ϕ^4 model under Dirichlet-Neumann boundary conditions

Daniel Dantchev[1,2], **Vassil Vassilev**[1]

[1] Institute of Mechanics, Bulgarian Academy of Sciences, Academic Georgy Bonchev St. building 4, 1113 Sofia, Bulgaria

[2] Max-Planck-Institut für Intelligente Systeme, Heisenbergstrasse 3, D-70569 Stuttgart, Germany

E-mail: `danieldantchev@gmail.com, vasilvas53@gmail.com`

Abstract. The minimization of the Ginsburg-Landau ϕ^4 functional is at core of the so-called ϕ^4 model, which is one of the basic models of statistical mechanics. The minimization leads to a second order nonlinear differential equation that has to be solved under specific boundary conditions. In the current article we consider a system with a film geometry with thickness L under Dirichlet-Neumann boundary conditions applied along the finite-direction. We study the modifications of the bulk phase diagram for the finite system, as well as the field-temperature behavior of the characterizing the system order parameter profile, as well as the connected to it corresponding response functions (local and total susceptibilities).

1. Introduction

Currently, there is a substantial interest in the behavior of low-dimensional systems undergoing phase transitions. This is both due to the internal needs of theory to be developed for such systems, but also due to the experimental interest of scaled down systems. One considers systems with finite geometry like fully finite systems, chains, films, etc.

In the current article we consider a system with a film geometry of width L at temperature T and exposed to some external ordering field h. In statistical mechanics the systems are described via some order parameter, which can be scalar, vector, tensor, etc. We specifically envisage a system described by scalar, i.e., Ising type mean-field order parameter under Dirichlet-Neumann boundary conditions. Let us assume that along the finite direction of length L the corresponding Cartesian coordinate is z. For such a system in the grand canonical ensemble the finite-size scaling theory [1–3] predicts:

- For the order parameter ϕ (e.g., magnetization) profile

$$\phi(z|T,h,L) \simeq a_h L^{-\beta/\nu} X_m\left(z|L,x_t,x_h\right) \tag{1}$$

where

$$x_t = a_t \tau L^{1/\nu}, \qquad x_h = a_h h L^{\Delta/\nu}. \tag{2}$$

Here $\tau = (T - T_c)/T_c$ is the dimensionless distance from the bulk critical point T_c of the infinite system. Under Dirichlet-Neumann boundary conditions in the current article we mean that

$$\phi(z=0|T,h,L)=0 \quad \text{and} \quad \frac{\partial}{\partial z}\phi(z|T,h,L)\Big|_{z=1}=0. \tag{3}$$

Obviously, this is a specific case of mixed boundary conditions problem in which the solution of a given differential equation is required to satisfy different boundary conditions on disjoint parts $\mathcal{B}_1$ and $\mathcal{B}_2$ of the boundary $\partial\Omega=\mathcal{B}_1\bigcup\mathcal{B}_2$ of the domain Ω where the condition is stated

$$\phi_{|\mathcal{B}_1}=f_1 \quad \text{and} \quad \frac{\partial}{\partial n}\phi_{|\mathcal{B}_2}=f_2. \tag{4}$$

Here ∂n means a derivative in a direction normal to the boundary $\mathcal{B}_2$. In the current article the case $f_1=f_2=0$ has been chosen and, because of the film geometry, the normal derivative is along the z axis.

A basic characteristic of the order parameter profile is its response to the external influence on the system described in the form of some external filed h, say a magnetic one. Thus, one defines the local and total response functions (susceptibilities). For them the finite-size scaling theory predicts:

- For the local (layer) susceptibility profile

$$k_BT\,\chi_l(z|T,h,L)\equiv\frac{\partial}{\partial h}\phi(z|T,h,L)\simeq a_h^2L^{\gamma/\nu}X_\chi\left(z|L,x_t,x_h\right) \tag{5}$$

with

$$X_\chi\left(z|L,x_t,x_h\right)=\frac{\partial}{\partial x_h}X_m\left(z|L,x_t,x_h\right); \tag{6}$$

- For the total susceptibility $\chi(T,h,L)\equiv L^{-1}\int_0^L\chi_l(z|T,h,L)dz$ one has

$$k_BT\,\chi(T,h,L)\simeq a_h^2L^{\gamma/\nu}X\left(x_t,x_h\right). \tag{7}$$

In the above equations (1) – (7), k_B is the Boltzmann constant, β and γ are the critical exponents for the order parameter and the susceptibility (compressibility), the quantities a_t and a_h are nonuniversal metric factors that can be fixed, for a given system, by taking them to be, e.g., $a_t=1/\left[\xi_0^+\right]^{1/\nu}$, and $a_h=1/\left[\xi_{0,h}\right]^{\Delta/\nu}$, where ξ_0^+ and $\xi_{0,h}$ are the respective amplitudes of the correlation length along the τ and h axes. In addition, ν is a critical exponent characterizing the behavior of the correlation length, while Δ is another exponent related to the behavior of, say, order parameter as a function of the external field h.

Let us recall that the Ising system with a film geometry $\infty^2\times L$ possesses a critical point $T_{c,L}$ of its own with coordinates $(x_t^{(c)},x_h^{(c)})$. The scaling functions X_m, X_χ and X will exhibit singularities near this point. For example

$$X(x_t,x_h^{(c)})\simeq X_{c,t}\,\left(x_t-x_t^{(c)}\right)^{-\gamma_2}, \qquad x_t\to x_t^{(c)}, \tag{8}$$

where the subscript in γ_2 reminds that γ_2 is the critical exponent of the two-dimensional infinite system that is to be distinguished from the corresponding exponent γ for the three dimensional bulk system.

In the current article we will derive new exact analytical results for the scaling functions X_m, X_χ and X for the Ginzburg-Landau Ising type mean-field model under Dirichlet-Neumann boundary conditions. Let us recall that in the mean-field approximation $\beta=\nu=1/2$, $\Delta=3/2$ and $\gamma=\gamma_2=1$. For the version of the model considered here $\tau=(T-T_c)/T_c\,(\xi_0^+)^{-2}$, $z\in[0,L]$, $\xi_0^+=1$, $\xi_{0,h}=1/\sqrt[3]{3}$, $a_t=1$ and $a_h=3$ [4–6].

2. The Ginzburg-Landau functional

In the present work we consider the standard ϕ^4 Ginzburg–Landau functional

$$\mathcal{F}[\phi|\tau, h, L] = \int_0^L \mathcal{L}(\phi, \phi'|\tau, h)\, \mathrm{d}z \tag{9}$$

with

$$\mathcal{L}(\phi, \phi'|\tau, h) = \frac{1}{2}\phi'^2 + \frac{1}{2}\tau\phi^2 + \frac{1}{4}g\phi^4 - h\phi. \tag{10}$$

Here L, $g \in \mathbb{R}^+$, while $\tau, h \in \mathbb{R}$, $z \in (0, L)$ and $\phi = \phi(z)$ are the independent and dependent variables, respectively, and the prime indicates differentiation with respect to the variable z.

This functional describes a critical system of Ising type in a film geometry $\infty^2 \times L$, where the film thickness L is supposed to be along the z axis. In Eq. (9), $\phi(z; \tau, h, L)$ is the order parameter of the system, g is the bare coupling constant, and, as before, τ is the bare reduced temperature and h is the external ordering field.

The physical state of the regarded system is described by the minimizers of the Ginzburg–Landau functional $\mathcal{F}[\phi; \tau, h, L]$ given above whose extremals are determined by the solutions of the corresponding Euler-Lagrange equation

$$\frac{d}{dz}\frac{\partial \mathcal{L}}{\partial \phi'} - \frac{\partial \mathcal{L}}{\partial \phi} = 0, \tag{11}$$

which, on account of Eq. (10), reads

$$\phi'' - \phi\left[\tau + g\,\phi^2\right] + h = 0. \tag{12}$$

Multiplying equation (12) by ϕ' and integrating once over z one obtains the following first integral of the system

$$\frac{1}{2}\phi'^2 - \frac{1}{2}\tau\phi^2 - \frac{1}{4}g\phi^4 + h\phi = c, \tag{13}$$

where c is the constant of integration. Another quantities of interest are the local $\chi_l(z, T, h, L)$ and total $\chi(z, T, h, L)$ susceptibilities

$$\chi_l(z|T, h, L) \equiv \frac{\partial}{\partial h}\phi(z|T, h, L) \quad \text{and} \quad L^{-1}\chi_l(z|T, h, L) = \int_0^L \chi_l(z|T, h, L)dz. \tag{14}$$

From Eq. (12) for χ_l one has

$$-\chi_l'' + \chi_l\left[\tau + 3g\,\phi^2\right] = 1. \tag{15}$$

It is convenient to introduce the following notations

$$\zeta = z/L, \quad x_t = \tau L^{1/\nu}, \quad \bar{x}_h = \sqrt{2g}hL^{\Delta/\nu}, \quad \nu = 1/2, \quad \Delta = 3/2 \tag{16}$$

and

$$\phi(z) = \sqrt{\frac{2}{g}}\, L^{-\beta/\nu} X_m(\zeta|x_t, \bar{x}_h). \tag{17}$$

In terms of the above variables the energy functional Eq. (9) and its Lagrangian density Eq. (10) read

$$\mathcal{F}[X_m|x_t, \bar{x}_h] = \frac{1}{gL^4}\int_0^1 \mathcal{L}[X_m, X_m'|x_t, \bar{x}_h]d\zeta, \tag{18}$$

with

$$\mathcal{L}[X_m, X_m'|x_t, \bar{x}_h] = X_m'^2(\zeta) + X_m^4(\zeta) + x_t X_m^2(\zeta) - \bar{x}_h X_m(\zeta). \tag{19}$$

The primes here and hereafter indicate differentiation with respect to the variable $\zeta \in [0,1]$. Accordingly, Eq. (12) and its first integral (13) become

$$X_m''(\zeta) = X_m(\zeta)\left[x_t + 2X_m^2(\zeta)\right] - \frac{\bar{x}_h}{2}. \tag{20}$$

and

$$X_m'^2(\zeta) = P[X_m], \qquad \text{with} \qquad P[X_m] = X_m^4(\zeta) + x_t X_m^2(\zeta) - \bar{x}_h X_m(\zeta) + \varepsilon, \tag{21}$$

respectively, where ε denotes the respective constant of integration.

We are looking for such a solution of Eq. (19) that

$$X_m(\zeta = 0|x_t, \bar{x}_h) = 0 \qquad \text{and} \qquad X_m'(\zeta = 1|x_t, \bar{x}_h) = 0, \tag{22}$$

i.e., we are looking for a solution of the problem under Dirichlet-Neumann boundary conditions.

3. Expression for the order parameter profile

Below we derive the corresponding result within two different approaches.

3.1. Results for the order parameter profiles in the case of zero field

In this case the expression for the order parameter profiles can be expressed in terms of Jacobi elliptic functions.

Let us look for a solution of Eq. (20) with $\bar{x}_h = 0$ of the type

$$X_m(\zeta|a,b,k) = a\,\mathrm{sn}\,(b\,\zeta\,|k\,)\,, \tag{23}$$

where $\mathrm{sn}(.|k)$ is the corresponding Jacobi elliptic function with $0 \le k \le 1$. Here a, b and k are parameters that are to be determined. Let us first check what restrictions the boundary conditions Eq. (22) impose on these parameters. First, it is clear that $X_m(\zeta = 0|a,b,k) = 0$ by the very form in which we have chosen to look for a solution. Next, the condition $X_m'(\zeta = 1|a,b,k) = 0$ leads to

$$ab\ \mathrm{cn}\,(b\,|k\,)\,\mathrm{dn}\,(b\,|k\,) = 0. \tag{24}$$

Solving for b, renouncing the trivial solution $b = 0$, we obtain

$$b = K\,(k)\,. \tag{25}$$

Plugging $a\,\mathrm{sn}\,(b\,\zeta\,|K\,(k)\,)$ into Eq. (20) (with $\bar{x}_h = 0$) and solving for x_t, we derive

$$x_t = \left(k^2 - 1\right) K\,(k)^2 - 2a^2\,\mathrm{sn}\,(\zeta\,K\,(k)\,|k)^2\,. \tag{26}$$

The above shall be valid for any ζ. Thus, from $\zeta = 0$ we conclude that

$$x_t(k) = -\left(k^2 + 1\right) K\,(k)^2\,, \tag{27}$$

while from $\zeta = 1$, with x_t given by Eq. (27), it follows that

$$a = \pm k\,K\,(k)\,. \tag{28}$$

Summarizing, we conclude that

$$X_m(\zeta) = \pm\,k\,K\,(k)\,\mathrm{sn}\left(\zeta K\,(k)\,\middle|k\right), \quad \text{with} \quad x_t = -\left(k^2 + 1\right) K\,(k)^2\,, \quad 0 \le k \le 1. \tag{29}$$

The phase diagram of the considered system follows from the above relations and its details are given in Figure 1 - on the left panel for the bulk system and for the finite film with Dirichlet-Neumann boundary conditions - on the right panel. From Eq. (27) it follows that the critical temperature of the finite system, below which the order parameter profile is nonzero, is

$$x_{t,\,\mathrm{crit}} = x_t(k = 0) = -\frac{\pi^2}{4}. \tag{30}$$

The last means that for $x_t \ge -\pi^2/4$ one has $X_m = 0$ and $X_m \ne 0$ for $x_t < -\pi^2/4 \simeq -2.4674$. Several order parameter profiles for different values of x_t are shown in Fig. 2.

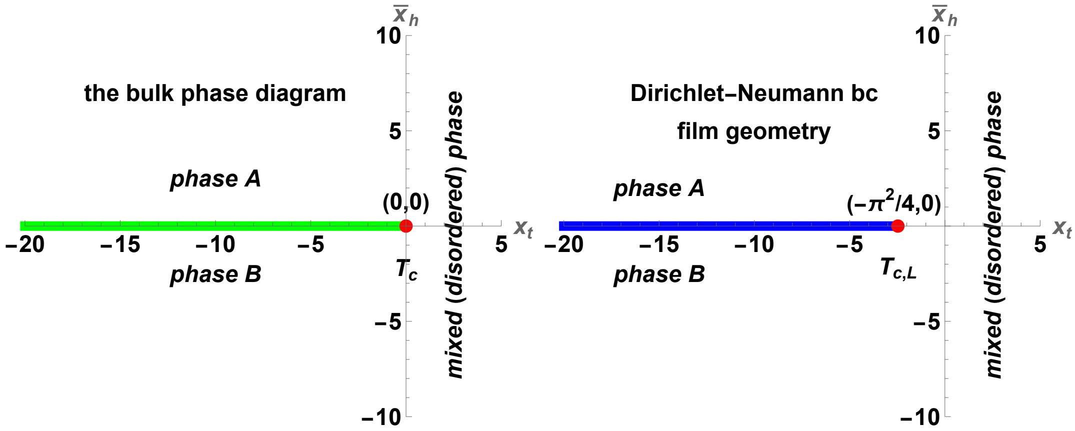

Figure 1. **Left panel**: The phase diagram of the bulk system (i.e., of the system in which the limit $L \to \infty$ has been performed, keeping all other parameters, T and h, fixed). **Right panel**: The phase diagram of the finite system with Dirichlet-Neumann boundary conditions. In the bulk system a phase transition of first order happens when crossing the phase coexistence line that is at $\bar{x}_h = 0$ and spans for $T \in (0, T = T_c)$. At $T = T_c$ the system exhibits a second order phase transition. In the finite system the coexistence line is at $\bar{x}_h = 0$ and spans for $T \in (0, T = T_{c,L})$. The second order phase transition happens again at $\bar{x}_h = 0$ but at, see Eq. (30), $T = T_{c,L} \equiv T_c(1 - x_{t,\text{crit}} L^{-2}) = T_c(1 - (\pi^2/4)L^{-2})$. Note the change with Dirichlet-Dirichlet boundary conditions where the critical point is at $T_{c,L} = T_c(1-\pi^2 L^{-2})$. We emphasize that in the finite system the second order phase transition does *not* happen at $T = T_c$ but at some other, L-dependent temperature $T_{c,L}$, such that $T_{c,L\to\infty} = T_c$.

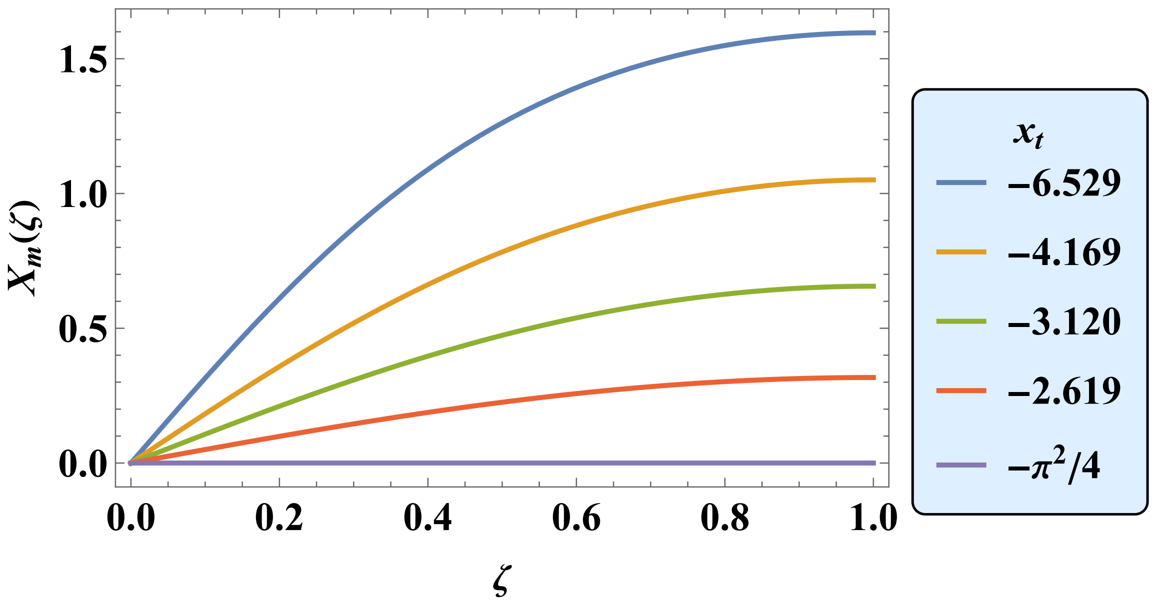

Figure 2. The behavior of the order parameter profile for $x_t = -6.529, -4.169, -3.120, -2.619$, and $x_t = -\pi^2/4$.

3.2. Results for the order parameter profile in the case of nonzero field

3.2.1. Approach I: Using the first integral. Let $X_m(\zeta = 1) = X_{m,r}$. Then, from Eq. (21) and Eq. (22) we obtain $P[X_{m,r}] = 0$, and thus

$$P[X_m] = X_m^4(\zeta) - X_{m,r}^4 + x_t \left[X_m^2(\zeta) - X_{m,r}^2\right] - \bar{x}_h \left[X_m(\zeta) - X_{m,r}\right]. \tag{31}$$

In addition Eq. (21) delivers

$$\zeta = \int_0^{X_m(\zeta)} \frac{dX_m}{\sqrt{X_m^4 - X_{m,r}^4 + x_t \left[X_m^2 - X_{m,r}^2\right] - \bar{x}_h \left[X_m - X_{m,r}\right]}}, \tag{32}$$

and

$$1 = \int_0^{X_{m,r}} \frac{dX_m}{\sqrt{X_m^4 - X_{m,r}^4 + x_t \left[X_m^2 - X_{m,r}^2\right] - \bar{x}_h \left[X_m - X_{m,r}\right]}}, \tag{33}$$

The algorithm for solving numerically the problem for finding the order parameter profile under Dirichlet-Neumann boundary conditions is now clear. From Eq. (33) one can determine $X_{m,r}$ as a function of x_t and $\bar{x}_h$. Then, from Eq. (32) one determines ζ as a function of X_m. Inverting this dependence, one shall arrive at the desired function $X_m(\zeta)$. If there is more than one solution obtained under the procedure described above, one shall choose this profile $X_m(\zeta)$ that provides the minimum of the free energy $\mathcal{F}$, see Eq. (18).

For $\bar{x}_h = 0$ one has $P[X_m] = P[-X_m]$. Thus, in this case there are two equally probable possibilities $X_m'(\zeta) > 0$ and $X_m'(\zeta) < 0$ which will lead to two order parameter profiles with the same free energy. If $h > 0$ since the physical solution has to minimize the functional Eq. (18) it is clear that $\bar{x}_h X_m(\zeta) > 0$, when $h > 0$. Next, the problem is symmetric under the *simultaneous* change of the signs of X_m and h. Therefore, it is enough to study the case $h \geq 0$ with $X_m(\zeta) \geq 0$.

Let us assume that $X_m'(\zeta) > 0$, where $X_m(\zeta)$ starts from $X_m(\zeta = 0) = 0$ and reaches its maximum at $X_m(\zeta = 1) = X_{m,r}$. Then, from Eq. (32) one obtains

$$\zeta = X_{m,r}^{-1} \int_0^{X_m(\zeta)/X_{m,r}} \frac{dy}{\sqrt{y^4 - 1 + x_{t,r}\left[y^2 - 1\right] - \bar{x}_{h,r}\left[y - 1\right]}}, \tag{34}$$

and

$$X_{m,r} = \int_0^1 \frac{dy}{\sqrt{y^4 - 1 + x_{t,r}\left[y^2 - 1\right] - \bar{x}_{h,r}\left[y - 1\right]}}, \tag{35}$$

where

$$y = X_m/X_{m,r}, \qquad x_{t,r} = x_t/X_{m,r}^2 \quad \text{and} \quad \bar{x}_{h,r} = \bar{x}_h/X_{m,r}^3. \tag{36}$$

Eqs. (34) - (36) provide an even simpler, than the described above, numerical algorithm for solving the problem about the determination of the order parameter profile. First, for any given set of values $\{x_{t,r}, \bar{x}_{h,r} \geq 0\} \in \mathbb{R}^2$, Eq. (35) delivers a *single* value of $X_{m,r} \in \mathbb{Z}$. Of course, we are only interested in $X_{m,r} \geq 0$. When this is the case, Eq. (34) delivers numerically $X_m(\zeta)$. Actually, we have shown that if for a given set of values $\{x_t, \bar{x}_h \geq 0\}$ the order parameter for the Dirichlet-Neumann boundary conditions exist, it is only one. Thus, we can prove the following:

Proposition *If the external magnetic field is nonzero, i.e., $\bar{x}_h \neq 0$, in the case when for given x_t and $\bar{x}_h$ the order parameter profile $X_m(\zeta)$ which minimizes the free energy exist under the Dirichlet-Neumann boundary conditions $X_m(0) = 0$, $X_m'(1) = 0$, it is a single one, monotonic on the interval $(0, 1)$, and for it $\bar{x}_h X_m(\zeta) \geq 0$.*

Several order parameter profiles for different values of x_t are shown in Fig. 2.

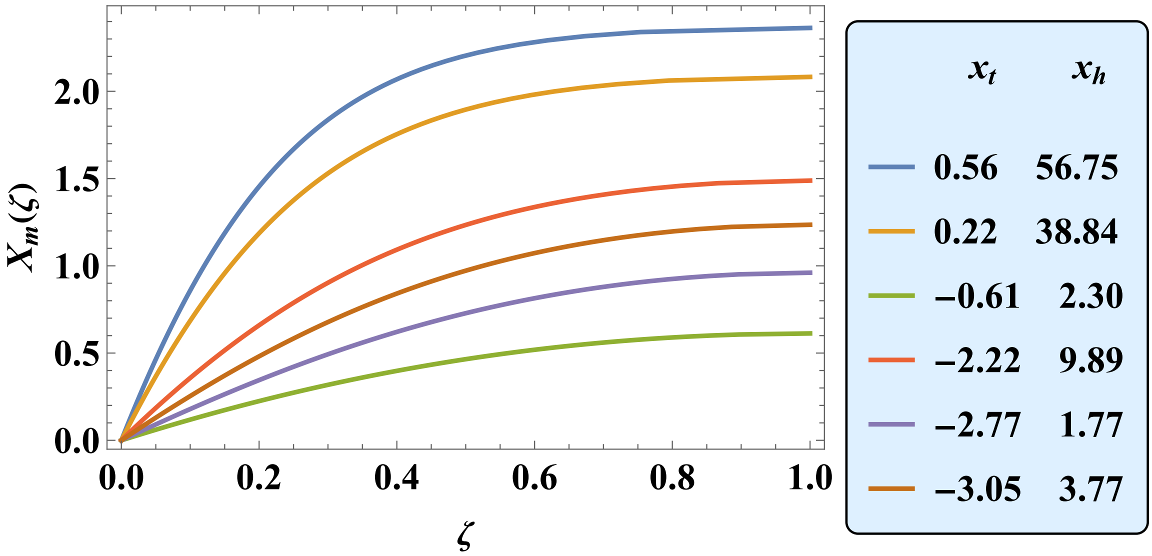

Figure 3. The behavior of the order parameter profile for $\{x_t = 0.56, x_h = 56.75\}$, $\{x_t = 0.22, x_h = 38.84\}$, $\{x_t = -0.61, x_h = 2.30\}$, $\{x_t = -2.22, x_h = 9.89\}$, $\{x_t = -2.77, x_h = 1.77\}$, $\{x_t = -3.05, x_h = 3.77\}$.

Let us demonstrate how from above expressions one can obtain the ones for the specific case of $\bar{x}_h = 0$. Then the integrals Eq. (34) and Eq. (35) can be calculated explicitly in terms of elliptic functions. From Eq. (35) one obtains

$$X_{m,r} = \frac{K\left[\left(-x_t/X_{m,r}^2 - 1\right)^{-1/2}\right]}{\sqrt{-x_t/X_{m,r}^2 - 1}} \tag{37}$$

while Eq. (34) delivers

$$\zeta X_{m,r} = \frac{F\left[\sin^{-1}\left(X_m(\zeta)/X_{m,r}\right)\Big|\left(-x_t/X_{m,r}^2 - 1\right)^{-1/2}\right]}{\sqrt{-x_t/X_{m,r}^2 - 1}}, \tag{38}$$

or, reverting the last result

$$X_m(\zeta)/X_{m,r} = \mathrm{sn}\left(\zeta\, X_{m,r}\sqrt{-x_t/X_{m,r}^2 - 1}\,\Big|\left(-x_t/X_{m,r}^2 - 1\right)^{-1/2}\right), \tag{39}$$

where $K(z)$ is the complete elliptic integral of the first kind, $F(z|m)$ gives the elliptic integral of the first kind, and $\mathrm{sn}(z|m)$ — the Jacobi elliptic function.

From Eq. (37) and Eq. (39) one derives

$$X_m(\zeta) = X_{m,r}\ \mathrm{sn}\left\{\zeta\ K\left[\left(-x_t/X_{m,r}^2 - 1\right)^{-1/2}\right]\Big|\left(-x_t/X_{m,r}^2 - 1\right)^{-1/2}\right\}. \tag{40}$$

Setting

$$k = \left(-x_t/X_{m,r}^2 - 1\right)^{-1/2} \tag{41}$$

from Eq. (40) one arrives at

$$X_m(\zeta) = X_{m,r}\ \mathrm{sn}(\zeta\ K(k)\big|k), \tag{42}$$

and from Eq. (37) it follows

$$X_{m,r} = k\, K(k). \tag{43}$$

Eq. (41) then delivers Eq. (27) from the previous approach. The inspection of the equations of the two approaches ensures as that they lead to the same result for the order parameter profile, as it shall be expected.

3.2.2. Approach II: Exact explicit results for the order parameter profile in the case of nonzero field via Weierstrass function. Following [7, p. 454] one obtains that the order parameter for given values of the temperature and the field reads

$$X_m\left(\zeta|x_t, \bar{x}_h, X_{m,r}\right) = X_{m,r} + \frac{6X_{m,r}\left(x_t + 2X_{m,r}^2\right) - 3\bar{x}_h}{12\wp\left(\zeta - 1; g_2, g_3\right) - \left(x_t + 6X_{m,r}^2\right)}, \tag{44}$$

where $X_{m,r} = X_{m,r}(x_t, x_h)$ is the value of the order parameter profile at the right end of the system. Note that $X_{m,r}$ is to be determined by the boundary conditions. Here $\wp\left(v; g_2, g_3\right)$ is the Weierstrass elliptic function whose invariants g_2 and g_3 read

$$\begin{aligned} g_2 &= \frac{1}{12}x_t^2 - X_{m,r}\left(X_{m,r}^3 + x_t X_{m,r} - \bar{x}_h\right), \\ g_3 &= -\frac{1}{432}\left[27\bar{x}_h^2 + 2x_t^3 + 72 x_t X_{m,r}\left(X_{m,r}^3 + x_t X_{m,r} - \bar{x}_h\right)\right]. \end{aligned} \tag{45}$$

The procedure for the explicit numerical determination of $X_m\left(\zeta|x_t, \bar{x}_h, X_{m,r}\right)$ is now clear. First, using that (see, e.g., [8]) $\wp(\zeta \to 0) \simeq \zeta^{-2}$, we immediately conclude that $X_m\left(1|x_t, \bar{x}_h, X_{m,r}\right) = X_{m,r}$, as it ought to be. It is also easy to show that $X_m'\left(\zeta \to 1|x_t, \bar{x}_h, X_{m,r}\right) = 0$. The only remaining requirement that $X_m\left(\zeta \to 0|x_t, \bar{x}_h, X_{m,r}\right) = 0$ leads to an transcendental equation from where we have to determine $X_{m,r}$. Normally, one obtains more than one solution of this equation. The one, that corresponds to the physical reality is the one which minimizes the energy given by Eq. (19).

4. Expression for the susceptibility

In terms of the notations of Eq. (16), for the local susceptibility (6) in the model under consideration (with $\nu = 1/2$, $\gamma = 1$) one derives

$$X_\chi(\zeta|x_t, \bar{x}_h) = 2\frac{\partial}{\partial \bar{x}_h} X_m(\zeta|x_t, \bar{x}_h). \tag{46}$$

From Eq. (20) one derives

$$-X_\chi'' + (x_t + 6X_m^2)X_\chi = 1. \tag{47}$$

This equation does not depend explicitly on x_h. It is possible to obtain its solution for $x_h = 0$ in terms of Jacobi elliptic functions.

Below we show that if one knows $X_m\left(\zeta|x_t, \bar{x}_h, X_{m,r}\right)$ one can determine the scaling function of the total susceptibility. Indeed, for a fixed x_t Eq. (46) implies

$$\frac{1}{2}X_\chi\left(\zeta|x_t, \bar{x}_h, X_{m,r}\right) = \frac{\partial}{\partial \bar{x}_h} X_m\left(\zeta|x_t, \bar{x}_h, X_{m,r}\right) + \frac{\partial}{\partial \bar{x}_h} X_{m,r}(\bar{x}_h) \frac{\partial}{\partial X_{m,r}} X_m\left(\zeta|x_t, \bar{x}_h, X_{m,r}\right). \tag{48}$$

Since for the local susceptibility at the end of the system one has

$$X_\chi(0|x_t, \bar{x}_h, , X_{m,r}) = 0, \tag{49}$$

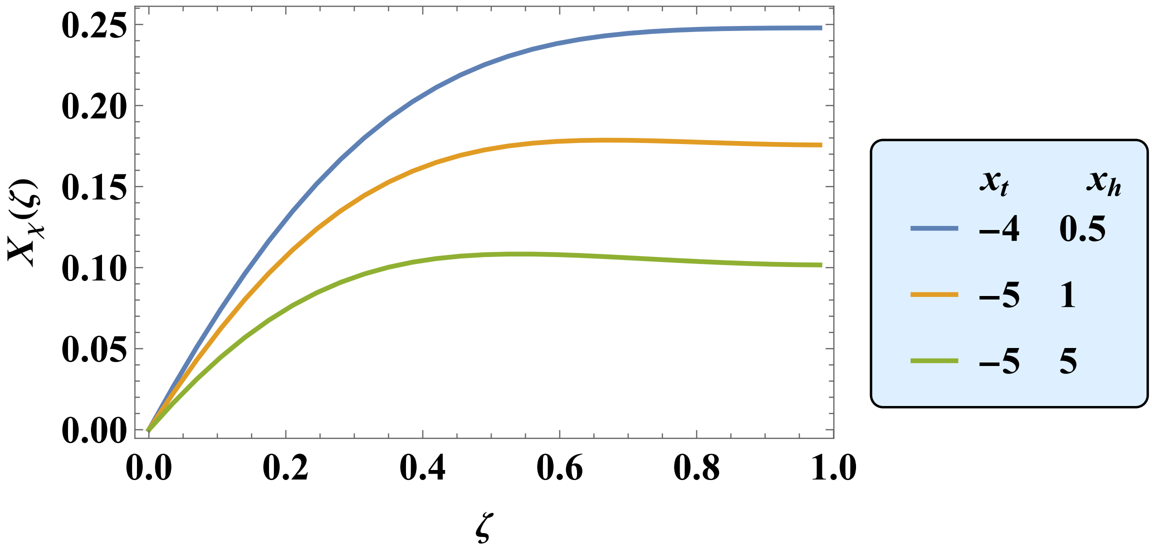

Figure 4. The behavior of the local susceptibility for $\{x_t = -4, x_h = 0.5\}$, $\{x_t = -5, x_h = 1\}$, $\{x_t = -1, x_h = 5\}$. Please note that for strong field and low temperatures the profile is *not* a monotonic function of ζ but becomes such for higher x_t and smaller x_h.

one derives

$$\frac{\partial}{\partial \bar{x}_h} X_{m,r}(\bar{x}_h) = -\frac{\frac{\partial}{\partial \bar{x}_h} X_m\left(0|x_t, \bar{x}_h, X_{m,r}\right)}{\frac{\partial}{\partial X_{m,r}} X_m\left(0|x_t, \bar{x}_h, X_{m,r}\right)}. \tag{50}$$

Thus, the total susceptibility

$$X(x_t, \bar{x}_h, X_{m,r}) = \int_0^1 X_\chi\left(\zeta|x_t, \bar{x}_h, X_{m,r}\right) d\zeta, \tag{51}$$

is determined by Eqs. (48) and (50) in terms of the scaling function of the order parameter profile $X_m(\zeta|x_t, \bar{x}_h, X_{m,r})$, given in analytic form by Eq. (44), and its partial derivatives with respect to $\bar{x}_h$ and $X_{m,r}$.

Using the procedure described above can determine the behavior of the local and total susceptibilities for given values of x_t and x_h The behavior of $X_\chi(\zeta|x_t, x_h)$ is shown in Fig. 4, while the behavior of the total susceptibility $X(x_t, x_h)$ is demonstrated in Fig. 5 One clearly observes the divergence of X for $x_h = 0$ when $x_t \to -\pi^2/4$.

4.1. On the analytical solution for the susceptibility in zero external field

In the current section we solve Eq. (47) for $X_\chi(\zeta|x_t) \equiv X_\chi(\zeta|x_t, \bar{x}_h = 0)$. When $\bar{x}_h = 0$ the order parameter profile X_m is given by Eq. (29) (see also Eq. (42)). Eq. (47) is a second order differential equation. According to the general theory [9] of the differential equations of the second order, the solution of such an equation is given by

$$X_\chi(\zeta|x_t) = c_1 y_1(\zeta|x_t) + c_2 y_2(\zeta|x_t) + c_i y_i(\zeta|x_t), \tag{52}$$

where $y_1(\zeta|x_t)$ and $y_2(\zeta|x_t)$ are linearly independent solutions of the homogeneous equation

$$-X_\chi'' + (x_t + 6X_m^2)X_\chi = 0, \tag{53}$$

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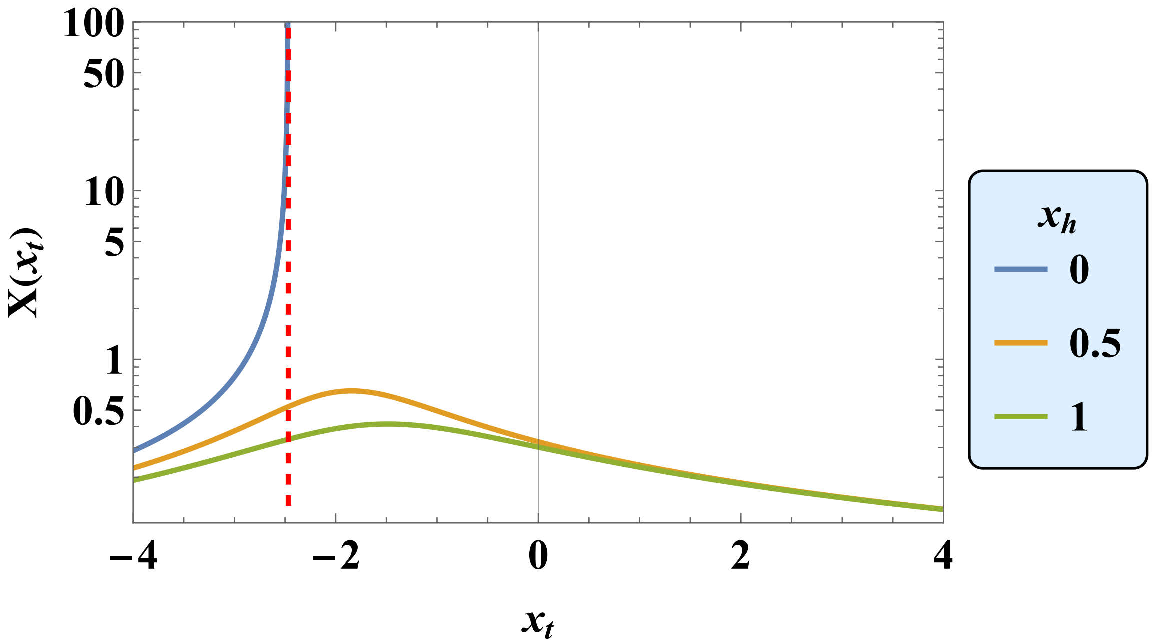

Figure 5. The behavior of the total susceptibility for $\{x_h = 0\}$, $\{x_h = 0.5\}$, and $\{x_h = 1\}$. Note that, as expected, larger the field, smaller the total susceptibility. It diverges near the critical point $\{x_t = -\pi^2/4, 0\}$ of the finite system.

while $y_i(\zeta|x_t)$ is a particular solution of the inhomogeneous Eq. (47); c_1, c_2 and c_i are constants.

We start with the determination of y_1. One can check that

$$y_1(\zeta|x_t) = \frac{d}{d\zeta} X_m(\zeta|x_t) \tag{54}$$

is a solution of Eq. (53). Performing the calculations, one obtains the explicit form for $y_1(\zeta|x_t)$

$$y_1(\zeta|x_t) = kK(k)^2 \,\mathrm{cn}\,[\zeta K(k)\,|k]\,\mathrm{dn}\,[\zeta K(k)\,|k]\,. \tag{55}$$

The behavior of $y_1(\zeta|x_t)$ for several values of k (i.e., of x_t) is shown in Fig. 6. Knowing y_1 one finds y_2 via [9] the construction:

$$y_2(\zeta|x_t) = y_1(\zeta|x_t) \int \frac{d\zeta}{[y_1(\zeta|x_t)]^2}. \tag{56}$$

From Eq. (56) it follows that

$$y_2''(\zeta|x_t) = y_1''(\zeta|x_t) \int \frac{d\zeta}{[y_1(\zeta|x_t)]^2}. \tag{57}$$

Thus, since $y_1(\zeta|x_t)$ is a solution of Eq. (53), it follows that $y_2(\zeta|x_t)$ is also a solution of Eq. (53). Having $y_1(\zeta|x_t)$ and $y_2(\zeta|x_t)$, one can determine the corresponding Wronskian

$$W = y_1(\zeta|x_t)y_2'(\zeta|x_t) - y_2(\zeta, x_t)y_1'(\zeta, x_t). \tag{58}$$

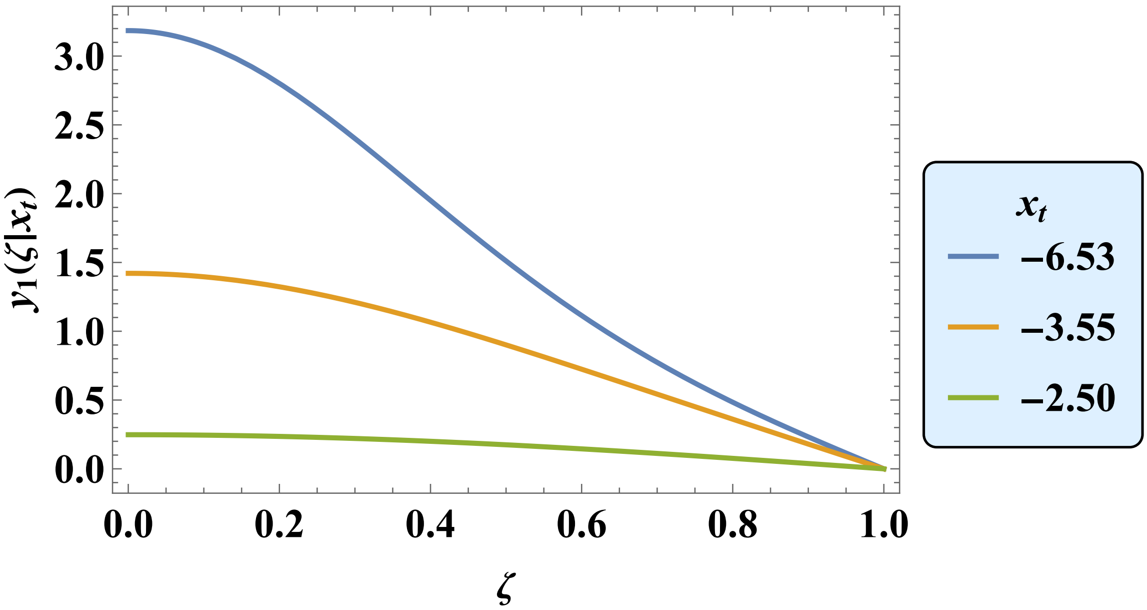

Figure 6. The behavior of $y_1(\zeta|x_t)$ as a function of ζ for $x_t = -6.53, -3.55$, and $x_t = -2.50$. We observe that it is a monotonically decreasing function equal to zero for $\zeta = 1$.

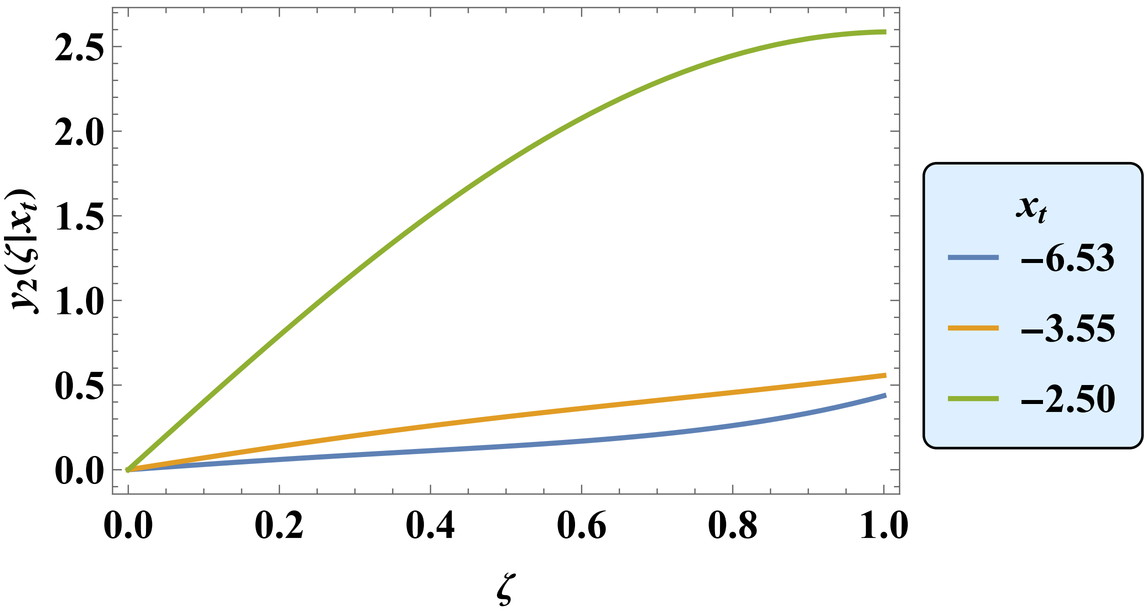

Figure 7. The behavior of $y_2(\zeta|x_t)$ as a function of ζ for $x_t = -6.53, -3.55$, and $x_t = -2.50$. We observe that it is a monotonically increasing function equal to zero for $\zeta = 0$.

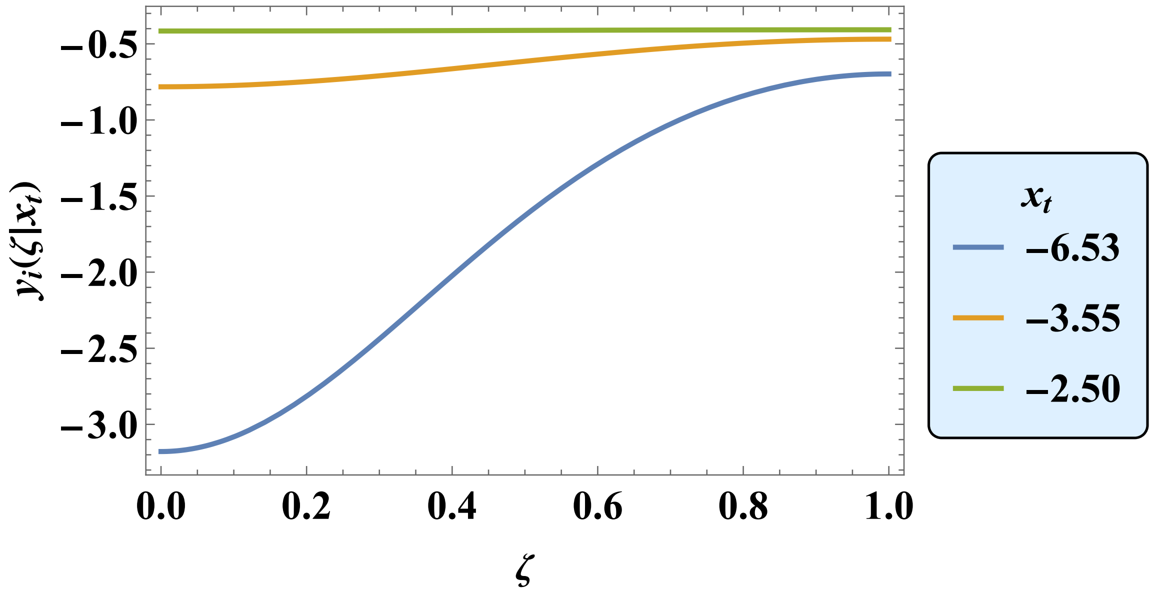

Figure 8. The behavior of $y_i(\zeta|x_t)$ as a function of ζ for $x_t = -6.53, -3.55$, and $x_t = -2.50$. We observe that it is a negative and monotonically increasing function of $\zeta = 0$.

From Eq. (56) it immediately follows that $W = 1$, which means that y_1 and y_2 are linearly independent solutions. The standard behavior of $y_2(\zeta)$ for several selected values of x_t is shown in Fig. 7.

According to the general recipe [9], for the particular solution of the homogeneous equation one has

$$y_i(\zeta|x_t) = y_1(\zeta|x_t)\int y_2(\zeta|x_t)d\zeta - y_2(\zeta|x_t)\int y_1(\zeta|x_t)d\zeta. \tag{59}$$

Having in mind Eq. (54) the above expression simplifies to

$$y_i(\zeta|x_t) = -y_1(\zeta|x_t)\int \frac{X_m(\zeta|x_t)}{[y_1(\zeta|x_t)]^2}d\zeta. \tag{60}$$

Performing the integration one obtains the explicit expression

$$y_i(\zeta|x_t) = \frac{1-k^2-2\text{dn}\left(\zeta K\left(k^2\right)|k^2\right)^2}{\left(k^2-1\right)^2 K\left(k^2\right)^2}. \tag{61}$$

The behavior of $y_i(\zeta)$ for selected values of x_t is shown in Fig. 8.

It is easy to check that $c_i y_i(\zeta|x_t)$ with $c_i = 1$ is a solution of Eq. (47). Requiring the the solution for X_χ preserves the symmetru due to the Dirichlet - Neumann boundary conditions we obtain that

$$c_1(k) = \frac{k^2+1}{k\left(k^2-1\right)^2 K\left(k^2\right)^4} \tag{62}$$

and

$$c_2(k) = \frac{k\left(k^2+1\right)K\left(k^2\right)}{\left(k^2-1\right)K\left(k^2\right)+\left(k^2+1\right)E\left(k^2\right)}. \tag{63}$$

The behavior of $X_\chi(\zeta|x_t)$ (shown in logarithmic scale) as a function of ζ for several values of x_t is shown in Fig. 9. The behavior of the total susceptibility is given in Fig. 10.

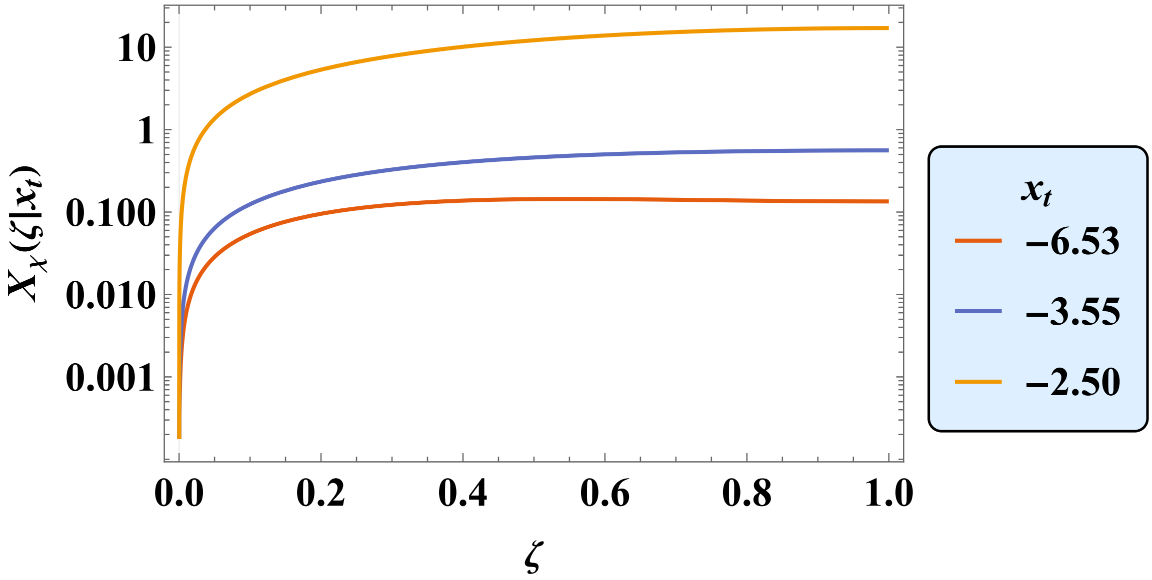

Figure 9. The behavior of $X_\chi(\zeta|x_t)$ (in logarithmic scale) as a function of ζ for $x_t = -6.53, -3.55$, and $x_t = -2.50$. We observe that the function sharply increases on approaching the critical point.

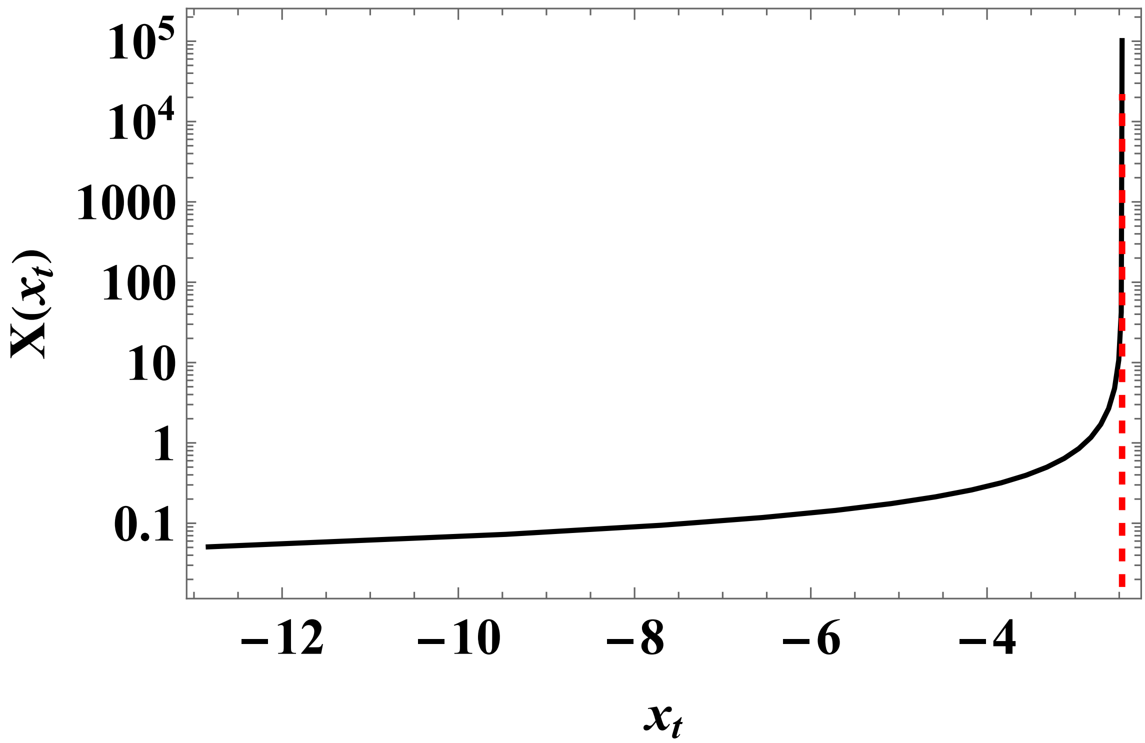

Figure 10. The behavior of the total susceptibility$X(x_t)$ as a function of x_t. We observe that the function dramatically increases upon approaching the critical point. The red vertical dashed line marks the position of the critical temperature $T_{c,L} = -\pi^2/4$.

5. Concluding Comments and Discussion

In the current article we study a system with a film geometry describing a critical fluid under Dirichlet-Neumann boundary conditions. We determine the order parameter profile, local and total susceptibilities as a function both of temperature T and the external ordering field h. As a result we obtained the phase diagram of the finite system shown in Fig. 1. We observe that the finite system possesses a critical point of its own at a temperature $T_{c,L} = -\pi^2/4$ *below* the bulk critical temperature T_c. The last implies that, for a zero field, the order parameter is zero for $T > T_{c,L}$. Its behavior is explicitly given, in terms of the Jacobi elliptic functions, in Eq. (29) (see also Eq. (42)). The behavior of the order parameter for several selected values of the scaled temperature x_t is shown in Fig. 2. The behavior of the order parameter profiles for non-zero external field h is determined in two independent ways - *i)* using the first integral of the system - see Eq. (34) — Eq. (36), and *ii)* via the via Weierstrass function - see Eq. (44) — Eq. (45). A visualization of the order parameter profile for the case of nonzero field for specific values of x_t and x_h is shown in Fig. 3. The response of the order parameter profile to the change of the xternal influence on the system, i.e., the external field, is reflected by the local and total susceptibilities. General analytic expression for the susceptibilities are given in Eq. (48) and Eq. (51). From these expressions it is clear, that if one knows analytically the behavior of the order parameter as a function of x_t and x_h, one, in principle, can also determine the behavior of the local $X_\chi(\zeta|x_t, x_h)$ and total $X(x_t, x_h)$ susceptibilities. The behavior of the local susceptibility is derived in Sec. 4.1. It is given as a linear combination of three components y_1, y_2 and y_i — see Eq. (55), Eq. (56) and Eq. (61), correspondingly. The coefficients of the linear combinations c_1 and c_2 are given in Eq. (62) and Eq. (63), while $c_i = 1$. The behavior of $X_\chi(\zeta|x_t, x_h = 0)$ as a function of ζ for several selected values of x_t i shown in Fig. 9. We observe that the function sharply increases on approaching the critical point. The behavior of $X(x_t, x_h = 0)$ as a function of x_t is given in Fig. 10. This function has a singularity at the critical temperature $T_{c,L}$ and tends to infinity upon approaching this point from below.

From the above it is clear that mathematically the problem for finding the order parameter profile and the susceptibilities reduces itself to a problem for solving a system of two nonlinear differential equations of second order in which the second equation involves the solution of the first one as an input. In the current article we have demonstrated how one can tackle this problem and obtain analytical solutions for these two equations.

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Appendix A. Some details for derivation of the expression with Weierstrass function

Let us explain some details of the derivation of Eq. (44).

In Ref. [7, 20.6] one considered integrals of the type

$$z = \int_a^x \frac{1}{\sqrt{f(t)}} dt, \tag{A.1}$$

with $f(t)$ a quartic polynomial with no repeated factors

$$f(t) = a_0 t^4 + 4a_1 t^3 + 6a_2 t^2 + 4a_3 t + a_4. \tag{A.2}$$

Then it is shown that the integral Eq. (A.1) can be inverted to represent x as a function of z.

The corresponding result is [7, 20.6, Example 2, p. 454]

$$x(z) = a + \frac{\sqrt{f(a)}\,\wp'[z] + \frac{1}{2}f'(a)\left[\wp(z) - \frac{1}{24}f''(a)\right] + \frac{1}{24}f(a)f'''(a)}{2\left[\wp(z) - \frac{1}{24}f''(a)\right]^2 - \frac{1}{48}f(a)f^{iv}(a)}. \tag{A.3}$$

Here, a is an arbitrary constant and $\wp(z) = \wp(z; g_2, g_3)$ is the Weierstrass elliptic function with invariants

$$\begin{aligned} g_2 &= a_0a_4 - 4a_1a_3 + 3a_2^2, \\ g_3 &= a_0a_2a_4 + 2a_1a_2a_3 - a_2^3 - a_0a_3^2 - a_1^2a_4. \end{aligned} \tag{A.4}$$

If a is a root of the polynomial $f(t)$, then (A.3) simplifies and reads

$$x(z) = a + \frac{f'(a)}{4\left[\wp(z) - \frac{1}{24}f''(a)\right]}. \tag{A.5}$$

Thus, when $a = X_{m,r}$ and $f = P[X_m]$, (A.5) leads to the expression (44) since $X_{m,r}$ is a zero of the polynomial $P[X_m]$, while the invariants (A.4) take the form (45).

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