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ALGORITHM FOR CALCULATION OF THE PARTITION FUNCTION OF FRUSTRATED $S = 1/2$ HEISENBERG CHAINS

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Abstract: The paper presents the algorithm for calculation of the maximum eigenvalue of the transfer matrix for one-dimensional $S=1/2$ Heisenberg model with nearest and next-nearest neighbours interactions. This value permits a calculation of the partition function and free energy of the quantum system. This algorithm is implemented in the mevnnn procedure written in FORTRAN 90. The procedure is available at the *Poznań Supercomputing and Networking Center* on Cray T3E supercomputer in the library /usr/local/lib/libms.a

1. INTRODUCTION

We studied $S = 1/2$ one-dimensional Heisenberg model with nearest neigbours (nn) and next-nearest neigbours (nnn) interactions described by Hamiltonian

$$H = -J\sum_{i=1}^{N} (S_i S_{i+1} + \alpha S_i S_{i+2}), \tag{1}$$

where N is the size of the chain, J and α are the nn exchange integral and the ratio of the nnn exchange integral to the nn one, respectively. This model and the algorithm presented in this paper have practical applications for some quasi-one dimensional systems and in this work they are exploited to evaluate thermodynamical properties of $CuGe0_3$ and $Pb[Cu(S0_4)(0H)_2]$ [1,2]. In this paper the numerical aspects of the algorithm are described and the binary code is supplied.

The partition function is the fundamental quantity in investigation of thermodynamical properties of a Heisenberg model and it is defined as

$$Z = \mathrm{Tr}\, e^{-\beta\mathcal{H}}, \tag{2}$$

where $\beta = 1/kT$.

2. THE QTM TECHNIQUE

When we solve the system with the nn exchange interaction only ($\alpha = 0$), we can use in simple way the QTM algorithm based on the Trotter formula [3]

$$Z = \lim_{m\to\infty} Z_m = \lim_{m\to\infty} \mathrm{Tr}\left(e^{-\frac{\beta}{m}\mathcal{H}} \right)^m. \tag{3}$$

It can be shown [4, 5] that Z_m is the partition function of a two-dimensional ($2m$ x N) system of Ising-like spin variables. It means that the value of the partition function Z of one-dimensional

quantum system can be found by calculating subsequent classical contributions Z_m and extrapolating these result to $m = \infty$.

This method fails for $\alpha \neq 0$. In order to perform the calculations for a macroscopic chain (infinite N), we need to reverse the transfer from the chain to the Trotter direction. We can accomplish this for $\alpha \neq 0$ in two steps [1],

The first step is to divide the Hamiltonian (1) into two non-commuting parts $H = H_A + H_B$

$$H_B = H_{3,6} + H_{7,10} + H_{11,14} + \dots , \tag{4}$$

where $H_{i,\ i+3}$ describes the interactions inside the four-spin block beginning at the i-th site of the quantum chain. Then we can use the Trotter expression to obtain the m-th classical approximation Z_m of the partition function Z

$$Z_m = \sum_{\{S_{r,i}\}} \prod_{r=1}^{m} \prod_{i=1}^{N/4} L_{2r-1,4i-3}(S)\, L_{2r,4i-1}(S), \tag{5}$$

where

$$L_{r,i}(S) = \left\langle S_{r,i\dots r,\ i+3} \left| e^{-\beta/m H_{i,\ i+3}} \right| S_{r+1,i} \dots S_{r+1,i+3} \right\rangle. \tag{6}$$

Z_m is now the partition function of the classical system of $2m$ x N spins, with the effective interactions grouped into eight-spin blocks. For this system, we define a global transfer matrix between the r-th and $(r + 1)$-th rows and expand it in the product of four-spin local transfer matrices $L_{r,\ i}(S)$.

In the second step we reduce spin variables by introducing an effective classical spin $\sigma = 3/2$ and replacing each pair of S=1/2 spins, distributed along a given row r, by the spin σ

$$\left(S_{r,i}, S_{r,i+1}\right) \rightarrow \sigma_{r,j} \quad \text{where} \quad j = 1 \dots N/2 . \tag{7}$$

At the same time, the local transfer matrix $L_{r,\ i}(S)$ can be expressed as $L_{r,j}(\sigma)$, i.e. it can be rewritten in the basis of σ. Now, we can reverse the transfer direction by defining new a local transfer matrix $V_{r,\ r+1}$

$$\begin{aligned} &\left\langle \sigma_{r,j}\sigma_{r+1,j} \left| V_{r,\ r+1} \right| \sigma_{r,j+1}\sigma_{r+1,j+1} \right\rangle \\ &\qquad \| \\ &\left\langle \sigma_{r,j}\sigma_{r,j+1} \left| e^{-\beta/m H_{j,j+1}} \right| \sigma_{r+1,j}\sigma_{r+1,j+1} \right\rangle. \end{aligned} \tag{8}$$

The global transfer matrices W_1 and W_2 (for odd and even columns of spins, respectively) can be expressed by the corresponding products of $V_{r,\,r+1}$

$$W_1 = V_{1,2} V_{3,4} V_{5,6} \cdots V_{2m-1,2m},$$
$$W_2 = V_{2,3} V_{4,5} V_{6,7} \cdots V_{2m,1}. \tag{9}$$

In this way the m-th classical approach to the partition function of (1) can be written in the form

$$Z_m = \mathrm{Tr}[W_1 W_2]^{N/4}. \tag{10}$$

For an infinite system (i.e. when $N \to \infty$) the free energy per spin is simply given by the maximum eigenvalue $\lambda_{\max}(m)$ of the transfer matrix $W_1 W_2$

$$f_m = -\log Z_m = -k_B T \log \lambda_{\max}(m), \tag{11}$$

which can be easily shown. When we denote eigenvalue of matrix **A** in decreasing order by $\lambda_{\max}$, λ_1, then

$$\lim_{N\to\infty} \mathrm{Tr}\mathbf{A}^N = \lim_{N\to\infty} \lambda_{\max}^N \left[1 + \left(\frac{\lambda_1}{\lambda_{\max}}\right)^N\right] = \lambda_{\max}^N. \tag{12}$$

The free energy of the initial quantum system can be found from f_m by extrapolation to $m \to \infty$, according to the formula

$$f_m = \sum_{n=1}^{\infty} \frac{a_n}{m^{2n}} + f_\infty. \tag{13}$$

3. CALCULATION OF THE LARGEST EIGENVALUE

In order to find $\lambda_{\max}(m)$ we iteratively use the eigenequation for the transfer matrix $W_1 W_2$

$$W_1 W_2 \,|\, \sigma\rangle = \lambda(m) \,|\, \sigma\rangle. \tag{14}$$

At each step of the iteration we calculate a product of the normalized to unity vector $|\sigma_i>$ and the transfer matrix $W_1 W_2$. Then we find a value of λ_{i+1} as a root from the norm of the resulting vector

$$W_1 W_2 \,|\, \sigma_i\rangle = |\, \sigma_{i+1}\rangle \tag{15}$$

$$\lambda_{i+1}^2(m) = \langle \sigma_{i+1} \,|\, \sigma_{i+1} \rangle. \tag{16}$$

When we normalize this vector, this procedure is repeated until difference between the values λ_{i+1} and λ_i is not greater then some δ parameter

$$|\lambda_{i+1}(m) - \lambda_i(m)| \leq \lambda \tag{17}$$

and at the same time

$$\langle \sigma_i | \sigma_{i+1} \rangle \leq \delta^2 . \tag{18}$$

It means that with a precision determined by δ, the vector $|\sigma_i> = |\sigma_{i+1}>$ is the eigenvector of transfer matrix W_1W_2 with the eigenvalue $\lambda_i(m) = \lambda_{i+1}(m)$.

We were able to calculate the aproximants f_m up to $m = 6$, which has taken 15 minutes on Cray J916. Then we calculated the thermodynamical properties by numerical differentiation of the free energy f_m and we extrapolated them to infinite Trotter number m according to the formula (13).

4. THE PROCEDURE CALL

The calculation of the highest eigenvalue can be carried out using the subroutine `mevnnn`. The subroutine `mevnnn` returns the maximum eigenvalue in the parameter `log_1`. This routine should be called with the argument which describes the physical model and limits of the calculations

```
call mevnnn(t, j1, j2, an, m, delta, nmax, log_1)
```

The parameters are characterized in the Table below.

Parameter	Type	Characteristics
t	REAL*8	temperature
j1	REAL*8	nearst neighbor exchange integral
j2	REAL*8	next-nearst neighbor exchange integral
an	REAL*8	ratio J_z/J_x ($J_x = J_y$)
m	INTEGER	Trotter's index (can take value from 2 to 13)
delta	REAL*8	δ factor
nmax	INTEGER	maximum number of iteration
log_1	REAL*8	logarithm of the maximum eigenvalue

A Fortran program calling the `mevnnn` subroutine located on the Cray T3E supercomputer can be compiled using the command

```
f90 -l/usr/local/lib/libms.a main.f
```

The subroutine supports the 03 compiler option. Here is an example program which calls `mevnnn` with the parameters explicitly specified.

```
program test
real*8 t,j1,j2,an,delta,log_l
integer m,nmax
t = 10.0
j1 = 100.0
j2 = 90.0
an = 0.9
delta = 0.1e-12
do m = 2,5
  nmax = 1000
  call mevnnn(t,j1,j2,an,m,delta,nmax,log_l)
  write(*,*)  m,log_l, nmax
end do
end
```

As result of execution of the `test` program the following values of the Trotter index, the logarithm of the maximum eigenvalue and the number of iterations should appear on the screen.

```
2,  19.604831496849986,  100
3,  19.518148198458604,  15
4,  19.470876797790815,  29
5,  19.442549173292296,  26
```

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