of the same order as of the standard Monte-Carlo method. Figure 3 represents temperature dependences of longitudinal uniform susceptibility of anti-ferromagnetic Ising chain with different values of transverse field. It can be seen that when $\Omega \to 0$ the curve is close to that for the zero transverse field, studied rigorously. When $\Omega/J(0) = 0.5$, the so-called "critical" field, the results asymptotically fit the zero-temperature result, computed by means of expressions taken from [6].

4 CONCLUSIONS

The above discussed methods appear to be practical for one-dimensional systems. We must mention, however, that all the procedures are universally appropriate for any kind of exchange. Of course, this must be carefully tested in each case, because theoretical applicability gives no warranty of a good convergence in the numerical experiment.

The procedures admit their generalization on different modifications of TIM. First of all, we can use them to study Ising systems in the random transverse field. Such a model describes, for instance, partially deuterated KDP-type ferroelectrics. The changes in representation (14) for this case are obvious.

Then, we can use the variant for short-range interactions for simulation of TIM with additional multi-spin exchange of following type:

$$(1/4!) \sum_{i,j,k,l}^{N\prime} I_{ijkl} S_z^i S_z^j S_z^k S_z^l. \tag{15}$$

This additional term in (1) produces new kinds of units in (8) – triades and the tethrades of $A^{\pm}_{k(\alpha)}$ operators. So, we can add new kinds of steps to stochastic procedure without radical changes in its structure.

Acknowledgements
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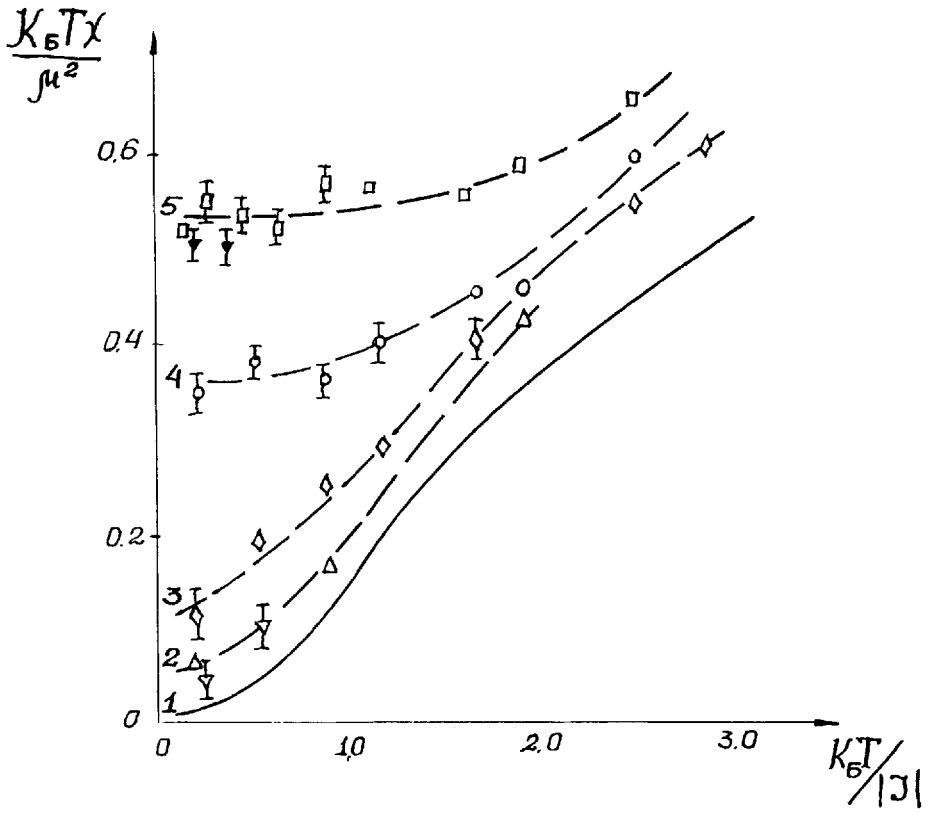

Figure 3 Starting uniform longitudinal susceptibility χ for the 1-dimensional antiferromagnetic TIM with nearest-neighbour interaction: 1, accurate solution, $\Omega/|J| = 0$; 2, MCH, $\Omega/|J| = 0.2$, $\triangle$, $N = 100$, ∇, $N = 200$; 3, MCH, $\Omega/|J| = 0.5$, $N = 100$; 4, MCH, $\Omega/|J| = 1.0$, $N = 100$; 5, MCH, $\Omega/|J| = 1.5$, $\square$, $N = 100$, ∇, $N = 200$; *, $k_B T\chi/\mu^2|_{T=0}$, $\Omega/|J| = 1.0$, according to [6].

APPENDIX

A stochastic procedure for TIM with long-range ferromagnetic interaction.
The basic set of Markov chain steps had been chosen as follows:

(1) $C_{2r} = \ldots \underset{l}{i\ i} \ldots \rightarrow \ldots \underset{l}{i\ k} \ldots \underset{m}{i\ k} \ldots \underset{r+1}{i\ k} = C_{2r+2} = C_{2r+2}$

– transformation of a pair into two diades;

(2) $C_{2r} = \ldots \underset{l}{i\ j} \ldots \rightarrow \ldots \underset{l}{i\ k} \ldots \underset{m}{i\ k} \ldots \underset{r+1}{j\ k} = C_{2r+2}$

– transformation of a diade into two diades;

(3) $C_{2r} = \ldots \underset{l}{k\ j} \ldots \rightarrow \ldots \underset{l}{k\ k} \ldots \underset{r+1}{k\ j} = C_{2r+2}$

– injection of a pair into the middle of the chain;

(4) $C_{2r} \to C_{2r}\underset{\underset{r+1}{\sqcup}}{k}\,k = C_{2r+2}$

– addition of a pair;

(5) $C_{2r} = C_{2r-2}\hat{g} \to \hat{g}C_{2r-2} = C'_{2r}$ – cyclic transposition.

Everywhere index k is assumed to be chosen randomly. The above presented set of steps can be proved to be complete. It is also convenient for recurrent calculation of contributions.

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