

## Scaling of solvation force in two-dimensional Ising strips

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(Received 25 August 2008; published 4 December 2008)

The solvation force for two-dimensional Ising strips is calculated via exact diagonalization of the transfer matrix in two cases: the symmetric case corresponds to identical surface fields and the antisymmetric case to exactly opposite surface fields. In the symmetric case the solvation force is always negative (attractive), while in the antisymmetric case the solvation force is positive (repulsive) at high temperatures and negative at low temperatures. It changes sign close to the critical wetting temperature characterizing the semi-infinite system. The properties of the solvation force are discussed, and the scaling function describing its dependence on temperature, surface field, and strip's width is proposed.

DOI: 10.1103/PhysRevE.78.060602

PACS number(s): 68.08.Bc, 05.50.+q

### I. INTRODUCTION

The properties of the solvation force in various condensed-matter systems have been the subject of very intensive research during recent years [1–10]. Lattice models play a special role among the considered systems. Although many important results were obtained in this field by different methods of taking into account fluctuations which determine the properties of the analyzed systems, the approach based on the exact evaluation of the partition function via the transfer matrix method still plays a distinguished role. Below we report our results on the properties of the solvation force for two-dimensional (2D) Ising strips. They are obtained via exact diagonalization of the transfer matrix, which is then followed by numerical solutions of equations for eigenvalues.

We consider an Ising model on a 2D square lattice consisting of  $M$  rows and  $N$  columns. There is no bulk magnetic field acting on the system, and there are two surface fields:  $h_1$  acts on spins in the first row and  $h_2$  acts on the  $M$ th row. The Hamiltonian of this model takes the standard form

$$\mathcal{H}(\{s_{ij}\}) = -J \sum_{n=1}^N \sum_{m=1}^{M-1} s_{n,m} s_{n,m+1} - J \sum_{n=1}^N \sum_{m=1}^M s_{n,m} s_{n+1,m} - h_1 \sum_{n=1}^N s_{n,1} - h_2 \sum_{n=1}^N s_{n,M}, \quad (1)$$

where  $s_{n,m} = \pm 1$  with  $n=1, \dots, N$ ,  $m=1, \dots, M$  denotes the spin located in the  $n$ th column and  $m$ th row, and  $J$  is the coupling constant. Periodic boundary conditions in the horizontal direction are imposed:  $s_{N+1,m} \equiv s_{1,m}$ .

Our purpose is to determine the properties of the solvation force experienced by the system boundaries. In the following we consider two cases: the symmetric case (S) corresponds to  $h_1=h_2$ , and for the antisymmetric case (AS) one has  $h_1=-h_2$ .

Although the strip of finite width experiences no phase transition, we shall often refer to two critical temperatures: the bulk critical temperature  $k_B T_c = 2J/\ln(1+\sqrt{2})$  and the

wetting temperature  $T_w$ , which characterizes the critical wetting transition in a semi-infinite system with surface field  $h_1$ . The wetting temperature fulfills the equation

$$\cosh 2K_1 = \cosh 2K - \sinh 2K e^{-2K}, \quad (2)$$

where  $K=J/(k_B T_w)$ ,  $K_1=h_1/(k_B T_w)$ , and  $k_B$  is the Boltzmann constant. For a small surface field  $h_1$  this equation leads to

$$\frac{T_c - T_w}{T_c} = \frac{1}{4} (1 + \sqrt{2}) \ln(1 + \sqrt{2}) \left( \frac{h_1}{J} \right)^2, \quad \frac{h_1}{J} \rightarrow 0. \quad (3)$$

For  $h_1 \geq J$  one has  $T_w=0$  and there is no wetting transition.

### II. SOLVATION FORCE

The dimensionless free energy per one column is defined as

$$f(T, h_1, M) = \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\mathcal{F}}{k_B T} = - \lim_{N \rightarrow \infty} \frac{\ln \mathcal{Z}}{N}, \quad (4)$$

where  $\mathcal{Z}$  is the canonical partition function for the Hamiltonian (1), which we evaluate using the exact transfer matrix method [11, 12]. The free energy may be separated into three types of contributions:

$$f(T, h_1, M) = M f_b(T) + f_s(T, h_1) + f_{\text{int}}(T, h_1, M), \quad (5)$$

where  $f_b$  is the bulk free energy per one spin [13] and  $f_s$  is the surface free energy; both  $f_b$  and  $f_s$  are  $M$  independent. The remaining term  $f_{\text{int}}$  describes the interaction between the system boundaries. It tends to 0 as  $M$  goes to infinity, and from this term the solvation force originates.

The solvation force is, in general, defined as the minus derivative of  $f_{\text{int}}$  with respect to  $M$ . In our case, because  $M$  takes only integer values, we use the definition

$$f_{\text{solv}}(T, h_1, M) = - [f_{\text{int}}(T, h_1, M+1) - f_{\text{int}}(T, h_1, M)], \quad (6)$$

which leads to the expression

$$f_{\text{solv}}(T, h_1, M) = f(T, h_1, M) - f(T, h_1, M+1) - f_b. \quad (7)$$

The solvation force for the 2D strip has been already analyzed in the  $T_w=0$  case [5] corresponding to  $h_1=J$ . Our analysis covers the whole spectrum  $T_w \geq 0$ —i.e.,  $h_1 \leq J$ . To

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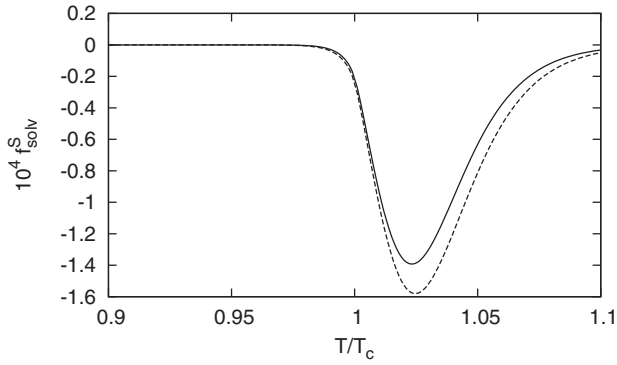


FIG. 1. Comparison of the solvation force  $f_{\text{sol}}^S$  for  $T_w=0.8T_c$  ( $h_1 \approx 0.60J$ ) (solid curve) and  $T_w=0$  ( $h_1=J$ ) (dashed curve) for the symmetric case  $h_1=h_2$ . Both curves correspond to the value  $M=50$ .

calculate the solvation force we used the methods described in [11,12,14,15]. The complete analysis (including also the inhomogeneous boundary fields) will be published elsewhere [16]; here, we discuss only the main results.

First, we briefly discuss the symmetric case (S). The corresponding solvation force  $f_{\text{sol}}^S$  is plotted in Fig. 1 for two cases:  $T_w > 0$  (solid curve) and  $T_w = 0$  (dashed curve). The difference between these two functions is only of quantitative nature—decreasing the surface field  $h_1$ , i.e., increasing the wetting temperature  $T_w$  results in decreasing the absolute value of the solvation force. The minimum of the solvation force  $f_{\text{sol}}^S$  is located at  $T_{\text{min}}^S > T_c$ .

For opposite surface fields (AS) the solvation force  $f_{\text{sol}}^{\text{AS}}$  in the  $T_w > 0$  case, i.e.,  $h_1 < J$ , differs substantially from the  $T_w = 0$ —i.e.,  $h_1 = J$ —case. Figure 2 presents a typical plot of  $f_{\text{sol}}^{\text{AS}}$  as a function of  $T$ . For low temperatures this force is negative (attractive) and has a minimum at  $T_{\text{min}}^{\text{AS}} < T_w$ . The solvation force is negative at the wetting temperature and has a zero at  $T^* > T_w$ . Above  $T^*$  the solvation force is positive (repulsive) and has a maximum at  $T_{\text{max}}^{\text{AS}} < T_c$  (for  $M$  large enough). This remains in contrast with the  $T_w = 0$  case in which the solvation force is positive for all temperatures.

Exactly at the bulk critical temperature  $T_c$  the dependence of the solvation force on  $M$  has been found using conformal invariance [17,18]:

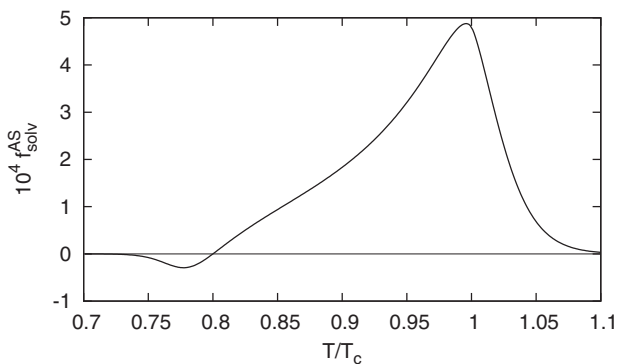


FIG. 2. The solvation force  $f_{\text{sol}}^{\text{AS}}$  as a function of temperature for  $T_w=0.8T_c$  (i.e.,  $h_1 \approx 0.60J$ ) and  $M=50$  in the antisymmetric case  $h_1=-h_2$ . Note that the difference between the zero of the solvation force  $T^*$  and the wetting temperature  $T_w$  is not visible in this scale.

$$f_{\text{sol}}^S(T_c, h_1, M) = -\frac{\pi}{48M^2} + O(1/M^3), \quad (8)$$

$$f_{\text{sol}}^{\text{AS}}(T_c, h_1, M) = \frac{23\pi}{48M^2} + O(1/M^3). \quad (9)$$

This result, in particular the universal values of the amplitudes, has been reproduced by our analysis. In the rest of this paper we exclusively discuss the antisymmetric case (AS).

First, we concentrate on the temperature  $T^*$  at which the solvation force becomes zero. We have found that for fixed  $h_1 > 0$  and for  $M \rightarrow \infty$  this temperature approaches the wetting temperature  $T_w$  exponentially:

$$\frac{T^* - T_w}{T_c} = A(h_1)e^{-B(h_1)M}, \quad M \rightarrow \infty, \quad (10)$$

where  $A(h_1)$  and  $B(h_1)$  are positive functions of the surface field  $h_1$ .<sup>1</sup> We have found that for  $h_1 \rightarrow 0$ —i.e.,  $T_w \rightarrow T_c$ —one has  $A(h_1) \rightarrow 0$ .

We note that this result is different from the corresponding result obtained within the mean-field theory where  $T^*$  is exponentially shifted *below*  $T_w$ . It is also different from the corresponding result obtained for the restricted solid-on-solid (RSOS) model, where  $T^*$  is *equal* to  $T_w$  [19].

### III. SCALING FUNCTION

In this section we discuss the scaling function that describes the behavior of the solvation force  $f_{\text{sol}}^{\text{AS}}(T, h_1, M)$  for large  $M$  and subcritical temperatures. The relevant scaling function  $\mathcal{X}(x)$  has already been proposed to describe  $f_{\text{sol}}^{\text{AS}}$  in the  $T_w = 0$  case [5]:

$$f_{\text{sol}}^{\text{AS}}(T, h_1 = J, M) = \frac{1}{M^2} \mathcal{X}\left(\frac{M}{\xi(T)}\right). \quad (11)$$

The correlation length for the 2D Ising model close to  $T_c$  is  $\xi(T) = \xi_0 t^{-1}$ , where  $t = (T_c - T)/T_c > 0$  and  $\xi_0 = [4 \ln(1 + \sqrt{2})]^{-1}$ . The scaling function  $\mathcal{X}(x)$  can be obtained numerically from the transfer matrix spectrum and some of its properties can be proved analytically [see Eq. (9) and [20]]—namely,

$$\mathcal{X}(0) = 23\pi/48, \quad (12)$$

$$\mathcal{X}(x) = 2\pi^2/x, \quad \text{for } x \rightarrow \infty. \quad (13)$$

Here we would like to extend this result to the  $h_1 < J$ —i.e.,  $T_w > 0$ —case.

For the 2D Ising model the gap exponent  $\Delta_1 = 1/2$  [19,21] and for  $T < T_c$  the scaling behavior

<sup>1</sup>In principle, these functions can be found by fitting Eq. (10) to our numerical results. However, for  $T_w > 0.5T_c$  and  $M \geq 10$  the difference between  $T^*$  and  $T_w$  is of the order of numerical errors and we were unable to precisely determine the functions  $A(h_1)$  and  $B(h_1)$ .

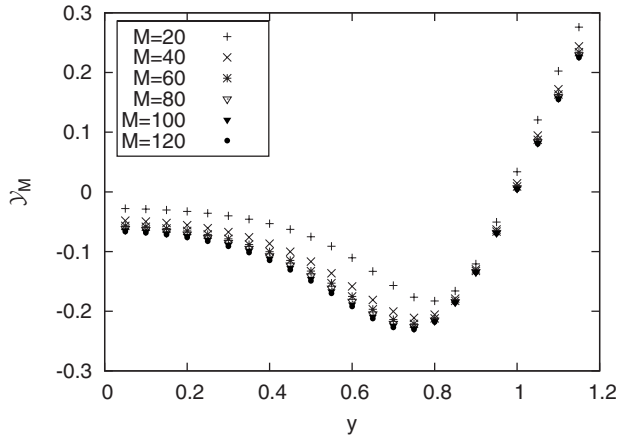


FIG. 3. Convergence of the scaling function. The function  $\mathcal{Y}_M$  is evaluated for  $x=1$  and for several values of  $y$  and  $M$  presented in the plot.

$$f_{\text{solv}}^{\text{AS}}(T, h_1, M) = \frac{1}{M^2} \mathcal{Y}(x, y), \quad (14)$$

where

$$x = \frac{M}{\xi_0 t^{-1}}, \quad y = \frac{A_0 h_1}{k_B T_c t^{1/2}} \quad (15)$$

come into play in the limit  $M \rightarrow \infty$  with  $x$  and  $y$  fixed. This implies additionally the  $t \rightarrow 0$ ,  $h_1 \rightarrow 0$  and  $T_w \rightarrow T_c$  limits. The coefficient  $A_0 = [(1 + \sqrt{2}) / \ln(1 + \sqrt{2})]^{1/2}$  in Eq. (15) has been introduced such that the value  $y=1$  corresponds to  $T=T_w$ , and then Eq. (3) is satisfied. For  $y < 1$ , Eq. (14) gives the solvation force  $f_{\text{solv}}^{\text{AS}}$  below the wetting temperature and for  $y > 1$  above  $T_w$ .

Equation (14) may be rewritten in the form leading to the scaling function

$$\mathcal{Y}(x, y) = \lim_{M \rightarrow \infty} \mathcal{Y}_M(x, y), \quad (16)$$

where

$$\mathcal{Y}_M(x, y) = M^2 f_{\text{solv}} \left( T_c \left( 1 - \frac{x \xi_0}{M} \right), k_B T_c y \left( \frac{x \xi_0}{M A_0^2} \right)^{1/2}, M \right). \quad (17)$$

Figure 3 presents plots of  $\mathcal{Y}_M$  for fixed value of  $x=1$  and selected values of  $y \in [0, 1.2]$  to exhibit the convergence of the series  $\mathcal{Y}_M$ . Typically, for  $M$  large enough one has

$$\mathcal{Y}_M(x, y) = \mathcal{Y}(x, y) + \frac{C(x, y)}{M} + O(M^{-2}). \quad (18)$$

To estimate the values of the function  $\mathcal{Y}$  we evaluated  $\mathcal{Y}_M$  for  $M=200$ . We note that a different way of obtaining the function  $\mathcal{Y}$ , based on the least-squares method [22] (details of our analysis will be explained in [16]) which allows us to calculate the functions  $\mathcal{Y}$  and  $C$  in Eq. (18), leads to similar results (the differences are not visible on the scale of our figures). The plots of function  $\mathcal{Y}$  are shown in Fig. 4.

Next, we investigate the relation between the scaling functions  $\mathcal{Y}(x, y)$  and  $\mathcal{X}(x)$ . The function  $\mathcal{X}(x)$  is calculated

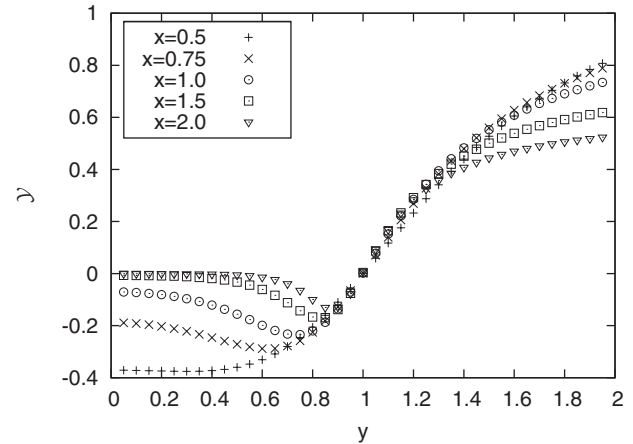


FIG. 4. Plots of the scaling function  $\mathcal{Y}$ . All plots were obtained from  $\mathcal{Y}_M$  for  $M=200$ .

in the limit  $M \rightarrow \infty$ ,  $t \rightarrow 0$  with  $h_1$  and  $Mt$  fixed. By applying this limit to Eqs. (14) and (11) one gets

$$\mathcal{X}(x) = \lim_{y \rightarrow \infty} \mathcal{Y}(x, y). \quad (19)$$

The functions  $\mathcal{X}(x)$  and  $\mathcal{Y}(x, y)$  plotted for selected values of  $y$  are presented in Fig. 5. Additionally we have found that  $\mathcal{X}(x) - \mathcal{Y}(x, y) \propto y^{-2}$  for large  $y$ .

The scaling function  $\mathcal{Y}(x, y)$  changes its sign; see Figs. 4 and 5. The zeros of the scaling function are denoted by  $y^*(x)$ —i.e.,  $\mathcal{Y}(x, y^*(x))=0$ . We have found that for large  $x$  the function  $y^*(x)$  approaches 1 exponentially from above. This allows us to show that in the scaling limit  $M \rightarrow \infty$ ,  $h_1 \rightarrow 0$ , and  $Mh_1^2$  fixed one has

$$\begin{aligned} \frac{T^* - T_w}{T_c} &= \frac{T_c - T_w}{T_c} - \frac{1}{M} f \left( \frac{Mh_1^2}{k_B^2 T_c^2} \right) + O(1/M^2), \\ &= \frac{1}{M} g \left( \frac{Mh_1^2}{k_B^2 T_c^2} \right) + O(1/M^2), \end{aligned} \quad (20)$$

where  $f(\zeta)$  and  $g(\zeta)$  are positive functions which can be determined via an implicit formula

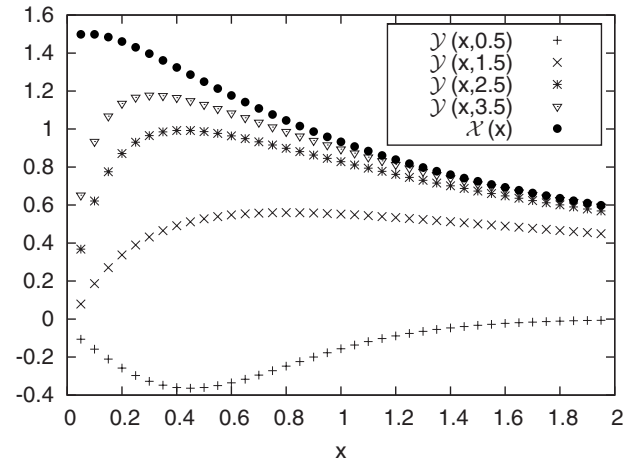


FIG. 5. The scaling function  $\mathcal{Y}$  plotted for  $y=0.5, 1.5, 2.5, 3.5$  and the scaling function  $\mathcal{X}$ . All points were calculated for  $M=200$ .

$$A_0 \xi^{1/2} = [f(\zeta)]^{1/2} y^*(f(\zeta)/\xi_0), \quad (21)$$

$$g(\zeta) = A_0^2 - f(\zeta). \quad (22)$$

We note that Eq. (20) is different from Eq. (10) because different limiting procedures were applied in these two cases.

#### IV. CONCLUSIONS

In the symmetric case of identical surface fields the solvation force is negative (attractive) and has a minimum at the supercritical temperature. The solvation force is calculated for system parameters such that  $T_w > 0$  differs only quantitatively from the one in the case  $T_w = 0$ ; see Fig. 1.

In the antisymmetric case of opposite surface fields the solvation force is positive at high temperatures and negative at low temperatures. It changes its sign at temperature  $T^* > T_w$ ; see Fig. 2. In the case of  $h_1$  fixed and  $M \rightarrow \infty$  the

difference  $T^* - T_w$  approaches 0 exponentially quickly in  $M$ .

The scaling function  $\mathcal{Y}(x, y)$  was proposed to describe the behavior of the solvation force for  $T < T_c$  in the limit  $h_1 \rightarrow 0$  and  $M \rightarrow \infty$ ; see Figs. 4 and 5. We checked that in the limit of high surface field [ $y \rightarrow \infty$  in Eq. (14)] this scaling function approached the scaling function describing the scaling behavior of the solvation force in the  $T_w = 0$  case. In addition, the zeros of the scaling function were investigated to find the formula for  $T^* - T_w$  in the  $h_1 \rightarrow 0$  limit.

#### ACKNOWLEDGMENTS

We thank A. Maciołek, D. Danchev, and S. Dietrich for many helpful discussions. This work has been financed from the funds provided by the Polish Ministry of Science and Higher Education for scientific research under Research Project No. N202 076 31/0108.

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- [1] R. Evans and U. Marini Bettolo Marconi, *J. Chem. Phys.* **86**, 7138 (1987).  
 [2] H. K. Christenson and C. E. Blom, *J. Chem. Phys.* **86**, 419 (1987).  
 [3] R. Evans, *J. Phys.: Condens. Matter* **2**, 8989 (1990).  
 [4] R. Evans, J. R. Henderson, D. C. Hoyle, A. O. Parry, and Z. A. Sabeur, *Mol. Phys.* **80**, 755 (1993).  
 [5] R. Evans and J. Stecki, *Phys. Rev. B* **49**, 8842 (1994).  
 [6] A. Hanke, F. Schlesener, E. Eisenriegler, and S. Dietrich, *Phys. Rev. Lett.* **81**, 1885 (1998).  
 [7] A. Drzewiński, A. Maciołek, and R. Evans, *Phys. Rev. Lett.* **85**, 3079 (2000).  
 [8] S. Kondrat, A. Poniewierski, and L. Harnau, *Eur. Phys. J. E* **10**, 163 (2003).  
 [9] F. Schlesener, A. Hanke, and S. Dietrich, *J. Stat. Phys.* **110**, 981 (2003).  
 [10] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, and C. Bechinger, *Nature (London)* **451**, 172 (2008).  
 [11] B. Kaufman, *Phys. Rev.* **76**, 1232 (1949).  
 [12] D. B. Abraham and A. Martin-Löf, *Commun. Math. Phys.* **32**, 245 (1973).  
 [13] L. Onsager, *Phys. Rev.* **65**, 117 (1944).  
 [14] J. Stecki, A. Maciołek, and K. Olaussen, *Phys. Rev. B* **49**, 1092 (1994).  
 [15] A. Maciołek and J. Stecki, *Phys. Rev. B* **54**, 1128 (1996).  
 [16] P. Nowakowski and M. Napiórkowski (unpublished).  
 [17] M. P. Nightingale and J. O. Indekeu, *Phys. Rev. Lett.* **54**, 1824 (1985); H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, *ibid.* **56**, 742 (1986).  
 [18] J. L. Cardy, *Nucl. Phys. B* **275**, 200 (1986).  
 [19] A. O. Parry and R. Evans, *Phys. Rev. Lett.* **64**, 439 (1990); *Physica A* **181**, 250 (1992).  
 [20] D. M. Danchev (private communication); see also J. G. Brankov, D. M. Danchev, and N. S. Tonchev, *Theory of Critical Phenomena in Finite-Size Systems, Scaling and Quantum Effects* (World Scientific, Singapore, 2000).  
 [21] K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8, p. 1.  
 [22] A. L. Talapov and H. W. Blöte, *J. Phys. A* **29**, 5727 (1996).