Physica A 457 (2016) 34–41

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

The numerical study of first order wetting transition with two defect lines

X.T. Wu

Department of Physics, Beijing Normal University, Beijing, 100875, China

ARTICLE INFO

Article history:
Received 17 January 2016
Available online 7 April 2016

Keywords:
Wetting transition
First order
Bond propagation algorithm

ABSTRACT

The first order wetting transition with two defect lines, one near a wall and another at a distance N_1, in the $d = 2$ Ising model is studied by the bond propagation algorithm. The numerical calculations are carried out on very large lattices with size up to $160^2 \times 160$. The finite size effects of the first order transition in that model are discussed. The magnetization profile is also calculated. The numerical results agree with the exact results very well.

1. Introduction

The wetting transition is a subject of considerable interest [1]. The first exactly solvable model for wetting transition is the two-dimensional (2D) model of Abraham (model A), which contains only short-range forces, leads to a continuous wetting transition [2]. Later, Forgacs et al. proposed a model (model AB) for first order wetting transition [3,4]. Exact solutions for first-order transitions, as opposed to second-order transitions are scarce. It is worth studying it further. In this paper, we study the model AB with bond propagation algorithm (BPA). On one hand, there is no numerical work such as Monte Carlo simulation on the AB model. Our study is a numerical investigation on this model. On the other hand, we hope to test the efficiency of BPA on this kind of problem by comparing with the exact solution. It is helpful for further study on wetting transition with BPA. For example, BPA can be used to study the disordered systems, which is usually beyond the exact solution.

BPA is very efficient, accurate and powerful to solve the two dimensional Ising model with various boundary conditions [5–7]. To study the wetting transition, BPA with a surface field is proposed in Ref. [7]. BPA is very accurate and can be carried on lattices with extremely large sizes, say 2000×2000. With it, we have verified the CFT predictions on the corner free energy with free boundary condition [8,9]. The result on the central charge of Ising model agrees with CFT in the precision of 10^{-10} [10–12]. We also recover the aspect ratio dependence of the corner free energy in CFT theory accurately [9,10]. The corner free energy with fixed boundary and mixed boundary condition has been studied by CFT recently [13–15]. With an extended BPA [7], we verified this CFT prediction in the accuracy 10^{-16} [16].

The AB model is depicted in Fig. 1. We consider a two-dimensional Ising model. The couplings connecting the substrate (the boundary with all spins down, denoted by a minus sign in Fig. 1) to the first layer (column) are given by $J_1 = a_1 J$, with $0 < a_1 < 1$, where J denotes the bulk interactions. The boundary conditions at the Nth ($N = N_1 + N_2$) layer favor all spins up (denoted by a plus sign in Fig. 1). At a distance N_1 from the substrate an additional column of defect bonds $J_2 = a_2 J$ is placed with $0 < a_2 < 1$.

According to the exact solution [3], for $a_1 < a_2$, the wetting transition at $T = T_1$ (which is given below) becomes sharp first order in the limit $N_1 \to \infty$, $N_2 \to \infty$, $M \to \infty$, and it is "finite-size rounded" for finite N_1.

E-mail address: wuxt@bnu.edu.cn.

http://dx.doi.org/10.1016/j.physa.2016.03.057
0378-4371/

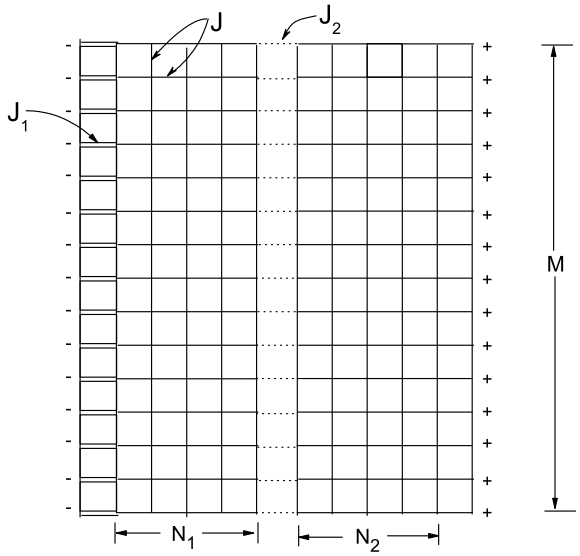

Fig. 1. Definition of the model. Double lines denote $J_1 = a_1 J$, solid-dashed lines denote $J_2 = a_2 J$. All the other couplings are J.

In our numerical study, we set $N_1 = N_2 = N/2$ for convenience. Due to the anisotropic character, we set $M = N^2$. Because the BPA is efficient, we study the lattices with size $N = 40, 80, 120, 160$ respectively. The free energy density, internal energy density and specific heat are calculated. As the lattice size increases, the first order transition singularity develops. The jumps of internal energy become more drastic as the lattices become larger. The peaks in the specific heat become sharper as the lattices become larger. We fix $a_1 = 0.3$ and choose four cases for $a_2 = 0.7, 0.6, 0.5, 0.4$ respectively. Through comparing these results, we can see how the first order characters develop and in what case they develop fast with the increasing of lattice size.

2. Numerical study of AB model

2.1. Brief review of AB model

In the numerical calculation, the fixed boundary condition for example at the left side (all the spins in first column are fixed to be negative) shown in Fig. 1 is replaced by a surface field applied on the spins in second column. The fixed boundary on the right side can be dealt similarly. Then the Hamiltonian is given by

$$\begin{aligned}\mathcal{H} = &-\sum_{m=1}^{M}\sum_{n=1}^{N_1-1} J[\sigma_{n,m}\sigma_{n+1,m} + \sigma_{n,m}\sigma_{n,m+1}] \\ &-\sum_{m=1}^{M}\sum_{n=N_1}^{N-1} J[\sigma_{n,m}\sigma_{n+1,m} + \sigma_{n,m}\sigma_{n,m+1}] \\ &-\sum_{m=1}^{M}[(a_2-1)J\sigma_{N_1,m}\sigma_{N_1+1,m} + H_L\sigma_{1,m} + H_R\sigma_{N,m}] \end{aligned} \tag{1}$$

where $\sigma_{n,m} = \pm 1$ are the Ising spins and we set $J = 1$. The coupling between the spin $\sigma_{N_1,m}$ and $\sigma_{N_1+1,m}$ is a_2. For $H_L = -a_1, H_R = 1$, the model gives the same boundary conditions as in AB model.

Generally we need to calculate the partition function

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

where $\beta = 1/T$.

In order to calculate the interfacial free energy, we consider two types of boundary conditions as done in Abraham's model [2]:

$$\begin{aligned} +-: &\quad H_L = -a_1, \qquad H_R = 1 \\ ++: &\quad H_L = a_1, \qquad H_R = 1. \end{aligned} \tag{3}$$