

# The algorithm for the partition function of the generalised Ising model on a square lattice

P. Kozłowski, G. Kamieniarz, G. Musiał

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

## Abstract

The paper presents the algorithm and description of a procedure **gim** written in the FORTRAN 90 language, for calculation of the partition function of the generalised Ising model on a square lattice. The procedure is available at *the Poznań Supercomputing and Networking Center* on a Cray J916 supercomputer in numerical procedure library **mestat**.

## 1 Introduction

Spontaneous ordering of atomic spins is one of the most interesting phenomena in solid state physics. Unfortunately, exact quantitative description of ferro- and antiferromagnetism is not possible in terms of the existing theories, therefore considerations are performed on models of these phenomena among which particularly important is *the Ising model* [1]. The main advantage of this model is the exact solvability of its two-dimensional version which is a non-trivial example of a system in which magnetic phase transitions can be analysed exactly.

In the Ising model only one order parameter is considered. A natural extension of the Ising model is *the Ashkin-Teller model* [2] which is based on three order parameters and two kinds of spin variables.

In this model a set of  $N$  fixed points, called the lattice sites, forming a 2-dimensional periodic lattice of regular structure, is considered. Each site is attributed with a spin variable (henceforth denoted as  $S_i$  or  $\sigma_i$ ,  $2 = 1, 2, \dots, N$ )

which is a *number* and can take values of +1 or -1. The system has no other degrees of freedom.

The partition function is defined by the expression:

$$\mathcal{Z} = \sum e^{-\beta H}, \quad (1)$$

where the summation runs over all configurations of spin variables  $S$  and  $\sigma$ ,  $H$  is the hamiltonian of the system,  $\beta = 1/k_B T$  is the inverse of the product of temperature  $T$  and the Boltzmann constant  $k_B$ . The partition function  $\mathcal{Z}$  is one of the fundamental quantities in the statistical physics as the logarithm of the partition function multiplied by  $-\beta^{-1}$  gives the free energy of the system which is necessary to obtain the thermodynamic functions of the system.

The **gim** procedure was written for a planar square lattice and permits a calculation of the partition function  $\mathcal{Z}$  for the Ising model per a single lattice site, taking advantage of the accurate algorithm based on the transfer matrix. Given the actual values of appropriate parameters, the procedure enables the calculations for the Ashkin-Teller or standard Ising models.

## 2 The Hamiltonian and the algorithm of calculations

The starting point for the calculations is the Hamiltonian of the system which for *the Ashkin-Teller model* takes the form:

$$\mathcal{H} = -\beta H = -\mathbf{pk1} \sum_{\langle i,j \rangle} S_i S_j - \mathbf{pk2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \mathbf{pk4} \sum_{\langle i,j \rangle} S_i \sigma_i S_j \sigma_j, \quad (2)$$

where the summation runs over pairs of the nearest neighbours on an  $L \times L$  size square lattice with periodic boundary conditions, and **pk1**, **pk2**, **pk4** are the reduced coupling constants which as the parameters of the procedure are written down by thick letters.

The hamiltonian of *the standard Ising model* is a particular case of hamiltonian (2) restricted to the first term:

$$\mathcal{H} = -\mathbf{pk1} \sum_{\langle i,j \rangle} S_i S_j. \quad (3)$$

In this model there is only one kind of spin variable.

To calculate the partition function we make use of the perturbation transfer matrix method [3] and the following relation [4]:

$$\mathcal{Z}_0 = \sum_n \langle n | \mathbf{T}^L | n \rangle, \quad (4)$$

where  $L$  is the number of sites in a column or a line,  $\mathbf{T}$  is the transfer matrix, and  $|n\rangle$  vectors form a  $4^L$  dimensional base of the transfer matrix  $\mathbf{T}$  of the *Ashkin-Teller model* and  $2^L$  dimensional base of the *Ising model*. The smaller base for the latter model permits calculations for larger systems.

The memory required to carry out this algorithm was minimised having recourse to the fact that only two  $|n\rangle$  vectors are needed for the calculations. The algorithm is based on the numerically exact calculations of the trace (4) where inaccuracies are only due to round-ups. It is estimated that about 12 significant digits of the result are accurate.

### 3 Description of the gim procedure

The **gim** procedure is written in FORTRAN 90 with the use of a vectorizable algorithm.

The call of the procedure:

```
call gim(l, pk1, pk2, pk4, zO, w)
```

The input parameters:

1 - an *integer* type variable which determines the number of sites in a line (column) and can take the values: 2, 3, ...,  $M_{\max}$ , where  $M_{\max}$  is 10 and 20 for the *Ashkin-Teller* and *Ising model*, respectively.

**pk1, pk2, pk4** - are *real\*8* type variables determining the values of the hamiltonian (2) parameters for the *Ashkin-Teller model*, whereas for the *Ising model* **pk1** determines the value of the hamiltonian (3) parameter.

**w** - a *character\*1* type variable whose value determines for which model the calculations are performed, i.e. when it takes a value *I* or *i* the calculations are for the standard Ising model, otherwise for the *Ashkin-Teller model*.

The output parameters:

**zO** - a *real\*8* type variable which contains the partition function in the zero field. It is the partition function per a single site of a 1 x 1 size lattice.

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