Scaling of solvation force in 2D Ising strip

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The solvation force for the 2D Ising strip 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.

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I. INTRODUCTION

Properties of the solvation force in various condensed matter systems have been the subject of very intensive research during recent years [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. Lattice models play special role among 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 2D Ising strip. They are obtained via exact diagonalization of the transfer matrix which is then followed by numerical solutions of equations for eigenvalues.

We consider Ising model on a two–dimensional 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

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

(1)

where $s_{n,m} = \pm 1$ with $n = 1, \ldots, N$, $m = 1, \ldots, M$ 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 $k_BT_c = 2J/\ln (1 + \sqrt{2})$, 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

$$
\cosh 2K_1 = \cosh 2K - \sinh 2Ke^{-2K},
$$

(2)

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

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

(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

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

(4)

where $Z$ 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

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

(5)

where $f_b$ is the bulk free energy per one spin [12] 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 $f_{\text{int}}$ wrt $M$. In our case, because $M$ takes only integer values, we use the definition

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

which leads to the following expression

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

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 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 $f_{\text{solv}}^S$ is plotted in Fig.1 for two cases: $T_w > 0$ (solid curve) and $T_w = 0$ (broken 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 $f_{\text{solv}}^S$ is located at $T_{\text{min}}^S > T_c$.

For opposite surface fields (AS) the solvation force $f_{\text{solv}}^AS$ in the $T_w > 0$ case, i.e., $h_1 < J$, differs substantially from the $T_w = 0$, i.e., $h_1 = J$ case. Fig.2 presents a typical plot of $f_{\text{solv}}^AS$ as a function of $T$. For low temperatures this force is negative (attractive) and has a minimum at $T_{\text{min}}^AS < T_w$. The solvation force is negative at wetting temperature and has a zero at $T^* > T_w$. Above $T^*$ the solvation force is positive (repulsive) and has a maximum at $T_{\text{max}}^AS < T_c$ (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 \[17, 18\]

$$f_{\text{solv}}^S(T_c, h_1, M) = -\frac{\pi^4}{48 M^2} + O(1/M^3), \quad (8)$$
$$f_{\text{solv}}^{AS}(T_c, h_1, M) = -\frac{\pi^4}{48 M^2} + O(1/M^3). \quad (9)$$

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 asymmetric 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 $M \to \infty$ this temperature approaches the wetting temperature $T_w$ exponentially

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

where $A(h_1)$ and $B(h_1)$ are positive functions of the surface field $h_1$ \[21\]. We have found that for $h_1 \to 0$, i.e., $T_w \to T_c$ one has

$$\lim_{h_1 \to 0} A(h_1) = 0. \quad (11)$$

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 (ROSO) 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 $f_{\text{solv}}^{AS}(T, h_1, M)$ for large $M$ and subcritical temperatures. The relevant
Here we would like to extend this result to $h/T < T_c$ (see Eq.(9) and [20]), namely some of its properties can be proved analytically (see Eq.(19) and (20)), namely

$$f_{\text{solv}}^\text{AS} (T, h_1 = J, M) = \frac{1}{M^2} \mathcal{X} \left( \frac{M}{\xi_0^{-1}(T)} \right).$$

The correlation length for 2D Ising model close to $T_c$ is $\xi_0^{-1}(T) = \xi_0^{-1} t^{-1}$, where $t = (T_c - T)/T_c > 0$ and $\xi_0^{-1} = [4 \ln (1 + \sqrt{2})]^{-1}$. 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.(19) and 20), namely

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

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

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

For 2D Ising model the gap exponent $\Delta_1 = 1/2$ and for $T < T_c$ the following scaling behavior

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

where

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

comes into play in the limit $M \to \infty$ with $x$ and $y$ fixed. This implies additionally the $t \to 0$, $h_1 \to 0$, and $T_w \to T_c$ limits. The coefficient $A_0 = (1 + \sqrt{2}) / \ln (1 + \sqrt{2})$ has been introduced such that the value $y = 1$ corresponds to $T = T_w$ and then Eq.(8) is satisfied. For $y < 1$ Eq.(15) gives the solvation force $f_{\text{solv}}^\text{AS}$ below the wetting temperature and for $y > 1$ above $T_w$.

Eq.(15) may be rewritten in the form leading to the scaling function

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

where

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

Fig.4 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

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

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 which allows to calculate the functions $\mathcal{Y}$ and $C$ in Eq.(19), leads to similar results (the differences are not visible on the scale of our figures). The plots of function $\mathcal{Y}$ are shown on 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 in the limit \( M \to \infty, t \to 0 \) with \( h_1 \) and \( M t \) fixed. By applying this limit to Eqs (15) and (12) one gets

\[
\mathcal{X}(x) = \lim_{y \to \infty} \mathcal{Y}(x, y).
\]

The functions \( \mathcal{X}(x) \) and \( \mathcal{Y}(x, y) \) plotted for selected values of \( y \) are presented on Fig.4. 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 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 form above. This allows us to show that in the scaling limit \( M \to \infty, h_1 \to 0, \) and \( M h_1^2 \) fixed one has

\[
\frac{T^* - T_w}{T_c} = \frac{T_c - T_w}{T_c} - \frac{1}{M} \left[ f \left( \frac{M h_1^2}{k_B T_c} \right) + O \left( 1/M^2 \right) \right],
\]

\[
= \frac{1}{M} g \left( \frac{M h_1^2}{k_B T_c^2} \right) + O \left( 1/M^2 \right),
\]

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

\[
A_0 \zeta^{1/2} = \left[ f(\zeta) \right]^{1/2} y^* \left( f(\zeta) / \xi_0 \right),
\]

\[
g(\zeta) = A_0^2 - f(\zeta).
\]

We note that Eq. (21) is different form 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 minimum at supercritical temperature. The solvation force calculated for system parameters such that \( T_w > 0 \) differs only quantitatively from the one in 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 \( h_1 \) fixed and \( M \to \infty \) 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 \( h_1 \to 0 \) and \( M \to \infty \), see Figs 4 5. We checked that in the limit of high surface field \( y \to \infty \) in Eq. (15) this scaling function approached the scaling function describing the scaling behavior of the for 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 \( h_1 \to 0 \) limit.

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