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Algorithm for calculation of the maximum eigenvalue of transfer matrix for the linear $S = 1/2$ Heisenberg model

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Abstract

The paper presents the algorithm and description of the **meigval** procedure written in FORTRAN 90 language which was designed for calculation of the maximum eigenvalue of transfer matrix for one-dimensional $S = 1/2$ Heisenberg model. The procedure is available at the *Poznań Supercomputing and Networking Centre* on a Cray J916 supercomputer in the numerical procedure library **/lib/mestat.a.**

1 Introduction

The **meigval** procedure enables a calculation of the maximum eigenvalue of the transfer matrix for one-dimensional 5 = 1/2 Heisenberg magnet characterised by the hamiltonian

$$\mathcal{H} = -\sum_{i=1}^{N-1} \left(J_x \mathrm{S}_i^x \mathrm{S}_{i+1}^x + J_y \mathrm{S}_i^y \mathrm{S}_{i+1}^y + J_z \mathrm{S}_i^z \mathrm{S}_{i+1}^z \right). \tag{1}$$

The constants J_x, J_y, J_z determine coupling between neighbouring spins in a chain of a length N. The procedure was constructed under the assumption that $\mathrm{J}_x = \mathrm{J}_y \neq J_z$, so it can be used to systems with isotropic interactions in the XY plane.

The fundamental quantity in investigation of thermodynamical properties of a Heisenberg model is the partition function $\mathcal{Z}$ defined as

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

where $\beta = 1/kT$. On the basis of the general Trotter formula [1], the above equation can be rewritten as

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

It can be shown [2] that $\mathcal{Z}_m$ 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 $\mathcal{Z}$ of a one-dimensional quantum system can be found by calculating subsequent classical contributions Z_m and extrapolating the results to m = ∞

The calculations necessary to determine the partition function can be considerably simplified using the transfer-matrix method [3, 4]. Such an approach can be followed for classical systems whose Hamiltonian structure enables a sep-aration of interactions into those within certain blocks and among the blocks. The transfer matrix can be defined as

$$\mathbf{T}_m(\sigma_i, \sigma_{i+1}) = e^{-\frac{\beta}{m}\mathcal{H}_{i,i+1}}, \tag{4}$$

where σ_i stands for a configuration of the i-th classical block. Now, the partition function of a classical system can be transformed into

$$\mathcal{Z}_m = \mathrm{Tr}\,(\mathbf{T}_m)^N. \tag{5}$$

It can be easily shown, that $\mathcal{Z}_m$ is related to the free energy (per a single spin site) through the formula

$$f_m = -\log \mathcal{Z}_m = -\lim_{N\to\infty} \log \lambda(m)_{max}, \tag{6}$$

where $\lambda(m)_{max}$ is the highest eigenvalue of the transfer matrix $\mathbf{T}_m$. The free energy of the quantum system is given by the equation

$$f = \lim_{m\to\infty} f_m. \tag{7}$$

2 The method of calculation

The method for determination of $\lambda(m)_{max}$ is based on the iterational use of the eigenequation for the transfer operator $\mathbf{T}_m$

$$\mathbf{T}_m|\sigma\rangle = \lambda(m)|\sigma\rangle. \tag{8}$$

The `meigval` procedure calculates in each step a product of the normalised to unity vector $|\sigma_i\rangle$ and the matrix $\mathbf{T}_m$, then finds a value of λ_{i+1} as a root from the norm of the resulting vector

$$\mathbf{T}_m|\sigma_i\rangle = |\sigma_{i+1}\rangle \qquad \lambda(m)^2_{i+1} = \langle\sigma_{i+1}|\sigma_{i+1}\rangle. \tag{9}$$

After normalisation of the vector, the procedure is repeated until the following conditions are met

$$|\lambda(m)_{i+1} - \lambda(m)_i| \leq \delta \quad \text{and} \quad \langle\sigma_i|\sigma_{i+1}\rangle \leq \delta^2. \tag{10}$$

It means that with the accuracy determined by δ, the vector $|\sigma_i\rangle = |\sigma_{i+1}\rangle$ is the eigenvector of the transfer matrix $\mathbf{T}_m$ with the eigenvalue of $\lambda(m)_i = \lambda(m)_{i+1}$.

Program gives a value of the logarithm of the maximum eigenvalue $\lambda(m)_{max}$, so the value of f_m from equation (6). In order to estimate the free energy f of a quantum system, the partial results f_m should be extrapolated to $m = \infty$, according to the formula

$$f = \sum_{n=1}^{\infty} \frac{a_n}{m^{2n}} + f_m. \tag{11}$$

In practice, for not too high temperatures, a satisfactory approximation of f can be obtained truncating in above the terms of an order higher than $n = 1$.

3 Initial parameters

The **maigval** subroutine is called by the instruction

call meigval(kx,kz,m,del,log.lambda,n)

In order to obtain correct results care should be taken to declare all subprogram parameters in the main program. The characteristics of the parameters is given in the table below.

parameter	type	characteristics
kx	REAL*8	reduced temperature $K_x = J_x/kT$ (equal to $K_y = J_y/kT$)
kz	REAL*8	reduced temperature $K_z = J_z/kT$
m	INTEGER	Trotter index m (can take values from 2 to 13)
del	REAL*8	accuracy δ of calculation of λ_{max}, (recommended $\delta \geq 10^{-13}$)
log_lambda	REAL*8	logarithm of the maximum eigenvalue
n	INTEGER	maximum number of iterations (after the calculations the final number is given)

The main program with the procedure code should be compiled in Fortran 90 standard using the instruction

```
f90 -l /lib/mestat.a main.f
```

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