

**Phase transitions in low dimensional  $\psi^4$  systems**

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# Phase transitions in low dimensional $\psi^4$ systems

Victor Bârsan

Department of Theoretical Physics, NIPNE (IFIN)  
Str. Atomistilor no.407, Bucharest-Magurele, Romania

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## Abstract

The phase transition in a planar array of weakly coupled Ginzburg-Landau chains with real order parameter is studied, using an original variant of the two level approximation. The results are extended to the quantum phase transition in a chain of quantum double well oscillators, coupled with an elastic interaction, using the matrix transfer method.

## 1 Introduction

The 1D discrete  $\psi^4$  model and its continuum limit, the  $\psi^4$  quantum field theory, have been widely investigated in many areas of physics, from elementary particles to solid state theory [1]. For the solid state physicist, the discrete  $\psi^4$  chain is important to the study of the dynamics of uniaxial ferroelectrics and hydrogen-bonded materials, to soliton excitations in trans-polyacetylene, etc.

The  $\psi^4$  Ginzburg-Landau functional is a central issue in almost all branches of condensed matter physics. In this paper, we shall restrict our investigation to 1D and 2D Ginzburg-Landau functionals, with real order parameter. They can describe quasi-1D materials or ultra-thin films deposited on crystal surfaces [2].

There is a deep connection between the 1D quantum discrete  $\psi^4$  chains and the system described by 2D  $\psi^4$  Ginzburg-Landau functionals. This connection is a consequence of a general theorem of statistical physics, asserting that a classical statistical mechanical system in  $D + 1$  dimensions is equivalent to a quantum mechanical system in  $D$  dimensions. The equivalence between the  $D+1$ -dimensional classical statistical mechanics system and the  $D$ -dimensional quantum mechanical system is assured by a "transfer matrix". We shall call the systems connected by a transfer matrix transformation, *dual* systems. The transfer matrix was firstly used in the early '40s, applied to the 2D Ising model by Schultz, Mattis and Lieb [3] and put in a form suitable for our discussion by Scalapino, Sears and Ferrell [4]. Scalapino and his co-workers showed [4] that the dual of a classical 1D statistical system, described by a  $\psi^4$  Ginzburg-Landau functional

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

is a zero-dimensional quantum mechanical system, namely a quantum anharmonic (quartic) oscillator, described by the Hamiltonian:

$$H = -\frac{1}{2m} \frac{d^2}{dx^2} + ax^2 + bx^4 \quad (2)$$

The meaning of the parameters  $\xi_0, a, b, c, m$  will be explained later on. The main point of [4] is that the free energy per unit length of the classical 1D system,  $f$  (not to be confused to the Ginzburg-Landau functional  $F^{(1D)}$ ) is proportional to the ground state energy  $\mathcal{E}_0$  of the quantum (zero-dimensional) system (2):

$$f = \frac{\mathcal{E}_0}{\xi_0} \quad (3)$$

Due to the connection between the partition function of (1), written as a functional integral over the fields  $\psi(x)$ ,

$$Z = \int \mathcal{D}\psi e^{-\beta F[\psi]} \quad (4)$$

and the free energy

$$f = -\frac{k_B T}{L} \ln Z \quad (5)$$

the equation (3) allows us to express thermodynamical quantities characterizing the statistical system (1) in terms of the solution of the quantum mechanical problem (2). For instance, the expectation value of the field intensity can be written as:

$$\langle \psi^2 \rangle = \frac{\partial \mathcal{E}_0}{\partial a} \quad (6)$$

One of the salient points of [4] is just the fact that the statistical physics of the 1D system can be obtained solving the quantum mechanical problem of its dual system, the quartic oscillator.

Stoeckly and Scalapino [5] extended the approach of [4] to a 2D generalization of (1), namely to a planar array of weakly coupled  $\psi^4$  Ginzburg-Landau chains, described by the functional:

$$F^{(2D)}[\psi] = \sum_{j=1}^N \int_0^L \frac{dx}{\xi_0} \left[ a\psi_j^2 + b\psi_j^4 + c \left( \frac{d\psi_j}{dx} \right)^2 + c_y (\psi_{j+1} - \psi_j)^2 \right] \quad (7)$$

where  $\psi_j(x)$  is the (real) order parameter on the chain  $j$ ;  $a, b, c, \xi_0$  are Ginzburg-Landau parameters; for a more detailed discussion, see for instance [6]. The

dual of this 2D statistical system is a 1D quantum system, namely a chain of anharmonic oscillators:

$$H = \sum_{j=1}^N \left[ -\frac{1}{2m} \frac{d^2}{dx_j^2} + ax_j^2 + bx_j^4 + c_y (x_{j+1} - x_j)^2 \right] \quad (8)$$

Stoekly and Scalapino [5] calculated the ground state energy of (8) using the so-called "two level approximation", valid when the first two energy levels of the single oscillator (2),  $\mathcal{E}_0$  and  $\mathcal{E}_1$ , are close each other, and the third one,  $\mathcal{E}_2$ , is much larger. In this way, they obtained the thermodynamics of (7), using formulae similar to (3) - (5), and found that the system exhibits a phase transition. The critical equation of this phase transition, giving the transition temperature in terms of the model parameters, is:

$$\mathcal{E}_1 - \mathcal{E}_0 = \frac{4c_y}{k_B T} \frac{\partial \mathcal{E}_0}{\partial a} \quad (9)$$

So, the transition temperature of the 2D system is determined in terms of quantities describing the 1D system (and, of course, the inter-chain coupling,  $c_y$ ).

The same critical equation (9) can be used to describe a quantum phase transition in (8), but Stoekly and Scalapino [5] did not discuss this issue.

Another advantage of the Stoekly-Scalapino approach is the fact that the "two level approximation" used by them consists in the replacement of the Hamiltonian (8) with a very simple effective one, which is a 1D Hamiltonian, bilinear in on-site fermionic operators; it can be easily diagonalized. Other authors who applied the "two level approximation" in similar investigations [7], [8], [9], [10], [1] [11] used, as effective Hamiltonian, a transverse Ising model, which is much more complicated (see for instance the monograph [12])

However, a disadvantage of the Stoekly-Scalapino approach - at least, of the variant described in their original paper [5] - is the fact that their results, expressed in terms of quantities characterizing the quartic oscillator, cannot be put in an analytical form, as functions of the parameters of the system,  $a, b, c$ , etc. They are "exact", as the authors claim, only in the sense that the precision of the numerical evaluation can be very high.

The dual of a statistical system is not just an auxiliary tool to study this system: it also presents interest in itself. As already mentioned, the chain of anharmonic quartic oscillators (8) is relevant for the physics of uniaxial ferroelectrics, of hydrogen-bonded polymers, etc. It provides a phenomenological description of the low-temperature properties of glassy materials (see references 1 and 2 in [11]). Recently, this system was studied via Monte Carlo simulations [13]. The approach of [13] was opposite to that used by Scalapino and his co-workers: the classical 2D system was studied with numerical methods, and the results were applied, via the transfer matrix method, to the 1D quantum system.

In order to avoid any confusions while toggling between statistical and quantum mechanical systems, let us make the following remark. When it is con-

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sidered the dual of a statistical system, the quantum oscillator(s) will have a temperature-dependent "mass" (see eq. (2) and (8)). However, we must keep in mind that the quantum mechanical problem is solved "at zero temperature", and the temperature dependence of the mass, coupling constant, energy levels etc. is just a parametric dependence, without any direct physical significance. The temperature keeps its genuine meaning only when we discuss the statistical systems.

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If the 2D statistical system exhibits an ordinary phase transition, its 1D quantum dual exhibits a quantum phase transition. This means that the properties of the ground state changes qualitatively, when the parameters  $a, b, c_y, m$  change "critically". This phase transition occurs at  $T = 0$ , due to the quantum fluctuations, which - unlike the thermal ones - are present at absolute zero too. They can restore a broken symmetry, which, in this case, is the  $x \rightarrow -x$  symmetry of the quartic potential. Classically, the on-site potential in (8) is, for  $a < 0$ , a two-well potential, with the particle at the bottom of one well or another. In the quantum ground state, the quantum fluctuations assure the tunneling between wells and restore the classically broken symmetry.

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As already mentioned, the chain of anharmonic oscillators (8) was studied with numerical methods [1], [13] [14], [15] and with analytical approximations [1]. Surprisingly enough, the fact that (8) is the dual of a 2D Ginzburg-Landau  $\psi^4$  system, for which a simple and elegant approach was proposed by Stoeckly and Scalapino [5] quite long time ago, remained unnoticed. In particular, the Stoeckly-Scalapino critical condition was never used to the study of the quantum phase transition in (8). As a general remark, we can mention that the analytical results were obtained mainly in older papers; the more recent ones are devoted, in general, to numerical investigations.

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**The contribution of the present paper to the study of the above topics consists of three steps.** *Firstly*, we shall adapt to the problem (2) the Hsue-Chern approach of the quartic oscillator. This approach allows us to obtain simple and accurate analytical expressions for the energy of the anharmonic oscillator. The benefit is that we can express the numerical results of Scalapino, Sears and Ferrell [4] in analytic form. *Secondly*, we shall use these results in order to obtain the thermodynamics of the 2D system. We shall determine the critical temperature in terms of the inter-chain coupling and **shall calculate** the average of the field intensity; this quantity is non-zero in the low-temperature phase and vanishes at the transition point. We shall study also the validity of the two-level approximation. *Thirdly*, taking advantage of the fact that the quantum  $\psi^4$  chain is dual to planar array of  $\psi^4$  Ginzburg-Landau chains, we shall apply the Stoeckly-Scalapino critical condition in order to obtain the phase diagram of the quantum phase transition. The agreement with the numerical results, obtained previously, is very good.

## 2 Hsue-Chern approach to the quartic anharmonic oscillator

We shall re-write the equation (2) in the form:

$$H = -\frac{1}{4} \frac{\xi_0^2}{\beta^2 c} \frac{d^2}{dx^2} + ax^2 + bx^4, \quad \frac{1}{\beta} = k_B T \quad (10)$$

where, out of the coefficients  $a, b, c$ , only  $a$  depends on temperature:

$$a = a'(t-1), \quad a' > 0, \quad t = \frac{T}{T_{MF}} \quad (11)$$

where  $T_{MF}$  is the "mean-field transition temperature", a parameter which, in fact, does not corresponds to any physical phase transition.  $\xi_0$  plays the role of a natural length unit, being defined as

$$\xi_0^2 = \frac{c}{a'} \quad (12)$$

Whith this convention, the inspection of (3) assures us that the coefficients  $a$  and  $b$  have dimensions of energy, assuming that the real field  $\psi(x)$  is dimensionless. However, the presence of  $\xi_0$  in (1) or (10) is mainly a question of convenience; in some cases, it will be preferable to take  $\xi_0 = 1$ ; with such a choice, the significance of parameters  $a, b, c$  will be slightly modified.

After a change of function, we can introduce the "reduced" Hamiltonian  $\mathcal{H}_\sigma$ ,

$$H = \frac{\xi_0}{\beta} \sqrt{\frac{|a|}{c}} \mathcal{H}_\sigma \quad (13)$$

where

$$\mathcal{H}_\sigma = -\frac{1}{2} \frac{d^2}{d\varphi^2} + \frac{1}{2} \sigma_a \varphi^2 + \lambda \varphi^4, \quad \sigma_a = \text{sgn } a = \text{sgn } (t-1) \quad (14)$$

The reduced Hamiltonian depends (besides a signum function) on one parameter only:

$$\lambda = \frac{b\xi_0}{4\beta} c^{-1/2} |a|^{-3/2} \quad (15)$$

or, equivalently,

$$\lambda = \frac{1}{4} \left( \frac{\Delta t}{2} \right)^{3/2} \frac{t}{|1-t|^{3/2}} \quad (16)$$

where

$$\frac{\Delta t}{2} = \left( \frac{b}{a'^2} k_B T_{MF} \right)^{2/3} = \left( \frac{b}{a'^2} \epsilon_{MF} \right)^{2/3}, \quad \epsilon_{MF} = k_B T_{MF} \quad (17)$$

The quantity  $\Delta t$  "measures the size of temperature region below  $T_c$  in which the thermal energy  $k_B T_{MF}$  is sufficient to drive the order parameter to zero over the mean-field coherence length" [4]. An almost identical quantity ( $\kappa$ ) is introduced by McKenzie ([16], eq. (7)) in the context of Ginzburg-Landau theory with a complex order parameter, with the remark that "most of physics" is determined by it.

As we shall immediately see, in some cases we must consider  $a$  as a simple, "structureless" parameter; in others, it will be considered a function of temperature, according to (11).

Our problem is the determination of the ground state energy of the reduced Hamiltonian (14). In the "sub-critical" regime (**the use of quotation marks is intended to remind that at  $t = 1$  no phase transition takes place in the 1D system described by (1)**),  $\sigma_a = -1$ ,  $t < 1$  and  $\mathcal{H}_\sigma$  describes a particle in a two-well potential:

$$\mathcal{H}_\sigma (\sigma = -1) = H_{2w} = -\frac{1}{2} \frac{d^2}{dx^2} - \frac{1}{2} x^2 + \lambda x^4 \quad (18)$$

In the "super-critical" regime,  $\sigma_a = 1$ ,  $t > 1$ , and  $\mathcal{H}_\sigma$  corresponds to a one-well potential:

$$\mathcal{H}_\sigma (\sigma = 1) = H_{1w} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \lambda x^4 \quad (19)$$

The minima of the two-well potential

$$V(x) = -\frac{1}{2} x^2 + \lambda x^4 \quad (20)$$

(or, in other words, the bottoms of the wells) are located at  $\pm x_m$ , with:

$$x_m = \left( \frac{2}{\Delta t} \right)^{3/4} \frac{(1-t)^{3/4}}{t^{1/2}} \quad (21)$$

and have the depth  $V_m = V(x_m)$ ,

$$V_m = \frac{1}{4} \left( \frac{2}{\Delta t} \right)^{3/2} \frac{(1-t)^{3/2}}{t} \quad (22)$$

The "depth/distance" ratio is:

$$\frac{V_m}{x_m} \sim \frac{(1-t)^{3/4}}{t^{1/2}} \quad (23)$$

So, for small temperatures,  $\frac{V_m}{x_m}$  is large: the potential consists of two deep and distant wells. For "critical" temperatures ( $t \lesssim 1$ ), the potential "shrinks", i.e. the wells become close each other and shallow.

Let us make a technical remark. Defining the reduced Hamiltonian  $\mathcal{H}_\sigma$  in the form (14), we chose to deal with an oscillator of mass  $m = 1$  and with a coefficient of the quartic term  $\lambda \neq 1$ . Some authors ([9], [10]) choose  $m \neq 1$  and

$\lambda = 1$ . Our option was determined by the fact that the Hsue-Chern approach, to be used later on, has been developed for the  $m = 1$  case.

The Hsue-Chern solution is described in detail in several papers ([17], [6]), so we shall give here only the final result. The ground state energy of the Hamiltonian  $\mathcal{H}_\sigma$  is:

$$\mathcal{E}_0 = \frac{3\omega^2 + \sigma_a}{8\omega} \quad (24)$$

where  $\omega$  is the real root of the equation

$$\omega^3 - \sigma_a\omega + 6\lambda = 0 \quad (25)$$

The excited states are given by the formula [18]:

$$\mathcal{E}_n = \mathcal{E}_0 + n\omega + \frac{3\lambda}{\omega^2}n(n-1) \quad (26)$$

So, the first excited state is  $\mathcal{E}_1 = \mathcal{E}_0 + \omega$ . The ground state energy of (10) is:

$$E_0 = \frac{\xi_0}{\beta} \sqrt{\frac{|a|}{c}} \mathcal{E}_0 = \epsilon_{MF} \cdot t \cdot \frac{3\omega^2 + \sigma_a}{8\omega} \quad (27)$$

Another useful formula is:

$$\frac{\partial E_0}{\partial a} = \frac{\xi_0}{4\beta\sqrt{|a|c}} \frac{1}{\omega} = \frac{1}{4} \frac{\epsilon_{MF}}{a'} \frac{t}{\sqrt{|1-t|}} \frac{1}{\omega} \quad (28)$$

The results (24), (26)-(28) can be fully exploited only if we determine the function  $\omega = \omega(\lambda)$ , according to (25). Let us discuss firstly the two limiting cases,  $\lambda \rightarrow 0$  (corresponding to low temperatures) and  $\lambda \rightarrow \infty$  (corresponding to "critical" temperatures,  $t \rightarrow 1$ ). For  $\lambda = 0$ , the cubic equation (25) gives:

$$\omega^3 - \sigma_a\omega = 0 \quad (29)$$

with the roots  $\omega = 0$ ,  $\omega^2 = \sigma_a$ . The first relation means that the equation has a solution which goes to zero when  $\lambda \rightarrow 0$ . The second one means that there are additional **real** roots only in the "super-critical" case,  $t > 1$ . For the case  $\lambda \rightarrow \infty$  ( $t \rightarrow 1$ ),  $\omega^3 \simeq 6\lambda$  and the equation has only **one** real root.

For arbitrary  $\lambda$ , the root  $\omega(\lambda)$  is:

$$\omega = \left[ 3\lambda + \left( -\frac{\sigma_a}{27} + 9\lambda^2 \right)^{1/2} \right] + \left[ 3\lambda - \left( -\frac{\sigma_a}{27} + 9\lambda^2 \right)^{1/2} \right] \quad (30)$$

This is the only real root for the "sub-critical" regime,  $\sigma_a = -1$ ,  $t < 1$ . For the "super-critical" regime,  $\sigma_a = 1$ ,  $t > 1$ , corresponding to small values of  $\lambda$ ,  $9\lambda^2 < \frac{1}{27}$ , or, equivalently, to small values of  $t$ . (The precise meaning of the term "small" depends on the value of the parameter  $\Delta t$ , see eq.(16).) However, in this case we cannot take the limit  $t \rightarrow 0$  (the only physically interesting situation, besides  $t \sim 1$ ), because it is incompatible with the condition  $t > 1$ . So, we shall



disregard these solutions, and (30) will be the only relevant root, for all range of  $t$ .

Let us give the form of  $\omega(\lambda)$  in the two physically interesting limiting cases:

1. small temperatures,  $t \simeq 0$  :

$$\omega(\lambda) = 6\lambda(1 - 2^2 3^2 \lambda^2 + 2^4 3^5 \lambda^4 + \dots) \quad (31)$$

$$\frac{1}{\omega(\lambda)} = \frac{1}{6\lambda} (1 + 2^2 3^2 \lambda^2 - 2^4 3^5 \lambda^4 - 2^6 3^{10} 5 \lambda^6 + \dots) \quad (32)$$

2. critical temperatures,  $t \sim 1$  :

$$\omega(\lambda) = (6\lambda)^{1/3} \left( 1 + \frac{\sigma_a}{3} (6\lambda)^{-2/3} - \sigma_a \frac{1}{81} (6\lambda)^{-2} + \frac{1}{3^5} (6\lambda)^{-8/3} - \frac{2^2}{3^8} (6\lambda)^{-4} + \dots \right) \quad (33)$$

$$\frac{1}{\omega(\lambda)} = (6\lambda)^{-1/3} \left( 1 - \sigma_a \frac{1}{3} (6\lambda)^{-2/3} + \frac{1}{9} (6\lambda)^{-4/3} - \sigma_a \frac{2}{3^4} (6\lambda)^{-2} + \sigma_a \frac{2}{3^6} (6\lambda)^{-10/3} - \frac{7}{3^8} (6\lambda)^{-4} + \dots \right) \quad (34)$$

The ground state energy of the reduced Hamiltonian (18) can be written as:

$$\mathcal{E}_0 = \frac{1}{2} \left[ -\frac{1}{24\lambda} + 3\lambda - 2(3\lambda)^3 + 112(3\lambda)^5 + \dots \right], \quad t \sim 0 \quad (35)$$

$$\mathcal{E}_0 = \frac{1}{8} (3\lambda)^{1/3} \left[ 3 + 2\sigma_a (6\lambda)^{-2/3} - \frac{1}{3} (6\lambda)^{-4/3} + \sigma_a \frac{2}{27} (6\lambda)^{-2} - \frac{1}{3^4} (6\lambda)^{-8/3} + \frac{2}{3^7} (6\lambda)^{-4} - \sigma_a \frac{7}{3^8} (6\lambda)^{-14/3} + \dots \right] \quad (36)$$

The Hsue-Chern solution can also provide an alternate approach to the evaluation of the free energy of a chain of classical anharmonic oscillators coupled via elastic forces. In a seminal paper, Krumhansl and Schrieffer [19] treated the order-disorder (deep-well) limit of this system with the transfer matrix method, following closely the Scalapino-Sears-Ferrell approach. They found that the system dual to the classical chain is an anharmonic oscillator; see eq. (30) of [19], almost identical to our equation (10). The evaluation of the ground state energy of the double-well problem was made by Krumhansl and Schrieffer using standard quantum-mechanical approach, and the tunneling splitting - using the WKB approximation. Finally, Krumhansl and Schrieffer were able to identify, in the expression obtained for the free energy of the chain, a contribution due to the phonons and another one, due to the motion of domain walls (solitons). The Hsue-Chern method could simplify this calculation, giving both the ground state energy ( $\mathcal{E}_0$ , our equation (24)) and the tunneling splitting ( $\omega = \mathcal{E}_1 - \mathcal{E}_0$ , our equation (26)), in a unitary approach.

### 3 The validity of the two-level approximation

As already mentioned, this approximation is satisfactory when the first two energy levels ( $\mathcal{E}_0, \mathcal{E}_1$ ) are close together, and the third one ( $\mathcal{E}_2$ ) is much larger. Clearly, this happens when the lowest energy level is situated deep inside the well. In our case, for small temperatures, according to (34),  $\mathcal{E}_0 \simeq -\frac{1}{48\lambda} < 0$  and, with (22),

$$\frac{|\mathcal{E}_0|}{V_m} \simeq \frac{1}{3} \quad (37)$$

$\mathcal{E}_0$  increases while  $t$  increases and reaches the top of the well ( $\mathcal{E}_0 = 0$ ) for  $\omega^2 = \frac{1}{3}$ , or, using the cubic equation (25), for  $6\lambda = \frac{4}{3\sqrt{3}}$ . With (16), this is an equation in  $t$ , with the solution:

$$t_0 \simeq 1 - \frac{3^{5/3}}{2^3} \Delta t \simeq 1 - 0.8 \cdot \Delta t \quad (38)$$

So, if the temperature approaches the "critical" region, the two-level approximation becomes poorer, and near  $t = 1$ , it breaks down. What means "near  $t = 1$ ", we can understand better considering the ratio (see (26) and (16)):

$$\frac{\mathcal{E}_1 - \mathcal{E}_0}{\mathcal{E}_2 - \mathcal{E}_1} = \frac{\omega^3}{3\lambda} \simeq 72\lambda^2 = \frac{9}{16} (\Delta t)^3 \frac{t^2}{|1-t|^3} \quad (39)$$

The function  $f(\lambda) = \frac{\mathcal{E}_1 - \mathcal{E}_0}{\mathcal{E}_2 - \mathcal{E}_1}$  increases monotonically with  $\lambda$  (and with  $t$ ). It remains small, for instance  $f(\lambda) < \frac{1}{10}$ , for  $\lambda < 0.04$  or

$$t < 1 - \left(\frac{1}{4}\right)^{1/3} \frac{\Delta t}{2} \simeq 1 - 0.3 \cdot \Delta t \quad (40)$$

If  $f(\lambda) = 1$ , then  $t \simeq 1 - 0.8 \cdot \Delta t$ , according to (37); so, on a temperature interval of  $\frac{\Delta t}{2}$ , the approximation becomes unusable.

The advantage of our analysis consists in the fact that we obtain a simple analytical formula for the separation between the first three energy levels, (39), in contrast with the numerical results produced by other approaches [1], [9].

### 4 The planar array of weakly coupled chains: critical temperature and averaged field intensity

The Stoeckly-Scalapino critical equation for the planar array of chains has the form:

$$\omega = 2\beta c_y < \psi_{1D}^2 > \quad (41)$$

where  $\psi_{1D}$  refers to the order parameter of the 1D system. With (28), the critical condition can be written as:

$$\omega^2 = c_y \frac{\xi_0}{\sqrt{|a|c}} \quad (42)$$

For small values of the inter-chain coupling, putting

$$\omega^2 = c_y \omega_0^2, \quad \omega_0 = \left( \frac{\xi_0}{\sqrt{|a|c}} \right)^{1/2} = \left( \frac{1}{a'} \frac{1}{\sqrt{|1-t|}} \right)^{1/2}, \quad (43)$$

replacing in the cubic equation (25) and keeping the lowest order term, we get:

$$\sigma_a c_y \omega_0 = -6\lambda \quad (44)$$

So, it has a solution only for  $\sigma_a = -1$ ,  $t < 1$ . In fact,

$$t_c \simeq \frac{2}{3} \left( \frac{2}{\Delta t} \right)^{3/2} \sqrt{\frac{c_y}{a'}} \quad (45)$$

Because  $t_c \sim c_y^{1/2}$ , the critical temperature tends to zero when the inter-chain coupling tends to zero, as expected. Indeed, if the inter-chain interaction is suppressed, the 2D array becomes a collection of non-interacting 1D chains, without any phase transition at  $t > 0$ .

A similar dependence of the transition temperature on the inter-chain coupling,  $t_c \sim c_y^{1/2}$ , was obtained by Scalapino, Imry and Pincus [20] for a planar array of weakly coupled classical Heisenberg spin chains (see eq. (59) of [20]) and Ginzburg-Landau chains with complex order parameter (see eq. (63) of [20]). The authors suggest a general behaviour of the form  $t_c \sim c_y^\alpha$ , with  $\alpha$  - an index depending on the number of components of the order parameter and the dimensionality of the array. However, for a planar array of Ising chains, and of Ginzburg-Landau chains with real order parameter, they obtained, in the mean field approximation, a different behaviour of the critical temperature,  $t_c \sim 1/\ln(c_y/c)$

Let us investigate now the behaviour of the averaged field intensity for this system,  $\langle \psi_{2D}^2 \rangle$ . The free energy of a planar array of chains was obtained recently using the Stoockly-Scalapino approach [21]. The relevant part of the free energy, near the transition temperature, is given by

$$f \sim (1 + \eta) E \left( \frac{2\sqrt{\eta}}{1 + \eta} \right) \quad (46)$$

The parameter  $\eta$  is defined as:

$$\eta = \frac{\omega}{2c_y \langle \psi_{1D}^2 \rangle} k_B T, \quad 0 < \eta < 1 \quad (47)$$

The restriction of  $\eta$  on the unit interval implies a restriction of  $T$  on the subcritical interval,  $0 < T < T_c$ .  $E$  is the complete elliptic integral of second kind; its second derivative has a logarithmic singularity, which corresponds,

physically, to an Ising-type singularity of the specific heat. Using a formula similar to (6), we obtain for the averaged field intensity  $\langle \psi_{2D}^2 \rangle$  the following behaviour:

$$\langle \psi_{2D}^2 \rangle \sim |1 - \eta| \ln |1 - \eta| \quad (48)$$

Near the critical temperature,  $\eta$  can be written as:

$$1 - \eta = \eta_1 \tau + \eta_2 \tau^2 + \dots, \quad \tau = \frac{T - T_c}{T_c} < 0 \quad (49)$$

It is easy to see that, using Stoeckly-Sacalapino notations (eq. (4.5) of [5]),  $\eta_1 = \frac{1}{2} (\epsilon_0 \Delta_1 - \epsilon_1 \Delta_0)$ . Consequently,

$$\langle \psi_{2D}^2 \rangle \sim |\tau| \ln |\tau|, \quad \tau < 0 \quad (50)$$

So, the intensity of the order parameter tends to zero when the temperature approaches the critical value, from below.

## 5 Quantum phase transition in a $\psi^4$ chain

In order to apply our approach to the problem of quantum phase transition in  $\psi^4$  chains, we shall consider the Hamiltonian (8), the dual of (7), where the "mass" is:

$$m = 2c\beta^2 \quad (51)$$

We shall write the Stoeckly-Scalapino critical equation for the system (8). In order to match our results with the numerical simulations of Wang et al. [13], it is convenient to modify slightly the calculations developed in the previous sections. So, instead of (27), let us write:

$$H_0 = \left( \frac{2|a|}{m} \right)^{1/2} \mathcal{H}_0 \quad (52)$$

with

$$\mathcal{H}_0 = -\frac{1}{2} \frac{d^2}{d\varphi^2} + \frac{1}{2} \sigma_a \varphi^2 + \lambda \varphi^4, \quad \lambda = \frac{b}{(2|a|)^{3/2} m^{1/2}} \quad (53)$$

In order to avoid too complicated notations, we shall use the same symbols  $\lambda, E_0, \mathcal{E}_0$  like in the previous sections, although their signification is slightly different. We hope this ambiguity will not produce any confusion.

The ground state energy of  $H_0$  ( $\mathcal{H}_0$ ) is  $E_0$  ( $\mathcal{E}_0$ ), and:

$$E_0 = \left( \frac{2|a|}{m} \right)^{1/2} \mathcal{E}_0 \quad (54)$$

also

$$\langle \psi^2 \rangle = \frac{1}{2^{3/2}} \frac{1}{\sqrt{m|a|}} \frac{1}{\omega} \quad (55)$$

The Stoeckly-Scalapino critical equation takes the form:

$$\omega^2 = \sqrt{2}\beta c_y \frac{1}{\sqrt{m|a|}} \quad (56)$$

The Hamiltonian used in [13] is:

$$H_W = \sum_n \left[ \frac{p_n^2}{2} + \frac{1}{2}w(\varphi_{n+1} - \varphi_n)^2 - \frac{1}{2}k\varphi_n^2 + \frac{1}{4}g\varphi_n^4 \right] \quad (57)$$

We shall introduce use new parameters, according to the natural energy scales of the system. The physical reason of this parametrization is linked to the fact that structural phase transitions, described by Hamiltonians like (57), can be frequently characterized by the competition of different energy scales, namely, multiple potential wells of local potential with degenerate ground state versus a coupling between neighboring local degrees of freedom. So, following [13], we shall note  $E_0 = \hbar\omega_0$ , with  $\omega_0 = \sqrt{w/m}$ , the characteristic frequency of a coupled chains of harmonic oscillators, and  $E_b = k^2/4g$ , the height of the energy barrier between wells. It is convenient to discuss the physics of our system in terms of two dimensionless parameters,

$$\epsilon = \frac{4E_b}{E_0}, \quad \gamma = \frac{w}{k} \quad (58)$$

It is interesting to note that, for the classical counterpart of (57), a popular dimensionless parameter is (see for instance [22], (II 2.8)):

$$s = \frac{k}{8dw} = \frac{1}{8d} \frac{1}{\gamma} \quad (59)$$

Here,  $d$  is the dimensionality of the system (in our case,  $d = 1$ ). The case  $s \gg 1$  (or  $\gamma \ll 1$ ) corresponds to the order-disorder limit, and the case  $s \ll 1$  (or  $\gamma \gg 1$ ) - to the displacive limit.

Our Hamiltonian (49) and Wang's one (57) are identical if we make the substitutions:

$$c_y = \frac{1}{2}w, \quad |a| = \frac{k}{2}, \quad b = \frac{g}{4} \quad (60)$$

In Wang's Hamiltonian (57), the coefficient of the quadratic term in the single oscillator Hamiltonian is negative, so, in our notations,  $\sigma_a = -1$ . Also,

$$\lambda = \frac{1}{4\hbar} \frac{1}{\epsilon\gamma^{1/2}} \quad (61)$$

and the Stoeckly-Scalapino critical equation becomes:

$$\omega^2 = \gamma^{1/2} \quad (62)$$

As  $\omega = \omega(\lambda)$  and  $\lambda = \lambda(\epsilon, \gamma)$ , according to (61), the critical condition gives a connection between the dimensionless parameters  $\epsilon$  and  $\gamma$  and defines the phase diagram (see Figure). It is similar to the phase diagram obtained using Monte Carlo simulations (see [13], fig. 2).

<Fig. 1. to be inserted here>

## 6 Conclusions

In this paper, we have proposed an analytic approximation, useful in the investigation of a phase transition in a planar array of weakly coupled Ginzburg-Landau ( $\psi^4$ ) chains, described by a real (one component) order parameter. We obtained a simple formula for the transition temperature (which is proportional to the square root of the inter-chain coupling) and for the average of the field intensity. We have also given an analytical estimation of the validity of the two level approximation. Using the matrix transfer method, this approach was applied to the quantum phase transition in a chain of  $\psi^4$  quantum oscillators coupled by elastic interaction. The phase diagram is similar to that obtained using Monte Carlo simulations.

An essential ingredient of our approach was the fact that we could express the numerical results of Scalapino and his co-workers [4], [5], referring to the statistical mechanics of low dimensional Ginzburg-Landau ( $\psi^4$ ) fields, in simple analytic form, using an analytical (approximate) solution of the single, one dimensional anharmonic (quartic) oscillator. Similar solutions can be obtained for two dimensional (planar) and three dimensional (spatial) quartic oscillator. Due to this fact, the approach described in this paper can be easily generalized to Ginzburg-Landau ( $\psi^4$ ) systems described by a multi-component order parameter, relevant for the study of CDWs and superconductivity (two components) or magnetism and ferroelectricity (three components).

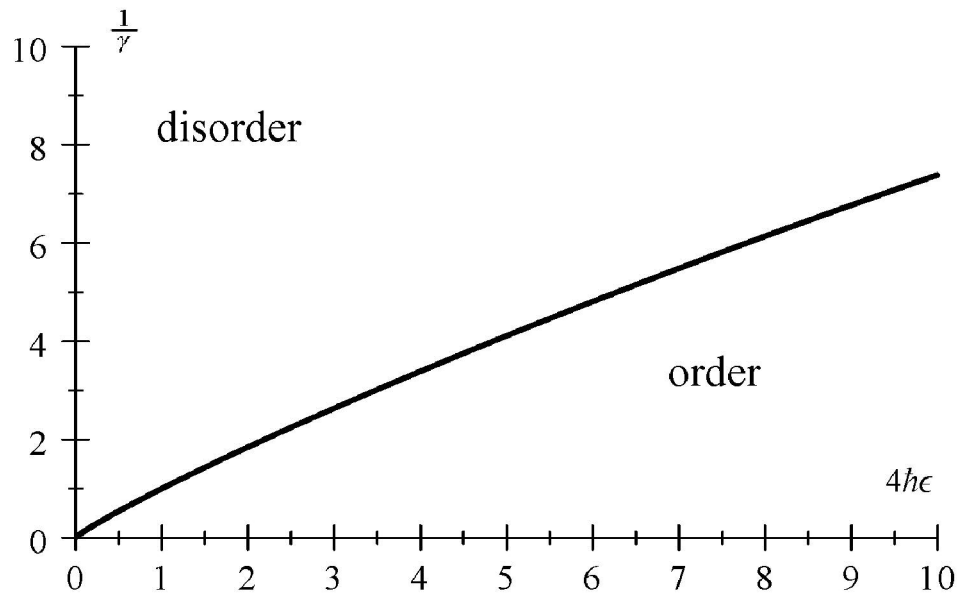
## References

- [1] Berman G. P., Bulgakov E. N., Campbell D. K., Gubernatis J. E., Sadreev A. F. and Wang, X., Phys. Rev. **B56** 11518 (1997)
- [2] Cai i., Qu H., Lu C., Ducharme S., Dowben P. A. and Zang J. Phys. Rev. **B70** 155411 (2004)
- [3] Schultz T.D., Mattis D.C. and Lieb E.H., Rev. Mod. Phys. **36** 856 (1964)

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7  
8 [4] Scalapino D.J., Sears M. and Ferrell R.A., Phys. Rev. **B6**, 3409 (1972)  
9  
10 [5] Stoeckly B. and Scalapino D. J. Phys. Rev. **B11** 205 (1975)  
11  
12 [6] Bârsan V., J. Phys.: Condens. Matter **18** 9286 (2006)  
13  
14 [7] Lajzerowicz J. and Pfeuty, J. Phys. (Paris) Suppl. **32**, C 5a-193 (1973)  
15  
16 [8] Dieterich W., Z. Phys. **270** 239 (1974)  
17  
18 [9] Bishop A. R. and Krumhansl J. A. Phys. Rev. **B12** 2824 (1975)  
19  
20 [10] Dieterich W., Adv. Phys. **25** 615 (1976)  
21  
22 [11] Kim D-H., Lin Y-C. and Rieger H. Phys. Rev. **E75** 016702 (2007)  
23  
24 [12] Chakrabarti B. K., Dutta A., Sen P., *Quantum Ising Phases and Transitions in Transverse Ising Models*, Springer, Berlin - Heidelberg - New York, 1996  
25  
26 [13] Wang X., Campbell D. K. and Gubernatis J. E. Phys. Rev. **B49** 15485 (1994)  
27  
28 [14] Toral R. and Chakrabarti A. Phys. Rev. **B42** 2445 (1990)  
29  
30 [15] Tröster A., Dellago C. and Schranz W. Phys. Rev. **B72** 094103 (2005)  
31  
32 [16] McKenzie R. H. Phys. Rev. **B52** 16428 (1995)  
33  
34 [17] Hsue C. S. and Chern J. L. Phys. Rev. **D29** 643 (1984)  
35  
36 [18] Patnaik P. K. Phys. Rev. **D33** 3145 (1986)  
37  
38 [19] Krumhansl J. A., Schrieffer J. R. Phys. Rev. **B11** 3535 (1975)  
39  
40 [20] Scalapino, D. J., Imry Y. and Pincus P. Phys. Rev. **B11** 2042 (1975)  
41  
42 [21] Bârsan V., Philos. Mag. **87** 1043 (2007)  
43  
44 [22] Bruce A. D. Adv. Phys. **29** 111 (1980)  
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**Figure caption:** The phase diagram as a function of  $\frac{1'}{\gamma}$  and  $4\hbar\epsilon$

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