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Ginzburg–Landau theory beyond the linear-chain approximation: the 2D case

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Abstract

Within the Ginzburg–Landau theory applied to a planar array of chains, characterized by a real order parameter, the inter-chain fluctuations are taken into account exactly. So, the ‘linear chain approximation’ is replaced by a rigorous treatment. The single-chain problem is addressed taking advantage of a precise and simple non-perturbative solution of the Schrödinger equation for the anharmonic oscillator.

1. Introduction

The Ginzburg–Landau (GL) theory was initially proposed in the frame of superconductivity (for a modern discussion, see for instance [1]), but was subsequently applied to a huge variety of systems and phase transitions, from Peierls transitions in quasi-one-dimensional systems [2] to rheological properties of self-assembling fluids [3] or tweed-like stripe modulation in magnetic materials [4].

Following a simple phenomenological approach introduced by Landau (see for instance [5]), a free energy functional is constructed by expanding the free energy density in powers of the order parameter ψ and its spatial gradient. The order parameter is a field with n components. For $n = 1$, ψ is real, and the GL functional may describe a solid–solid structural transformation [6, 7], in particular a martensitic transformation [8], or the phases of complex fluids, like a ternary mixture of oil, water and amphiphile [9]. For $n = 2$, ψ is complex, describing superconductivity, superfluidity, metal–insulator transitions, etc. For $n = 3$, ψ may describe magnetic systems, etc.

As GL theory is mainly an approach to critical phenomena, its success depends essentially on how the fluctuations are taken into consideration. A mean-field treatment predicts incorrect results, like an unphysical phase transition in one-dimensional (1D) systems, or incorrect temperature dependence of the order parameter. However, the fluctuations can be properly treated by taking into account all order-parameter configurations with a weight given by the Boltzmann factor, $\exp\{-\beta\mathcal{F}[\psi]\}$. For example, the partition function is given by a functional integral of $\exp\{-\beta\mathcal{F}[\psi]\}$ over all possible $\psi(x)$.

The main technical problem of this approach is that the functional integrals could be very difficult to evaluate. One of the most successful mathematical treatments is the transfer matrix technique [10], that allows one to reduce the functional integral in n dimensions to a quantum mechanical problem in $n - 1$ dimensions. More exactly, this ‘quantum mechanical problem’ consists in the evaluation of the energy spectrum of a so-called ‘transfer matrix Hamiltonian’. For a 1D system, described by a ψ^4 functional (see below), the ‘matrix transfer Hamiltonian’ is a one-particle anharmonic (quartic) oscillator Hamiltonian.

So, the statistical mechanics of such a 1D system is described by the energy spectrum (mainly, by the ground state energy) of an anharmonic oscillator. The first to take advantage of this analogy and to use this fact in order to develop a detailed description of 1D systems were Scalapino *et al* [11]. Although the fluctuations are treated correctly, even in this 1D case, the final result is not ‘exact’ (as generally claimed), as long as the energy spectrum of the anharmonic oscillator cannot be obtained exactly.

The theory was extended to the study of quasi-1D materials (planar or spatial arrays of weakly coupled chains), within the so-called ‘linear chain approximation’. It treats the correlations along the chain exactly, while introducing inter-chain coupling via effective fields. This ‘linear chain approximation’ provided a method of incorporating the 3D effects in the ‘exact’ 1D solution. A necessary condition of its validity is the strong anisotropy of the system: the intra-chain interactions must be much larger than the inter-chain ones.

Let us outline the main results of this approach. Applying the Scalapino–Sears–Ferrell theory [11] to higher dimensions, Stoeckly and Scalapino [12] studied a planar array of weakly coupled chains. They reduced the functional integration to the evaluation of the energy spectrum (essentially, to the first two levels) of the transfer-matrix Hamiltonian, describing, in this case, a chain of weakly coupled anharmonic oscillators. This eigenvalue problem was solved in the case of strong anisotropy, associating with this Hamiltonian a fermionic bilinear Hamiltonian, that can be solved exactly. Similar systems—planar arrays of weakly coupled chains—were transformed, by similar methods and under similar assumptions, into a pseudo-spin Hamiltonian, or into an Ising chain in transverse field, by Dietrich [13] and Lajzerovicz and Pfeuty [14], respectively.

The 2D and 3D problems were also addressed by Scalapino *et al* [15]. Using a mean-field approximation, the coupled chain problem is reduced to that of a single chain in an effective field. The physical systems under examination were Ising, classical Heisenberg, real and complex ψ^4 chains. A quite similar extension of the description of 1D behaviour to very anisotropic 2D and 3D systems was given by Bishop and Krumhansl [6]. They restricted their work to the structural phase transitions, but also gave a detailed analysis of the ‘strong anisotropy’ approximation, called sometimes the ‘two-level approximation’.

More recently, McKenzie [16] re-examined some fundamental aspects of the GL theory in quasi-1D systems, for a complex order parameter. The author emphasizes that the accurate description of the commonly studied CDW materials cannot be achieved without an exact treatment of the inter-chain fluctuations (see conclusions, point (3)).

In spite of some differences existing between the results of the aforementioned theories for a real or complex order parameter ψ , it is clear that the weaknesses of all these approaches have two sources, at the ‘intra-chain’ and at the ‘extra-chain’ level. The ‘intra-chain’ errors are due to the lack of an exact solution of the ‘transfer matrix Hamiltonian’. In almost all interesting cases, it corresponds to a quartic anharmonic oscillator. The ‘inter-chain’ errors are due to a mean-field treatment of fluctuations. Smaller errors correspond to higher anisotropy.

In the present paper, we shall avoid these difficulties as follows. The ‘intra-chain errors’ can be minimized taking advantage of the significant progress in understanding the anharmonic oscillator, reflected in a vast literature produced after the publication of the main contributions

of Scalapino and his co-workers, just mentioned in the preceding paragraphs. In the last two decades, several precise (but however approximate) expressions for the ground state energy of the anharmonic oscillator have been proposed. Out of these, we have chosen in the present paper the Hsue–Chern approach, which is, at the same time, analytically simple and mathematically accurate. The ‘inter-chain errors’ will be eliminated using a Green’s function method, allowing an exact determination of the thermodynamic potentials. No anisotropy restriction is imposed.

In order to illustrate our approach as clearly as possible, we have chosen the simplest relevant physical system: a planar array of chains, characterized by a real order parameter. In this way, we have replaced the ‘linear chain approximation’ with an exact treatment. The errors in the solution of the 2D system are entirely produced by the approximate character of the anharmonic oscillator eigenvalues. These errors can be controlled and minimized. The paper is mainly intended to introduce a new method rather than to produce new results.

The outline of the paper is as follows. In section 2, we define the Ginzburg–Landau functional and briefly describe the transfer matrix method. The mean-field results of the GL theory are also mentioned. In section 3, we adapt to our problem an operator approach (due to Hsue and Chern) in order to study the anharmonic oscillator; in this way, a precise and analytically simple expression for the ground state energy is obtained. In section 4, these results are used to calculate the thermodynamics of the 1D chain. In section 5, the transfer matrix method is applied to a 2D system—a planar array of chains. The transfer matrix Hamiltonian obtained in this way describes a chain of coupled anharmonic oscillators. Its ground state energy is calculated exactly, using a Green’s function method, and the thermodynamics of the physical system can be obtained rigorously. The specific heat has a logarithmic singularity at the transition point, showing an Ising-like behaviour of the 2D system. The final section is devoted to conclusions and comments.

2. The Ginzburg–Landau functional and the transfer matrix equation

Let us consider a 1D system, characterized by a real order parameter $\psi(x)$. The simplest form of the GL functional (called sometimes the ψ^4 functional) is

$$F^{(1D)}[\psi] = \int_0^L \frac{dx}{\xi_0} \left[a\psi^2 + b\psi^4 + c \left(\frac{d\psi}{dx} \right)^2 \right]. \quad (1)$$

The only relevant temperature dependence is contained in the coefficient a :

$$a = a'(t - 1), \quad t = \frac{T}{T_c}, \quad a' > 0 \quad (2)$$

where the ‘mean field transition temperature’ T_c does not correspond to any real phase transition. The parameters b, c are positive, and $\xi_0 = \left(\frac{c}{a}\right)^{1/2}$ is a temperature-independent coherence length.

The expression of the coefficients a, b, c can be obtained from a microscopic analysis [17].

Let us recall the most important results of the mean field theory for the GL functional. If ψ is position independent, the minimum of $F^{(1D)}$ is achieved for

$$\psi_{\text{MF}} = \begin{cases} (-a/2b)^{1/2} = (a'/2b)^{1/2} \sqrt{1-t}, & t < 1 \\ 0, & t > 1. \end{cases} \quad (3)$$

So, the critical index of the order parameter has the value $\frac{1}{2}$. The free energy is

$$F^{(1D)} = \begin{cases} -\frac{a^2 L}{4b \xi_0} = \frac{a'}{4b \xi_0} (1-t)^2, & t < 1 \\ 0, & t > 1. \end{cases} \quad (4)$$

The specific heat has a jump

$$\Delta C_V = \frac{La'^2}{2\xi_0 b T_c}. \quad (5)$$

A fractional measure of the temperature width of the critical region is the parameter

$$\Delta t = 2 \left(\frac{b}{\beta_c a'^2} \right)^{2/3}, \quad \frac{1}{\beta_c} = k_B T_c. \quad (6)$$

The mean field solutions are only approximate, predicting, for instance, an incorrect $\psi(t)$ dependence. As Scalapino *et al* have shown [11], this difficulty is generated by the inappropriate treatment of fluctuations near T_c , rather than by the form of the functional (1), and can be overcome using a functional integral approach. According to [11], the thermodynamics of the system described by (1) is given by the partition function, evaluated as a path integral:

$$Z = \int e^{-\beta F^{(1D)}[\psi]} D\psi. \quad (7)$$

The transfer matrix theory allows one to write Z as

$$Z = \sum_n \exp\left(-\beta \frac{L}{\xi_0} \epsilon_n\right), \quad \beta = \frac{1}{k_B T} \quad (8)$$

where ϵ_n are the eigenvalues of the anharmonic oscillator Hamiltonian (1D transfer matrix Hamiltonian)

$$H_{\text{TM}}^{(1D)} = -\frac{1}{4} \frac{\xi_0^2}{\beta^2 c} \frac{\partial^2}{\partial \psi^2} + a\psi^2 + b\psi^4. \quad (9)$$

In the thermodynamic limit, only the smallest eigenvalue, $\epsilon_0^{(1D)}$, is important:

$$f^{(1D)} = -\frac{k_B T}{L} \ln Z = \frac{\epsilon_0^{(1D)}}{\xi_0}. \quad (10)$$

So, the thermodynamics of (1) can be easily evaluated, if we know the spectrum of the anharmonic oscillator (9).

3. The anharmonic oscillator: Hsue–Chern approach

The anharmonic oscillator is ‘a long standing difficult problem’ [18]. Understanding its properties is however vital to many physical domains, e.g. thermal expansion, phonon softening, field theory. The failure of the Rayleigh–Schrödinger (RS) perturbation method, demonstrated in the classical paper of Bender and Wu [19], pushed the development of more subtle approaches: path integral perturbation theory [20], supersymmetric quantum mechanics based methods [21], analytic methods generating exact solutions for specific potentials (quasi-exactly soluble systems) [22–25], the ‘two-step approach’ [26], etc.

The ‘two-step procedure’, proposed by Hsue and Chern [26], has the advantage of being, at the same time, simple and accurate. This approach offers a basis for the RS perturbation series, which is important, because the RS series for the energy of the anharmonic oscillator,

formed using the harmonic basis, is divergent. We shall outline here the Hsue–Chern method and we shall adapt it to our problem, (9).

Let us consider the Hamiltonian:

$$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \lambda x^4, \quad \lambda > 0. \quad (11)$$

In the second quantization language, it takes the form:

$$\mathcal{H} = \frac{1}{2} + \alpha^+\alpha + \frac{\lambda}{4}(\alpha + \alpha^+)^4. \quad (12)$$

If $|0\rangle$ is the ground state of (12), the state vector $|\Phi\rangle$ defined by

$$|\Phi\rangle = e^{\frac{\theta}{2}(\alpha^+)^2}|0\rangle \quad (13)$$

has the property

$$\alpha|\Phi\rangle = \theta\alpha^+|\Phi\rangle. \quad (14)$$

So, it is natural to define new boson operators, γ, γ^+ :

$$\gamma = \frac{\alpha - \theta\alpha^+}{\sqrt{1 - \theta^2}}, \quad (15)$$

which are annihilation and creation operators for the new vacuum $|\Phi\rangle$. The parameter θ is determined from the minimization of the ‘ground state’ energy, $\mathcal{E}_0(\theta)$:

$$\mathcal{E}_0(\theta) = \frac{\langle\Phi|\mathcal{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle}. \quad (16)$$

Reversing (15)

$$\alpha = \frac{\gamma + \theta\gamma^+}{\sqrt{1 - \theta^2}} \quad (17)$$

and using the identity [26]

$$(\gamma + \gamma^+)^4 = :(\gamma + \gamma^+)^4: + 6 :(\gamma + \gamma^+)^2: + 3$$

(the columns means normal ordering), the Hamiltonian (11) becomes

$$\begin{aligned} \mathcal{H} = \mathcal{E}_0 + & \left[\frac{\theta}{1 - \theta^2} + \frac{3\lambda}{2} \left(\frac{1 + \theta}{1 - \theta} \right)^2 \right] (\gamma^2 + (\gamma^+)^2) \\ & + \left[\frac{1 + \theta^2}{1 - \theta^2} + 3\lambda \left(\frac{1 + \theta}{1 - \theta} \right)^2 \right] \gamma^+\gamma + \frac{\lambda}{4} \left(\frac{1 + \theta}{1 - \theta} \right)^2 :(\gamma + \gamma^+)^4: . \end{aligned} \quad (18)$$

The ground state energy \mathcal{E}_0 of (18) can be written in the new variable

$$\omega = \frac{1 - \theta}{1 + \theta} \quad (19)$$

as

$$\mathcal{E}_0 = \frac{3\omega^2 + 1}{8\omega}, \quad (20)$$

ω being also the (only) real root of the equation:

$$-\omega^3 + \omega + 6\lambda = 0. \quad (21)$$

In order to adapt the HC method to the transfer matrix Hamiltonian (9), let us write it in a more suitable form:

$$H_{\text{TM}}^{(1D)} = \frac{\xi_0}{\beta_c} \sqrt{\frac{|a|}{c}} \mathcal{H}_{\text{TM}}^{(1D)} \quad (22)$$

where

$$\mathcal{H}_{\text{TM}}^{(1D)} = -\frac{1}{2} \frac{d^2}{d\varphi^2} - \frac{1}{2} \varepsilon \varphi^2 + \lambda \varphi^4 \quad (23)$$

and

$$\varepsilon = \text{sgn}(1 - t), \quad \lambda = \frac{b}{4\beta_c a^2} |t - 1|^{-3/2} \quad (24)$$

$\varepsilon = 1$ ($\varepsilon = -1$), or $t < 1$ ($t > 1$), corresponds to the subcritical (supercritical) regime. Following the Hsue–Chern approach, we get for the ground state energy of $\mathcal{H}_{\text{TM}}^{(1D)}$

$$\mathcal{E}_0 = \frac{3\omega^2 - \varepsilon}{8\omega} \quad (25)$$

with ω the real root of the equation:

$$-\omega^3 + \varepsilon\omega + 6\lambda = 0. \quad (26)$$

With (24)–(26), it is easy to obtain compact analytical formulae for thermodynamic quantities. As our interest is focused on the critical region, we shall give only the corresponding series expansions, near ‘the critical point’.

For the ground state of the Hamiltonians $\mathcal{H}_{\text{TM}}^{(1D)}$, (23), we get

$$\begin{aligned} \mathcal{E}_0^{TM} = \frac{(6\lambda)^{1/3}}{8} & \left\{ 3 - 2\varepsilon(6\lambda)^{-2/3} - \frac{1}{3}(6\lambda)^{-4/3} - \frac{2\varepsilon}{3^3}(6\lambda)^{-2} \right. \\ & \left. - \frac{1}{3^4}(6\lambda)^{-8/3} + \frac{2}{3^7}(6\lambda)^{-4} + \dots \right\} \end{aligned} \quad (27)$$

and for the ground state energy of (9)

$$\begin{aligned} \epsilon_0^{(1D)} = \frac{3}{8} \left(\frac{3}{2}\right)^{1/3} k_B T_c \left(\frac{\Delta t}{2}\right)^{1/2} & \left\{ 1 + \left(\frac{2}{3}\right)^{5/3} \tau - \frac{1}{3^2} \left(\frac{2}{3}\right)^{4/3} \tau^2 + \frac{1}{3^3} \left(\frac{2}{3}\right)^3 \tau^3 \right. \\ & \left. - \frac{1}{3^5} \left(\frac{2}{3}\right)^{8/3} \tau^4 + \frac{2^5}{3^{12}} \tau^6 + \dots \right\} \end{aligned} \quad (28)$$

where the ‘scaled temperature’ τ is

$$\tau = \frac{2(t - 1)}{\Delta t}. \quad (29)$$

This is the starting point in the study of the thermodynamic properties of the 1D system described by the GL functional (1). For the computation of some averages, for instance the mean value of the order parameter, an expression for $\epsilon_0^{(1D)}$ in which ξ_0 , a , b , c are independent parameters, is useful:

$$\begin{aligned} \epsilon_0^{(1D)} = \frac{1}{8} \frac{\xi_0}{\beta_c} (Ac)^{-1/2} \\ \times \left\{ 3 + 2Aa - \frac{1}{3}(Aa)^2 + \frac{2}{27}(Aa)^3 - \frac{1}{81}(Aa)^4 + \frac{2}{3^7}(Aa)^6 + \dots \right\}; \end{aligned} \quad (30)$$

$$A = \frac{2}{3} \frac{\beta_c c^{1/2}}{\xi_0 b}. \quad (31)$$

According to [26], this method allows the computation of the ground state energy with an error less than 2%, for any value of λ .

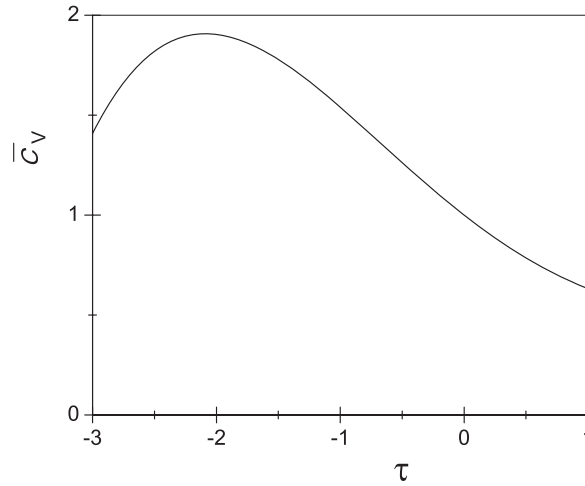


Figure 1. ‘Scaled specific heat’ \bar{c}_V , equation (35), as a function of the ‘scaled temperature’ τ .

4. The thermodynamic properties of the 1D system

As indicated in section 2, we can evaluate the free energy per unit length, $f^{(1D)} = \epsilon_0^{(1D)}/\xi_0$ (10), using expression (28) for the ground state energy $\epsilon_0^{(1D)}$. The specific heat of the length unit is

$$c_V = -T \frac{\partial^2 f}{\partial T^2} = -\left(\frac{2}{\Delta t}\right)^2 \frac{1}{\xi_0 T_c} \left(1 + \frac{1}{2} \tau \Delta t\right) \frac{d^2 \epsilon_0^{(1D)}}{d\tau^2}. \quad (32)$$

Using the jump of the specific heat (per length unit) predicted by the mean field theory (5),

$$\frac{\Delta C_V}{L} = \Delta c_V = \frac{k_B}{2\xi_0} \left(\frac{2}{\Delta t}\right)^{3/2} \quad (33)$$

we can define a ‘scaled specific heat’, \bar{c}_V ,

$$\bar{c}_V = 9 \frac{c_V}{\Delta c_V} \quad (34)$$

which retains only the relevant temperature dependence:

$$\bar{c}_V = \left(1 + \frac{1}{2} \tau \Delta t\right) \left\{ 1 - \frac{2^2}{3^2} \left(\frac{3}{2}\right)^{1/3} \tau + \frac{2^2}{3^3} \left(\frac{2}{3}\right)^{1/3} \tau^2 - \frac{2^4 \times 5}{3^8} \left(\frac{3}{2}\right)^{1/3} \tau^4 + \dots \right\}. \quad (35)$$

For small values of Δt ($\Delta t \lesssim 0.1$), equation (35) describes a peak of the specific heat (see figure 1). It is similar to the specific heat anomaly ([27] (figure 19)) observed in TTF-TCNQ or in other quasi-1D materials ([28] (figure 2)). In TTF-TCNQ, the anomaly is significant in a temperature range $\Delta T/T_c$ of about 0.1 [27]. A similar behaviour of the specific heat is predicted by molecular dynamics results [30].

For the expectation value of ψ^2 , we find, with (30),

$$\langle \psi^2 \rangle = \frac{\partial \epsilon_0^{(1D)}}{\partial a} = \frac{1}{4} \frac{\xi_0}{\beta_c} \sqrt{\frac{A}{c}} \times \left\{ 1 - \frac{1}{3} \left(\frac{2}{3}\right)^{2/3} \tau + \frac{2}{3^3} \left(\frac{2}{3}\right)^{1/3} \tau^2 - \frac{2^3}{3^6} \tau^3 + \frac{2^4}{3^9} \left(\frac{2}{3}\right)^{1/3} \tau^5 + \dots \right\}. \quad (36)$$

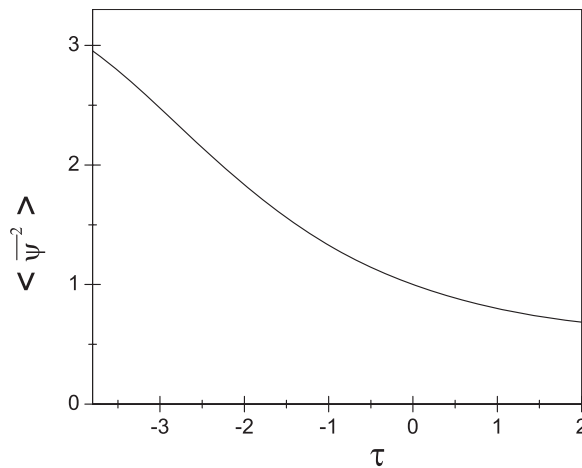


Figure 2. Expectation value of ‘scaled field’ intensity $\langle \bar{\psi}^2 \rangle$, equation (38), versus ‘scaled temperature’ τ .

We shall use the mean field value (3)

$$\langle \psi_{\text{MF}}^2 \rangle = \frac{a'}{2b} = \psi_{\text{MF}}^2(t=0)$$

in order to define a ‘scaled order parameter’ or ‘scaled field’ $\bar{\psi}$ through the relation

$$\langle \bar{\psi}^2 \rangle = \left(\frac{3}{2}\right)^{1/3} \frac{4}{\Delta t} \frac{\langle \psi^2 \rangle}{\langle \psi_{\text{MF}}^2 \rangle}. \quad (37)$$

We get for the expectation value of the scaled field intensity $\bar{\psi}^2$

$$\langle \bar{\psi}^2 \rangle = 1 - \frac{1}{3} \left(\frac{2}{3}\right)^{2/3} \tau + \frac{2}{3^3} \left(\frac{2}{3}\right)^{1/3} \tau^2 - \frac{2^3}{3^6} \tau^3 + \frac{2^4}{3^9} \left(\frac{2}{3}\right)^{1/3} \tau^5 + \dots \quad (38)$$

(see figure 2). Figure 2 is specially relevant for the phenomenon which is produced in a 1D material: instead of a neat phase transition, there is a smooth passage from a regime in which the order parameter is significantly nonzero and is growing with the lowering of temperature to a regime in which it is very small and becomes smaller for larger temperatures [11]. The agreement with the ‘exact results’ of Scalapino *et al* is very good (see [11] (figure 3); see also [29] (figure 3)). Of course, the results predicted by (35) and (38) cannot be taken into consideration too far away from the origin.

5. The coupled chain problem

The planar array of chains was studied by Lajzerowicz and Pfeuty [14], Dietrich [13], Stoeckly and Scalapino [12], and Scalapino *et al* [15], in the frame of the ‘linear chain approximation’, i.e. treating the inter-chain interaction in the mean-field approximation. Using molecular dynamics methods, Kerr and Bishop [30] studied a rectangular 2D lattice with interparticle interactions that are very different in strength along the two lattice directions; it may describe a system of weakly coupled chains with strong interaction within each chain. It is, also, a 2D, one-component order parameter model. All such models are in the same universality class (Ising) and have the same critical exponents, independent of anisotropy. In this section, we shall give an exact solution for the 2D coupled chain problem.

We shall study here the coupled chain problem using the GL theory. Let us consider a planar array of chains of length L , each of them characterized by a real order parameter $\psi_j(x)$, $j = 1, \dots, N$, and by a free energy functional given by (1). The free energy of the whole system is

$$F^{(2D)}[\psi] = \sum_{j=1}^N \int_0^L \frac{dx}{\xi_0} \left\{ a\psi_j^2 + b\psi_j^4 + c \left(\frac{d\psi_j}{dx} \right)^2 + c_{\perp}(\psi_{j+1} - \psi_j)^2 \right\} \quad (39)$$

where cyclic boundary conditions have been imposed:

$$\psi_{N+1} = \psi_1. \quad (40)$$

In general, one considers that the coupling between chains is small,

$$c_{\perp} \ll \frac{c}{\xi_0^2} \quad (41)$$

with ξ_0 as before. The coefficients a, b, c have the same significance as in section 2. With the transfer matrix method, one obtains the following associated Hamiltonian:

$$H_{\text{TM}}^{(2D)} = \sum_{j=1}^N \left\{ -\frac{1}{2m} \frac{\partial^2}{\partial \psi_j^2} + a\psi_j^2 + b\psi_j^4 + c_{\perp}(\psi_{j+1} - \psi_j)^2 \right\} \quad (42)$$

where

$$m = \frac{2\beta^2 c}{\xi_0^2}. \quad (43)$$

In the thermodynamic limit, the free energy per unit length of the coupled chains is, essentially, the ground state energy of the transfer Hamiltonian $H_{\text{TM}}^{(2D)}$, (42):

$$f^{(2D)} = \frac{\epsilon_0^{(2D)}}{\xi_0}. \quad (44)$$

So, the 2D statistical mechanics problem is reduced to a 1D quantum mechanics problem of N coupled anharmonic oscillators. By finding its ground state energy, we shall give, at the same time, a rigorous derivation of the free energy of the coupled chain problem, for a real order parameter, without any use of a restriction like (41).

Let us remark that (42) can be written as

$$H_{\text{TM}}^{(2D)} = \left(\frac{2\bar{a}}{m} \right)^{1/2} \mathcal{H}_{\text{TM}}^{(2D)} \quad (45)$$

where

$$\mathcal{H}_{\text{TM}}^{(2D)} = \sum_{j=1}^N \left\{ -\frac{1}{2} \frac{\partial^2}{\partial \varphi_j^2} + \frac{1}{2} \varphi_j^2 + \lambda \varphi_j^4 - \mu \varphi_{j+1} \varphi_j \right\} \quad (46)$$

with

$$\bar{a} = a'(t-1) + 2c_{\perp}, \quad \lambda = \frac{mb}{(2m\bar{a})^{3/2}}, \quad \mu = \frac{2c_{\perp}}{\bar{a}}. \quad (47)$$

Because we are not only interested in the regime $t \sim 1$, we shall maintain the temperature dependence of the ‘mass’ (43).

We shall compute the ground state energy of $\mathcal{H}_{\text{TM}}^{(2D)}$, (46), following closely a Green’s function approach described in [31]. Let

$$G_{ij}(\xi, t) = -i \langle T \tilde{\varphi}_i(\xi, t) \tilde{\varphi}_j(\xi, 0) \rangle \quad (48)$$

where

$$\tilde{\varphi}_i(\xi, t) = e^{iH_\xi t} \varphi_i e^{-iH_\xi t} \quad (49)$$

$$H_\xi = H_0 + \xi H_{\text{int}} \quad (50)$$

$$H_0 = \sum_{j=1}^N \left\{ -\frac{1}{2} \frac{\partial^2}{\partial \varphi_j^2} + \frac{1}{2} \varphi_j^2 + \lambda \varphi_j^4 \right\} \quad (51)$$

$$H_{\text{int}} = \frac{1}{2} \sum D_{ij} \varphi_i \varphi_j \quad (52)$$

$$D_{ij} = -\mu(\delta_{i,j+1} + \delta_{i,j-1}). \quad (53)$$

The shift of the ground state energy of H_ξ , (50), compared to the $c_\perp = 0$ case, is ([31] (equation (1.4.10)))

$$\Delta E_G = \lim_{t \rightarrow 0^+} \frac{i}{2} \sum_{i=j} D_{ij} \int_0^1 d\xi G_{ij}(\xi, t). \quad (54)$$

$G_{ij}(\xi, t)$ may be evaluated using the Dyson equation:

$$\begin{aligned} G_{ij}(\xi, t) &= G_0(t) \delta_{ij} + \int_{-\infty}^{\infty} dt' G_0(t-t') \sum_l \xi D_{il} G_{lj}(\xi, t') \\ &= G_0(t) \delta_{ij} + \xi \int_{-\infty}^{\infty} dt' G_0(t-t') D_{ij} G_0(t') \\ &\quad + \xi^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dt' dt'' \sum_{i'} G_0(t-t') D_{i'i'} G_0(t'-t'') D_{i'j} G_0(t'') + \dots \end{aligned} \quad (55)$$

It is convenient to introduce the time Fourier transform of the Green's function $G(t)$ (the indices, as well as the ξ dependence, will be dropped out, as irrelevant for these definitions):

$$G(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} G(\omega) e^{-i\omega t} d\omega, \quad G(\omega) = \int_{-\infty}^{+\infty} G(t) e^{i\omega t} d\omega. \quad (56)$$

In terms of $G(\omega)$, the series (55) becomes

$$G_{ij}(\xi, \omega) = G_0(\omega) \delta_{ij} + \xi \sum_l D_{il} G_{lj}(\xi, \omega) \quad (57)$$

$$= G_0(\omega) \delta_{ij} + \xi [G_0(\omega)]^2 D_{ij} + \xi^2 [G_0(\omega)]^3 \sum_k D_{ik} D_{kj} + \dots \quad (58)$$

Taking advantage of the translational invariance, assured by the cyclic boundary conditions, we Fourier transform again $G(\omega)$, in the reciprocal lattice space:

$$G_{ij}(\omega) = \frac{1}{N} \sum_k G_k(\omega) e^{ik(R_i - R_j)}, \quad G_k(\omega) = \sum_i G_{ij}(\omega) e^{-ik(R_i - R_j)}. \quad (59)$$

We have a similar relation for D :

$$D_k = \sum_j D_{ij} e^{-ik(R_i - R_j)}, \quad D_{ij} = \sum_k D_k e^{ik(R_i - R_j)}. \quad (60)$$

Finally, the Dyson equation (55), written in terms of $G_k(\omega)$, becomes a geometric series, with the sum

$$G_k(\xi, \omega) = \frac{G_0(\omega)}{1 - \xi G_0(\omega) D_k} = \frac{1}{G_0(\omega)^{-1} - \xi D_k} \quad (61)$$

where the ξ -dependence of the Green's function has been explicitly reintroduced. Taking into consideration the definition (53), the specific form of D_k is

$$D_k = -2\mu \cos kd \quad (62)$$

with d the lattice constant. We have ([31] ((1.6.9)))

$$G_0(\omega)^{-1} = \omega^2 - \Omega_0^2 + i\eta, \quad \eta > 0 \quad (63)$$

with Ω_0 the ground state energy of the single anharmonic oscillator. So, with (61), we obtain

$$G_k(\xi, \omega) = [G_0(\omega) - \xi D_k]^{-1} = (\omega^2 - \Omega_k^2 + i\eta)^{-1} \quad (64)$$

with the definition

$$\Omega_k^2 = \Omega_0^2 - 2\xi\mu \cos kd. \quad (65)$$

Also ([31] ((1.6.11))),

$$G_k(\xi, t) = -\frac{i}{2\Omega_k} e^{-i\Omega_k|t|}. \quad (66)$$

Finally, (54) becomes

$$\Delta E_G = \frac{1}{4} \int_0^1 d\xi \sum_k \frac{D_k}{\Omega_k} = \frac{1}{2} \sum_k \left(\sqrt{\Omega_0^2 + D_k} - \Omega_0 \right) \quad (67)$$

and the ground state energy of (46) is

$$E_G = \frac{1}{2} \sum_k \Omega_k = \frac{N}{2\pi} \int_0^\pi \sqrt{\Omega_0^2 - 2\mu \cos x} dx. \quad (68)$$

The integral in (68) is proportional to the complete elliptic integral of second kind [32], so

$$E_G = \frac{N}{\pi} (\Omega_0^2 + 2\mu)^{1/2} \mathbf{E} \left(2 \left(\frac{\mu}{\Omega_0^2 + 2\mu} \right)^{1/2} \right). \quad (69)$$

The free energy per unit length of the coupled chain system is

$$f^{(2D)} = \frac{1}{\beta} \left(\frac{\bar{a}}{c} \right)^{1/2} \frac{N}{\pi} (\Omega_0^2 + 2\mu)^{1/2} \mathbf{E} \left(2 \left(\frac{\mu}{\Omega_0^2 + 2\mu} \right)^{1/2} \right). \quad (70)$$

This is an exact formula. From here we can obtain the specific heat and the averages of ψ^2 and ψ^4 . The specific heat is proportional to the second derivative of $\mathbf{E}(r)$, which has a logarithmic singularity for $r = 1$. This condition means

$$\Omega_0^2 = 2\mu = \frac{2c_\perp}{a'(t-1) + 4c_\perp}. \quad (71)$$

The equation (71) determines the critical temperature of the transition. This behaviour of the specific heat (logarithmic singularity) confirms the inclusion of the system (planar array of chains) in the Ising universality class. This result was firstly obtained by Lajzerovicz and Pfeuty [14]. It was also supported by numerical calculations by Stoeckly [33].

For explicit calculations, the expression of Ω_0^2 is needed. Considering, in the first approximation, according to (27), that

$$\Omega_0 \simeq \frac{3}{8} (6\lambda)^{1/3} = \frac{3}{8} \frac{(6mb)^{1/3}}{(2m\bar{a})^{1/2}} \quad (72)$$

equation (71) can be written as

$$f(t) \equiv \frac{a'(t-1) + 4c_\perp}{a'(t-1) + 2c_\perp} = B \frac{c_\perp}{t^{2/3}}, \quad B = \text{constant}. \quad (73)$$

The left-hand side of (73) is a monotonically and slowly decreasing function of t , which takes the value 2 for $t = 1$; the rhs is a quickly decreasing function of t , which, at $t = 1$,

takes the value Bc_{\perp} ; as c_{\perp} is a ‘small parameter’, we can presume $Bc_{\perp} < 1$. Their crossing determines the critical temperature t_c ; it is smaller than unity and decreases with the interchain coupling.

In order to be more specific, let us introduce an ‘anisotropy factor’ n , and put, instead of (41),

$$c_{\perp} = \frac{1}{n} \frac{c}{\xi_0^2} = \frac{a'}{n}. \quad (74)$$

Equation (73) takes the form

$$0.092 \left(\frac{b}{\beta a'^2} \right)^{2/3} = \frac{1}{n} \frac{t - 1 + \frac{2}{n}}{t - 1 + \frac{4}{n}}. \quad (75)$$

In order to get a numerical value, we have to replace the Ginzburg–Landau parameters in (75) for a specific substance. ‘The derivation of these coefficients is a subtle matter’ [16], and their values should be considered mainly estimations, not exact results. We shall use the estimation of Lee *et al* [45] for TTF-TCNQ. According to equation (3) of [45],

$$a' = D_0, \quad b = D_0 b_1 \quad \text{for } t \simeq 1 \quad (76)$$

with D_0 the electronic density of states. Reference [45] uses the values

$$\frac{D_0}{kT_c} = \frac{5}{2} \frac{\pi}{\sin 0.15\pi} \simeq 5.8 \times 10^{-2}; \quad b_1 = \frac{7\zeta(3)}{16\pi^2} \simeq 5.3 \times 10^{-2} \quad (77)$$

with which (75) becomes

$$\frac{t - 1 + \frac{4}{n}}{t - 1 + \frac{2}{n}} = \frac{500}{n} t^{-2/3}. \quad (78)$$

For $n = 10$, $t = 0.8$; for $n = 5$, $t = 0.6$. For a 3D TTF-TCNQ sample, [45] gives $T_c^{(3D)} \simeq \frac{1}{4}T_c$. (Similar estimations give $T_c^{(3D)} \simeq \frac{1}{3}T_c$ for KCP— [2] (p 647).) Two dimensional TTF-TCNQ samples have not been manufactured, so we do not have experimental data for a planar array of TTF-TCNQ chains, but clearly the effect of the 2D ordering should be weaker than in the 3D case, so a value of $t = 0.6, \dots, 0.8$ for an anisotropy factor $n = 5, \dots, 10$ seems reasonable.

6. Conclusions and comments

In this paper we have applied the Ginzburg–Landau theory to low dimensional (1D and 2D) systems, taking into account the fluctuations exactly. No anisotropy condition, like (71), has been used. In this way, our approach goes beyond the ‘single chain approximation’, currently used in the literature, where the inter-chain fluctuations are treated within the mean field method. This is the main contribution of our work. Accurate analytic expressions for the thermodynamic functions describing the 1D and 2D systems have been calculated. The approximative character of these expressions is entirely due to the approximative character of the solutions of the Schrödinger equations for the anharmonic oscillator. The specific ansatz used in this paper (Hsue–Chern approach) is just an option, used in order to illustrate how the method works. More accurate (or even exact) solutions will produce more accurate (or even exact) results.

The present work can be easily improved at least in two directions: to replace the Hsue–Chern solution with a more accurate one; and to apply the method to a system described by a complex order parameter.

As already stated, the use of the Hsue–Chern solution for the anharmonic oscillator is just an option, motivated by the accuracy of this simple approximation. There is, however, a number of improved versions of the Hsue–Chern approach [34–36]. But there are also some even more powerful methods, developed in recent years.

Turbiner [37] proposed an extremely fast convergent perturbation theory for the quartic anharmonic oscillator and the double-well potential. Other interesting approaches (alternative approximation methods) have been proposed in [18] and [38]. The development of non-perturbative approaches led to several quasi-exactly solvable models [39, 40]. All these results could improve the solution of our transfer matrix Hamiltonian for a single chain with real order parameter.

For the complex order parameter case, the transfer matrix Hamiltonian corresponds to a 2D isotropic anharmonic oscillator, which can be transformed into a Schrödinger equation with centrifugal term and quartic potential [11, 16]. Its eigenvalues can be evaluated using the results of Seetharaman and Vasani [41] and [42, 43]. Quasi-exactly solvable models for this potential have been proposed by Znojil [44]. These results can be used to obtain accurate results for 1D systems described by complex fields.

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