

THERMODYNAMICS OF A PLANAR ARRAY OF GINZBURG-LANDAU
CHAINS WITH NEXT-NEAREST-NEIGHBOR INTERACTION

VICTOR BARSAN

Horia Hulubei National Institute for Physics and Nuclear Engineering,
Bucharest-Magurele, 077125, Romania

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Abstract. The thermodynamics of a planar array of Ginzburg-Landau chains with nn and nnn interaction is obtained analytically. The interaction term is treated exactly, while the quartic on-site potential is considered in a mean-field approximation. The free energy is expressed in terms of an Appell function. The specific heat can be calculated exactly, its singular term being proportional with the complete elliptic integral of first kind. It has a logarithmic singularity - the fingerprint of the Ising universality class. The equivalence of the ψ^4 models with Ising models is analyzed and its possible applications in microemulsions and adsorption of atoms on crystal surfaces are briefly discussed.

1. INTRODUCTION

The largest part of theoretical models used in solid state physics consider that the interaction of their constituents occurs only between nearest neighbors. The seminal paper of Montroll [1], where the transfer matrix concept was firstly introduced in physics, puts in a mathematical form the fact that, in a perfect crystal, the interaction is transferred from an atom to the next one (for an 1D system), from a row of atoms to the next one (for a 2D system), or from a plane to the next one (for a 3D system). The same concept was independently introduced by Kramers and Wannier [2, 3], and it was one of the ways of attack used by Onsager in order to find his celebrated solution of the Ising model [4].

With the renormalization group theory [5], it became largely accepted that, for the critical properties of a system, the inclusion of the more distant neighbors in the interaction potential is a "detail" which does not change its critical behavior [6]. However, for a more precise description of the thermodynamics of various solids and liquids, a more careful consideration of the inter-particle interaction could be essential.

This issue is more important for liquids, especially for liquid mixtures and microemulsions [7]; however, the model considered in the theory of microemulsions

is not a conventional liquid, but an Ising model, with next-nearest-neighbor (nnn) interaction. This model is not exactly soluble - like any model going beyond the variant worked out by Onsager - but some interesting results could be obtained [8, 9]. Interesting applications of Ising model in the study of phase diagram of binary and ternary solutions have been obtained by Lungu, Buzatu and coworkers [10, 11]. Due to the equivalence between Ising models and anisotropic ψ^4 models, at the level of the statistical sum [12], the results obtained for the ψ^4 models can be transferred to the Ising model, and vice-versa.

In this paper, we shall investigate the thermodynamics of ψ^4 models, namely of a planar array of Ginzburg-Landau chains, for the case of a nearest-neighbor (nn) and a next-nearest-neighbor (nnn) interaction. We shall consider the so-called pseudo-ferro-magnetic case, when the nn and nnn interaction are both attractive. The pseudo-anti-ferromagnetic case has been analyzed elsewhere [13]. We shall obtain an analytic result, which can be transferred to the Ising models. We shall evaluate the free energy of the planar arrays of Ginzburg-Landau chains using the transfer matrix method, *i.e.* calculating the ground state energy of a chain of quantum anharmonic oscillators; this is the dual of the classical 2D system. We shall use a Green function method, which has a simple form for bilinear Hamiltonians; the price paid for this is the fact that the anharmonicities of the on-site oscillator have to be treated in a mean field approximation. However, the interaction part is treated exactly. In this way, we obtain the free energy of the 2D system (the ψ^4 model) and its specific heat, which has a logarithmic singularity. This is the fingerprint of the Ising universality class, to which the ψ^4 model belongs. The equation for the critical temperature is also obtained. The relevance of this results for equivalent models, mainly for 2D Ising models, is discussed in detail.

2. THE PLANAR ARRAY OF CHAINS AND ITS DUAL

The system to be studied in this paper is a continuous variant of a model of a parallel array of chains of anharmonic classical oscillators. If $\psi_j(x)$ is the order parameter along the chain j , the Ginzburg-Landau functional of the model has the form

$$\mathcal{F}_{GL}[\psi] = \sum_{j=1}^N \int_0^L \frac{dx}{\xi_0} \times \left[a\psi_j^2 + b\psi_j^4 + c \left(\frac{d\psi_j}{dx} \right)^2 + c_1 (\psi_{j+1} - \psi_j)^2 + c_2 (\psi_{j+2} - \psi_j)^2 \right] \quad (1)$$

The field ψ_j is supposed to be real and to satisfy cyclic boundary conditions, $\psi_j(x) = \psi_{j+N}(x)$. The parameters a, b, c, ξ_0 have their usual significance, see for instance [14, 15] for details. The constants c_1, c_2 denote the nm and nmn interchain interaction, respectively.

Using the approach of Scalapino, Sears and Ferrell [16], we shall transform the classical statistical problem for (1) to a quantum mechanical problem of its dual system, a chain of quantum anharmonic oscillators, described by the Hamiltonian:

$$H = \sum_{j=1}^N \left[-\frac{1}{2m} \frac{\partial^2}{\partial \psi_j^2} + a\psi_j^2 + b\psi_j^4 + c_1(\psi_{j+1} - \psi_j)^2 + c_2(\psi_{j+2} - \psi_j)^2 \right] \quad (2)$$

The "mass" in (2) is temperature-dependent

$$m = \frac{2a'}{k_B^2 T^2}, \quad a' = a + c_1 + c_2 \quad (3)$$

As demonstrated in [16], the free energy of the 2D system of classical oscillators is equal to the ground state energy of the 1D system of quantum oscillators. Our immediate goal will be to evaluate this ground state energy, as a first step for obtaining the free energy of (1).

It is convenient to scale the Hamiltonian (2) to a simpler one

$$\begin{aligned} H_{nmn} &= \sum_{j=1}^N \left[-\frac{1}{2m} \frac{\partial^2}{\partial \psi_j^2} + a\psi_j^2 + b\psi_j^4 + c_1(\psi_{j+1} - \psi_j)^2 + c_2(\psi_{j+2} - \psi_j)^2 \right] \\ &= \sum_{j=1}^N \left[-\frac{1}{2m} \frac{\partial^2}{\partial \psi_j^2} + a_1\psi_j^2 + b\psi_j^4 - 2c_1\psi_j\psi_{j+1} - 2c_2\psi_j\psi_{j+2} \right], \end{aligned} \quad (4)$$

with

$$a_1 = a + c_1 + c_2. \quad (5)$$

We shall consider that the mass is temperature-dependent, that $a_1, c_1, c_2 > 0$. With a scaling given by

$$\psi_j = \alpha\varphi_j \quad (6)$$

and choosing

$$\alpha^2 = (2m|a_1|)^{-1/2}, \quad m\alpha^2 = \left(\frac{m}{2|a_1|} \right)^{1/2} \quad (7)$$

the Hamiltonian can be written as

$$H = \left(\frac{m}{2|a_1|} \right)^{1/2} \sum_{j=1}^N \left(-\frac{1}{2} \frac{\partial^2}{\partial \varphi_j^2} + \frac{1}{2} \sigma \varphi_j^2 + b_1 \varphi_j^4 - c'_1 \varphi_j \varphi_{j+1} - c'_2 \varphi_j \varphi_{j+2} \right), \quad (8)$$

where

$$\sigma = \text{sign}(a_1), \quad b_1 = \frac{b}{2^{3/2}m^{1/2}|a_1|^{3/2}}, \quad c'_1 = \frac{c_1}{|a_1|}, \quad c'_2 = \frac{c_2}{|a_1|}. \quad (9)$$

Splitting the scaled Hamiltonian into an on-site and an interacting term

$$H_\sigma = \sum_{j=1}^N \left(-\frac{1}{2} \frac{\partial^2}{\partial \varphi_j^2} + \frac{1}{2} \sigma \varphi_j^2 + b_1 \varphi_j^4 - c'_1 \varphi_j \varphi_{j+1} - c'_2 \varphi_j \varphi_{j+2} \right) \quad (10)$$

$$= H_{\sigma, \text{on site}} + H_{\sigma, \text{int}},$$

$$H_{\sigma, \text{on site}} = \sum_{j=1}^N \left(-\frac{1}{2} \frac{\partial^2}{\partial \varphi_j^2} + \frac{1}{2} \sigma \varphi_j^2 + b_1 \varphi_j^4 \right), \quad (11)$$

$$H_{\sigma, \text{int}} = - \sum_{j=1}^N (c'_1 \varphi_j \varphi_{j+1} + c'_2 \varphi_j \varphi_{j+2}) \quad (12)$$

and taking the Fourier transform of the interaction, according to the formulas

$$D_k = \sum_j D_{ij} e^{-ik(R_i - R_j)} = \sum_J D_J e^{-ikaJ} \quad (13)$$

$$D_J = -c'_1 (\delta_{J,1} + \delta_{J,-1}) - c'_2 (\delta_{J,2} + \delta_{J,-2}), \quad (14)$$

we get

$$D_k = -2c'_1 \cos ka - 2c'_2 \cos 2ka. \quad (15)$$

Replacing the anharmonic term in the on-site Hamiltonian by $x^2 \langle x^2 \rangle$, the full Hamiltonian is quadratic and we can use a Green function approach in order to calculate the ground state energy [17]:

$$\sum_k \sqrt{\Omega_0^2 + D_k} = \sum_k \sqrt{\Omega_0^2 - 2c'_1 \cos ka - 2c'_2 \cos 2ka}. \quad (16)$$

In the continuum limit, it is proportional to the integral:

$$I(A, B) = \int_0^\pi \sqrt{1 - A \cos x - B \cos 2x} dx, \quad (17)$$

with

$$A = \frac{2c'_1}{\Omega_0^2} > 0, \quad B = \frac{2c'_2}{\Omega_0^2} \geq 0. \quad (18)$$

The integrand

$$f(x) = 1 - A \cos x - B \cos 2x \quad (19)$$

can be written as

$$P(s) = -8Bs^2 + 2(A + 4B)s + 1 - A - B, \quad (20)$$

where

$$s = \sin^2 \frac{x}{2}. \quad (21)$$

It is easy to see that the radical is real if

$$-\sqrt{2} \leq A \leq \sqrt{2}; \quad -1 \leq B \leq 1. \quad (22)$$

We can write

$$P(s) = P(s) = 8B(s + |s_-|)(s_+ - s) > 0, \quad s_+ > 1, \quad B > 0, \quad (23)$$

where

$$s_{\pm} = \frac{(A + 4B) \pm \sqrt{8B + A^2 + 8B^2}}{8B}. \quad (24)$$

The integral is real for the "ferromagnetic" case, $B > 0$. Putting

$$s_+ = \frac{1}{k_1^2}, \quad |s_-| = \frac{1}{k_2^2}, \quad (25)$$

we have

$$P(s) = 8B \left(s + \frac{1}{k_2^2} \right) \left(\frac{1}{k_1^2} - s \right) = \frac{8B}{k_1^2 k_2^2} (1 - k_1^2 s) (1 + k_2^2 s) > 0. \quad (26)$$

We have to evaluate the integral

$$I(A, B) = \frac{2\sqrt{2B}}{k_1 k_2} \int_0^1 \sqrt{\frac{(1 - k_1^2 s)(1 + k_2^2 s)}{s(1 - s)}} ds \quad (27)$$

We shall adapt the formula

$$\int_0^1 x^{\lambda-1} (1 - x^{\mu-1}) (1 - ux)^{-\rho} (1 - vx)^{-\sigma} dx = \\ = B(\lambda, \mu) F_1(\lambda, \rho, \sigma, \lambda + \mu; u, v) \quad (28)$$

to our case

$$\lambda = \mu = \frac{1}{2}, \rho = -\frac{1}{2}, \sigma = -\frac{1}{2}, u = k_1^2, v = -k_2^2. \quad (29)$$

The result is

$$\int_0^1 \sqrt{\frac{(1 - k_1^2 s)(1 + k_2^2 s)}{s(1 - s)}} ds = \pi F_1 \left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 1; k_1^2, -k_2^2 \right), \quad (30)$$

where F_1 is the Appell function:

$$F_1(\lambda, \rho, \sigma, \lambda + \mu; u, v) = \sum_{m,n} \frac{(\lambda)_{m+n} (\rho)_m (\sigma)_n}{(\lambda + \mu)_{m+n} m! n!} x^m y^n. \quad (31)$$

Consequently,

$$I(A, B) = \frac{2\pi\sqrt{2B}}{k_1 k_2} F_1\left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 1; k_1^2, -k_2^2\right) \quad (32)$$

The Appell function can be reduced to a Gaussian hypergeometric function if:

$$\rho + \sigma = \lambda + \mu. \quad (33)$$

In our case,

$$\rho + \sigma = -1, \quad \lambda + \mu = 1, \quad (34)$$

so the sum $\rho + \sigma$ should increase with 2 in order to fulfill this condition.

Finally, we get for the ground state energy (GSE) of the Hamiltonian (2):

$$GSE = \frac{L}{2} \left(2m \frac{\Omega_0^2 (a + c_1 + c_2) - 2c_1 - 2c_2}{a + c_1 + c_2} \right)^{1/2} F_1\left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 1; k_1^2, -k_2^2\right), \quad (35)$$

$$s_+ = \frac{1}{k_1^2}, \quad |s_-| = \frac{1}{k_2^2}$$

supposing that the condition

$$a + c_1 + c_2 = a_1 > 0 \quad (36)$$

is fulfilled. The energy of the on-site Hamiltonian can be written in the harmonic approximation as [14]:

$$\Omega_0^2 = 1 + \frac{\lambda}{\omega(\lambda)}, \quad (37)$$

where $\omega(\lambda)$ is the real root of the following cubic equation:

$$\omega^3 - \sigma_a \omega - 6\lambda = 0. \quad (38)$$

3. THE SPECIFIC HEAT

As the specific heat is essentially the second derivative of the free energy F of the 2D system,

$$C = -T \frac{\partial^2 F}{\partial T^2}$$

and $F = GSE$, it can be calculated from the second derivatives of the Appell functions. Using the formula ([18], eq. 07.36.20.0009.01)

$$\frac{\partial^n}{\partial z_1^n} z_1^{n+b_1-1} F_1(a; b_1, b_2; c; z_1, z_2) = (b_1)_n z_1^{b_1-1} F_1(a; n+b_1, b_2; c; z_1, z_2) \quad (39)$$

and ([18], eq. 07.36.20.0010.01)

$$\frac{\partial^n}{\partial z_2^n} z_2^{n+b_2-1} F_1(a; b_1, b_2; c; z_1, z_2) = (b_2)_n z_2^{b_2-1} F_1(a; b_1, n+b_2; c; z_1, z_2) \quad (40)$$

for $n = 2$

$$\frac{\partial^2}{\partial z_1^2} z_1^{b_1+1} F_1(a; b_1, b_2; c; z_1, z_2) = b_1(b_1+1) z_1^{b_1-1} F_1(a; 2+b_1, b_2; c; z_1, z_2) \quad (41)$$

$$\frac{\partial^2}{\partial z_2^2} z_2^{b_2+1} F_1(a; b_1, b_2; c; z_1, z_2) = b_2(b_2+1) z_2^{b_2-1} F_1(a; b_1, 2+b_2; c; z_1, z_2) \quad (42)$$

and $a = \frac{1}{2}$; $b_1 = -\frac{1}{2}$, $b_2 = -\frac{1}{2}$; $c = 1$

$$\frac{\partial^2}{\partial z_1^2} z_1^{1/2} F_1\left(\frac{1}{2}; -\frac{1}{2}, -\frac{1}{2}; 1; z_1, z_2\right) = -\frac{z_1^{-3/2}}{4} F_1\left(\frac{1}{2}; \frac{3}{2}, -\frac{1}{2}; 1; z_1, z_2\right), \quad (43)$$

$$\frac{\partial^2}{\partial z_2^2} z_2^{1/2} F_1\left(\frac{1}{2}; -\frac{1}{2}, -\frac{1}{2}; 1; z_1, z_2\right) = -\frac{z_2^{-3/2}}{4} F_1\left(\frac{1}{2}; -\frac{1}{2}, \frac{3}{2}; 1; z_1, z_2\right), \quad (44)$$

we obtain two reducible F_1 functions ([18], eq. 07.36.03.0006.01)

$$F_1(a; b_1, b_2; b_1+b_2; z_1, z_2) = (1-z_2)^{-a} {}_2F_1\left(a, b_1; b_1+b_2; \frac{z_1-z_2}{1-z_2}\right) \quad (45)$$

or, for symmetry reasons, ([18], eq. 07.36.04.0004.01)

$$F_1(a; b_1, b_2; c; z_1, z_2) = F_1(a; b_2, b_1; c; z_2, z_1), \quad (46)$$

which leads to an equivalent formula

$$F_1(a; b_2, b_1; c; z_2, z_1) = (1-z_1)^{-a} {}_2F_1\left(a, b_2; b_1+b_2; \frac{z_2-z_1}{1-z_1}\right). \quad (47)$$

So

$$F_1\left(\frac{1}{2}; \frac{3}{2}, -\frac{1}{2}; 1; z_1, z_2\right) = (1-z_2)^{-1/2} {}_2F_1\left(\frac{1}{2}, \frac{3}{2}; 1; \frac{z_1-z_2}{1-z_2}\right) \quad (48)$$

and

$$F_1\left(\frac{1}{2}; -\frac{1}{2}, \frac{3}{2}; 1; z_1, z_2\right) = (1-z_2)^{-1/2} {}_2F_1\left(\frac{1}{2}; -\frac{1}{2}; 1; \frac{z_1-z_2}{1-z_2}\right). \quad (49)$$

Using again a symmetry property:

$$F_1\left(\frac{1}{2}; \frac{3}{2}, -\frac{1}{2}; 1; z_1, z_2\right) = F_1\left(\frac{1}{2}; -\frac{1}{2}, \frac{3}{2}; 1; z_2, z_1\right) \quad (50)$$

we can express the reduced form of F_1 in terms of ${}_2F_1\left(\frac{1}{2}; -\frac{1}{2}; 1; \frac{z_1-z_2}{1-z_2}\right)$ only. We have ([18], eq. 07.23.03.0112.01)

$${}_2F_1(a, 1-a; c; z) = (1-z)^{(c-1)/2} z^{-(c-1)/2} \Gamma(c) P_{-a}^{1-c}(1-2z). \quad (51)$$

For $a = 1/2$, $c = 1$, this gives

$${}_2F_1\left(\frac{1}{2}; -\frac{1}{2}; 1; z\right) = P_{-1/2}(1-2z) \quad (52)$$

In our notations,

$${}_2F_1\left(\frac{1}{2}; -\frac{1}{2}; 1; \frac{z_1 - z_2}{1 - z_2}\right) = P_{-1/2}\left(\frac{1 - 2z_1 + z_2}{1 - z_2}\right). \quad (53)$$

The Legendre function can be expressed in terms of the complete elliptic integral of first kind:

$$P_{-1/2}(x) = \frac{2}{\pi} \sqrt{\frac{2}{x+1}} K\left(\sqrt{\frac{x-1}{x+1}}\right), \quad (54)$$

which has a logarithmic singularity when its argument equals 1. This means that the specific heat has a logarithmic singularity at the transition point T_c , which can be determined from the equation

$$2z_1 - z_2 = 1. \quad (55)$$

Comparing the present case ($c_2 > 0$) with the pseudo-anti-ferromagnetic case ($c_2 < 0$), studied in [13], we can notice that the pseudo-ferromagnetic one is more complex mathematically, as, for $c_2 < 0$ the free energy is expressed in terms of complete elliptic integrals of first, second and third kind, which are much simpler than the Appell function.

4. THE 2D ISING MODEL WITH nmn INTERACTION

All the attempts of finding an exact solution of the Ising model beyond the limits of the Onsager variant have failed. Neither the introduction of an external field, nor a nmn interaction in the model could not be exactly described. However, interesting analytic results have been obtained by Fan and Wu [8], Grynberg and Tanatar [9], Lungu and Buzatu [10], [11]. The model has been investigated with Monte Carlo simulations by Aguilera-Granja *et al.* [19, 20] and Lee [21]. Finite-size effect have been evaluated by Zandvliet [22], in a controversial paper; see also [23]. Studying the adsorption of Hydrogen on Pd(100), Binder and Landau [24] considered a lattice gas and an Ising model with three-body interaction, nm repulsion and nmn interaction. Widom [7] used several variants of the Ising model in order to describe the behavior of microemulsions, one of the most investigated being the ANNNI (anisotropic next-nearest-neighbor Ising) model.

The equivalence, at the level of partition sums, between ψ^4 models and Ising models [12] can be used in order to transfer results from a class of models to another one. For a ψ^4 models with a quadratic term proportional to A , a quartic one proportional to B and an interaction term of the form

$$V_{int} = \sum_{l,m} c_{xy}^{(l,m)} u_x^{(l)} u_y^{(m)}, \quad (56)$$

where $u_\alpha^{(l)}$ means the displacement of an atom belonging to the l -th wire in the α direction, this equivalence means

$$\lim_{A \rightarrow \infty, A/B = -1} Z(\psi^4) = Z(\text{Ising}) = \sum_{\{\sigma_x^l\}} \sum_{\{\sigma_y^m\}} \exp\left(-\beta \sum_{l,m} c_{xy}^{(l,m)} \sigma_x^l \sigma_y^m\right), \sigma_{x,y}^m = \pm 1. \quad (57)$$

So, in this way, Ising models with arbitrary long interactions between spins are statistically equivalent with anharmonic solids with very deep on-site potentials. The consequences of this equivalence will be studied in a future work.

5. CONCLUSIONS

A planar array of Ginzburg-Landau chains with attractive nn and nnn interaction (the so-called pseudo-ferromagnetic case) has been studied using the transfer matrix method. The ground state energy of its dual system, an chain of quantum anharmonic oscillators interacting through elastic forces, has been evaluated using a Green function method. In order to avoid an infinite hierarchy of Green functions, the quartic term of the on-site Hamiltonian was treated in a mean field approximation. The ground state energy of the 1D system, and the free energy of the 2D one, have been obtained, in terms of an Appell function. The specific heat, which is mainly the second derivative of the Appell function, corresponds to a case when this function can be reduced to a Gaussian one, and, further one, to a complete elliptic integral of first kind. Its logarithmic singularity is the fingerprint of the Ising universality class, to whom the ψ^4 model belongs. This investigation completes the understanding of a 2D Ginzburg-Landau system with nnn interactions, as the present paper is devoted to the pseudo-ferromagnetic case, and the situation of the pseudo-anti-ferromagnetic case had been studied previously.

In fact, the Ising model is equivalent to ψ^4 models with very deep on-site two-well potentials, and this equivalence, which holds at the level of the statistical sums, can be exploited in order to transfer results from a model to another. Possible applications to the physics of microemulsions and adsorption of atoms on crystal surfaces are briefly discussed.

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