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HSUE-CHERN APPROACH TO THE QUANTUM ANHARMONIC OSCILLATOR WITH APPLICATIONS TO THE STATISTICAL PHYSICS OF LOW DIMENSIONAL GINZBURG-LANDAU SYSTEMS

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Abstract. An accurate analytic approximation of the energy eigenstates of a quartic anharmonic oscillator is analyzed in detail and applied to the statistical mechanics of 1D Ginzburg-Landau systems, using the transfer matrix theory. Applications to the theory of structural and quantum phase transitions are briefly mentioned.

Key words: quantic anharmonic oscillator, Ginzburg-Landau theory, 1D systems.

1. INTRODUCTION

The Ginzburg-Landau (GL) theory, initially proposed as a phenomenological approach to superconductivity [1], proved its usefulness in a huge number of problems. In the quasi-1D physics, it is relevant for structural phase transitions, uniaxial ferroelectrics, polymers, etc. The simplest form of the GL functional is:

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

where $\psi(x)$ is a real field, defined in each point of a physical system of length L. In the most popular choice, a has a simple temperature dependence:

$$a = a'(t-1), \qquad a' > 0, \quad t = \frac{T}{T_{MF}}, \tag{2}$$

and the parameters a', b, c are positive constants; their expression, as function of microscopic characteristics of the physical system, can be obtained, at least in principle, from a microscopic theory. However, in some cases, it is convenient to consider that a is a simple, structureless constant, rather that the function given by (1). The parameter ξ_0 is defined as:

$$\xi_0^2 = \frac{c}{a'}, \tag{3}$$

and can be viewed as a natural length unit. However, some authors define $F[\psi]$ taking $\xi_0 = 1$. A detailed discussion of various choices for a and ξ_0 will be given in a separate subsection of the present paper. T_{MF} is the so-called mean-field transition temperature; it does not correspond to any real phase transition (which cannot occur in 1D), but is just another parameter of the GL theory. In the same time, the mean field theory predicts a (spurious) phase transition at $t = 1$.

As GL theory is mainly an approach to critical phenomena, its success depends essentially on how the fluctuations are taken into account. A mean-field treatment predicts incorrect results, like an unphysical phase transition in 1D, or incorrect critical indices, in higher dimensions. However, Scalapino, Sears and Ferrell [2] showed that, at least in 1D, this failure is due to an improper treatment of fluctuations. So, the evaluation of the partition function of a physical system as a path integral of $\exp\left(-\beta F[\psi]\right)$ over all possible $\psi(x)$ fields should lead to correct results.

The main technical problem of this approach is that path integrals could be very difficult to evaluate. The method used by Scalapino, Sears and Ferrell is the transfer matrix technique, which reduces the evaluation of the path integral of $\exp\left(-\beta F[\psi]\right)$ to the calculation of the ground state energy of an anharmonic oscillator:

$$H = -\frac{1}{4}\frac{\xi_0^2}{\beta^2 c}\frac{d^2}{d\psi^2} + a\psi^2 + b\psi^4, \quad \frac{1}{\beta} = k_B T. \tag{4}$$

In fact, the first energy levels of the anharmonic oscillators, E_0, E_1, E_2 give the free energy and the correlation functions of the 1D system. For instance, the free energy of the 1D system is:

$$f = \frac{E_0}{\xi_0}. \tag{5}$$

For more details about the physics of the problem, the reader is referred to [2].

So, the determination of the first energy levels of the anharmonic oscillator (4) gives the statistical physics of the 1D system. This is a particular case of a general theorem of statistical mechanics, asserting that a classical statistical mechanical system in $D+1$ dimensions is equivalent to a quantum mechanical system in D dimensions. Another aspect of this theorem is the fact that, if we start the study of a classical statistical mechanics problem for a chain of anharmonic oscillators, with the Hamiltonian

$$H = \int \frac{dx}{l}\left[\frac{p(x)^2}{2m} + \frac{A}{2}u(x)^2 + \frac{B}{4}u(x)^4 + \frac{mc_0^2}{2}\left(\frac{du}{dx}\right)^2\right] \tag{6}$$

instead of the GL functional, and we follow the same approach, the transfer operator equation obtained in this way is almost identical to (4) (see [3], eq. (2) and (30)). So, the equation (4) is relevant not only for GL systems, but also for the investigation of microscopic models of structural phase transitions [4].

Recently, a simple method for the calculation of the free energy for a 2D [5] and 3D [6]array of GL chains with near neighbor interaction, and for a 2D array with next-near-neighbor interaction [7] have been proposed. For practical calculations, a clear understanding of the properties of a single anharmonic oscillator is essential.

The main goal of this paper is to provide a detailed study of the spectrum of (4), as a basis for the investigation of the behavior of the 1D system. The applications to the higher dimensional systems will not be explicitly discussed. We shall use an approach proposed by Hsue and Chern [10], who developed an analytic approximation for the study of the anharmonic oscillator.

The structure of this paper is the following. In Sec. 2, we shall discuss some preliminary aspects of the transfer matrix Hamiltonian, which is a quantum anharmonic oscillator. In Sec. 3, we shall present in detail the Hsue-Chern solution. In Sec. 4, a quantitative analysis of the validity of the two-level approximation, very popular in the context of the anharmonic oscillator, is given. In Sec. 5, the main physical applications of the transfer matrix theory to the statistical physics of the 1D GL systems are exposed. Explicit expressions for several interesting quantities, like correlation lengths, are given. The last section is devoted to conclusions and comments.

2. THE QUARTIC ANHARMONIC OSCILLATOR

In this section we shall discuss some general aspects concerning the anharmonic Hamiltonian (4). Let us note that it can be written in a simpler form, with a change of variable $\psi = \alpha x$; indeed,

$$H = 2|a|\alpha^2 \left(-\frac{1}{8}\frac{\xi_0^2}{\beta^2 c}\frac{1}{|a|\alpha^4}\frac{d^2}{dx^2} + \frac{1}{2}\sigma_a x^2 + \frac{b\alpha^2}{2|a|}x^4 \right), \tag{7}$$

where we have put:

$$\sigma_a = \mathrm{sign}a. \tag{8}$$

Imposing the condition that the coefficient of the derivative be $-\frac{1}{2}$, we obtain:

$$\alpha^2 = \frac{\xi_0}{2\beta}\left(c|a|\right)^{-1/2}. \tag{9}$$

The coefficient of the quartic term is:

$$\lambda = \frac{b\xi_0}{4\beta} c^{-1/2} |a|^{-3/2} = \frac{k_B T_{MF} b\xi_0}{4} c^{-1/2} |a|^{-3/2} t \tag{10}$$

or, replacing a according to (2),

$$\lambda = \frac{\epsilon_{MF} b\xi_0}{4} c^{-1/2} |a'|^{-3/2} \frac{t}{|1-t|^{3/2}}, \tag{11}$$

where

$$\epsilon_{MF} = k_B T_{MF}. \tag{12}$$

Another useful parameter is Δt, defined as:

$$\frac{1}{2}\Delta t = \left(\frac{b k_B T_{MF}}{a'^2} \right)^{2/3}. \tag{13}$$

Δt "measures the size of temperature region below T_c in which the thermal energy kT_c is sufficient to drive the order parameter to zero, over the mean-field coherence length" [2]. Δt is quite similar to the parameter κ, introduced by McKenzie [8], eq, (7)) in the context of the GL theory with a complex order parameter, with the remark that "most of physics" is determined by it. Finally, we can write:

$$\lambda = \frac{1}{4}\left(\frac{\Delta t}{2}\right)^{3/2} \frac{t}{|1-t|^{3/2}}. \tag{14}$$

It is convenient to introduce a reduced Hamiltonian $\mathcal{H}$:

$$H = \frac{\xi_0}{\beta}\sqrt{\frac{|a|}{c}}\,\mathcal{H} \tag{15}$$

$$\mathcal{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\sigma_a x^2 + \lambda x^4.$$

Let us be more specific and define a reduced Hamiltonian $\mathcal{H}_{1w}$ for the "post-critical" regime, which is characterized by an one-well potential

$$\sigma_a = 1 \Leftrightarrow a > 0 \Longleftrightarrow t > 1 \tag{16}$$

$$\mathcal{H}_{1w} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\sigma_a x^2 + \lambda x^4, \tag{17}$$

and another one, $\mathcal{H}_{2w}$, for the "pre-critical" regime, with a two-well potential:

$$\sigma_a = -1 \Leftrightarrow a < 0 \Longleftrightarrow t < 1 \tag{18}$$

$$\mathcal{H}_{2w} = -\frac{1}{2}\frac{d^2}{dx^2} - \frac{1}{2}x^2 + \lambda x^4. \tag{19}$$

The quotation marks mean that, in fact, at $t = 1$, no phase transition occurs in the 1D system. Such a transition is predicted by the mean field theory, but it is a spurious one.

The two-well potential

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

has two minima, located at $\pm x_m$, with

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

The well depth is:

$$V_m = -V(x_m) = \frac{1}{16\lambda} = \frac{1}{4}\left(\frac{2}{\Delta t}\right)^{3/2} \frac{(1-t)^{3/2}}{t} \tag{22}$$

and the ratio between the well depth and the distance between well bottoms:

$$\frac{V_m}{2x_m} = \frac{1}{16\sqrt{\lambda}} \sim \frac{(1-t)^{3/4}}{t^{1/2}}. \tag{23}$$

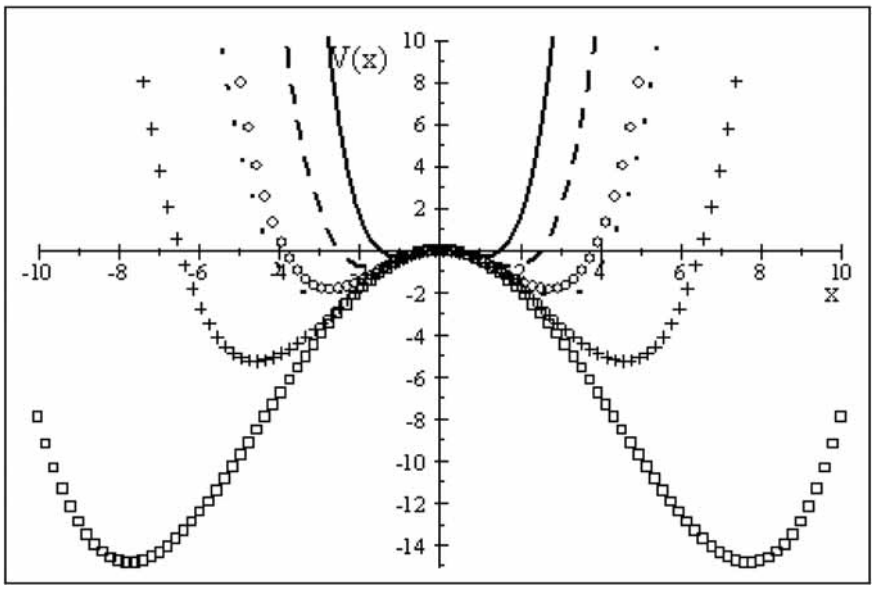

Fig. 1 – The two-well potential for several values of t and Δt. $V(x, \lambda(t = 0.9, \Delta t))$, $\Delta t = 0.2$ line, 0.1 dash, 0.05 dots; $V(x, \lambda(t = 0.7, \Delta t))$, $\Delta t = 0.2$ circle; 0.10 cross; 0.05 box.

So,

$$\frac{V_m}{x_m} \to 0 \text{ if } t \to 1 \tag{24}$$

$$\frac{V_m}{x_m} \to \infty \text{ if } t \to 0. \tag{25}$$

At small temperature, the potential consists of two distant and deep wells, and at $t \lesssim 1$, it "shrinks", *i.e.* the wells become close each other and shallow. This behavior can be seen in Fig. 1.

Some authors [9] use a different "effective Hamiltonian", with a mass $m \neq 1$ and a coefficient of the quadratic term equal to 1. Our choice is determined by the fact that it is the natural frame to use the Hsue-Chern approach to the anharmonic oscillator [10].

3. HSUE-CHERN APPROACH TO THE QUANTUM ANHARMONIC OSCILLATOR

In this section, we shall expose the Hsue-Chern solution of the quartic oscillator [10]. Let us introduce the second quantization formalism, putting:

$$a = \frac{x + ip}{\sqrt{2}}; \qquad a^+ = \frac{x - ip}{\sqrt{2}} \tag{26}$$

$$x = \frac{a + a^+}{\sqrt{2}}; \qquad p = i\frac{a^+ - a}{\sqrt{2}}. \tag{27}$$

The effective Hamiltonians can be written as:

$$\mathcal{H}_{1w} = a^+ a + \frac{1}{2} + \lambda \frac{\left(a + a^+\right)^4}{4} \tag{28}$$

$$\mathcal{H}_{2w} = -\frac{1}{2}\left(a^{+2} + a^2\right) + \lambda \frac{\left(a + a^+\right)^4}{4}. \tag{29}$$

The main point of the Hsue-Chern approach is to notice that if we define the state $|\varphi\rangle$ as

$$|\varphi\rangle = e^{(t/2)\left(a^+\right)^2}|0\rangle \tag{30}$$

then:

$$a|\varphi\rangle = ta^+|\varphi\rangle. \tag{31}$$

Consequently:

$$\left(a - ta^{+}\right)\left|\varphi\right\rangle = 0, \tag{32}$$

and $\left|\varphi\right\rangle$ represents the vacuum state for the boson operators b, b^{+}:

$$b = \frac{a - ta^{+}}{\sqrt{1-t^2}}; \qquad b^{+} = \frac{a^{+} - ta}{\sqrt{1-t^2}}. \tag{33}$$

Using the identities (the colons mean normal ordering)

$$\left(a^{+} + a\right)^2 =: \left(a^{+} + a\right)^2 : +1$$

$$\left(a^{+} + a\right)^4 =: \left(a^{+} + a\right)^4 : +6 : \left(a^{+} + a\right)^2 : +3,$$

and reversing (33)

$$a = \frac{b + tb^{+}}{\sqrt{1-t^2}}; \qquad a^{+} = \frac{b^{+} + tb}{\sqrt{1-t^2}} \tag{34}$$

we find easily that:

$$a^{+}a = \frac{1}{1-t^2}\left[\left(1+t^2\right)b^{+}b + t\left(b^{+2} + b^2\right) + t^2\right]$$

$$a^{+2} + a^2 = \frac{1}{1-t^2}\left[\left(1+t^2\right)\left(b^{+2} + b^2\right) + 4tb^{+}b + 2t\right]$$

$$a^{+} + a = \sqrt{\frac{1+t}{1-t}}\left(b + b^{+}\right)$$

$$\left(a^{+} + a\right)^4 = \left(\frac{1+t}{1-t}\right)^2\left[:\left(b^{+} + b\right)^4 : +6 : \left(b^{+} + b\right)^2 : +3\right] =$$

$$= \left(\frac{1+t}{1-t}\right)^2\left[:\left(b^{+} + b\right)^4 : +6\left(b^{+2} + b^2 + 2b^{+}b\right) + 3\right].$$

So, the Hamiltonians $\mathcal{H}_{1w}, \mathcal{H}_{2w}$ can be expressed in terms of b, b^{+} as follows:

$$\begin{aligned}\mathcal{H}_{1w} = \mathcal{E}_{1w}^{0} + \left[\frac{t}{1-t^2} + \frac{3\lambda}{2}\left(\frac{1+t}{1-t}\right)^2\right]\left(b^{+2} + b^2\right) + \left[\frac{1+t^2}{1-t^2} + 3\lambda\left(\frac{1+t}{1-t}\right)^2\right]b^{+}b + \\ + \frac{\lambda}{4}\left(\frac{1+t}{1-t}\right)^2\left[:\left(b^{+} + b\right)^4 :\right],\end{aligned} \tag{35}$$

where we have put:

$$\mathcal{E}_{1w}^{0} = \frac{1}{2} + \frac{t^2}{1-t^2} + \frac{3\lambda}{4}\left(\frac{1+t}{1-t}\right)^2 \tag{36}$$

Introducing the variable ω through the relation:

$$\omega = \frac{1-t}{1+t}; \qquad t = \frac{1-\omega}{1+\omega} \tag{37}$$

the parameter $\mathcal{E}_{1w}^{0}$ becomes:

$$\mathcal{E}_{1w}^{0} = \frac{\omega}{4} + \frac{1}{4\omega} + \frac{3\lambda}{4}\frac{1}{\omega^2}. \tag{38}$$

We shall determine the value of ω (or t) imposing the minimum condition:

$$\frac{d\mathcal{E}_{1w}^{0}}{d\omega} = 0. \tag{39}$$

This gives the following equation:

$$\omega^3 - \omega - 6\lambda = 0. \tag{40}$$

The coefficient of the term $\left(b^{+2} + b^2\right)$ in (50) is:

$$\frac{t}{1-t^2} + \frac{3\lambda}{2}\left(\frac{1+t}{1-t}\right)^2 = \frac{1}{4\omega^2}\left(\omega^3 - \omega - 6\lambda\right) = 0.$$

This is an essential simplification. It means that operators b, b^{+} correspond to normal modes, and is a general request for the Hartree approximation. Finally, we obtain:

$$\mathcal{H}_{1w} = \mathcal{E}_{1w}^{0} + \omega b^{+} b + \frac{\lambda}{4}\frac{1}{\omega^2}\left[:\left(b^{+} + b\right)^4:\right] \tag{41}$$

$$\mathcal{E}_{1w}^{0} = \frac{3\omega^2 + 1}{8\omega}; \qquad \sigma_a = 1, \quad a > 0 \Longleftrightarrow t > 1 \tag{42}$$

with ω – a root of eq. (55). Similarly, we obtain:

$$\mathcal{H}_{2w} = \mathcal{E}_{2w}^{0} + \omega b^{+} b + \frac{1}{24}\left(\omega + \frac{1}{\omega}\right)\left[:\left(b^{+} + b\right)^4:\right] \tag{43}$$

$$\mathcal{E}_{2w}^{0} = \frac{3\omega^2 - 1}{8\omega}, \qquad \sigma_a = -1, \qquad a < 0, \qquad t < 1 \tag{44}$$

with ω – a root of the equation

$$\omega^3 + \omega - 6\lambda = 0. \tag{45}$$

It is important to notice that the operators b, b^{+}, entering in $\mathcal{H}_{1w}$, $\mathcal{H}_{2w}$ are different. Formally, they have the same definition (42), but the parameter t has

different values in the "pre-critical" and "post-critical" regime. Indeed, $t=\frac{1-\omega}{1+\omega}$, with ω – a root of eq. (55) for 1*w*, respectively (61), for 2*w*.

The ground state energy of the Hamiltonian (3) is:

$$E_{1w}^0=\frac{\xi_0}{\beta}\sqrt{\frac{|a|}{c}}\frac{3\omega^2+1}{8\omega};\qquad \omega^3-\omega-6\lambda=0;\qquad \sigma_a=1,\qquad a>0\Longleftrightarrow t>1, \tag{46}$$

$$E_{2w}^0=\frac{\xi_0}{\beta}\sqrt{\frac{|a|}{c}}\frac{3\omega^2-1}{8\omega};\qquad \omega^3+\omega-6\lambda=0;\qquad \sigma_a=-1,\qquad a<0\Longleftrightarrow t<1. \tag{47}$$

The cubic equation can be written in a unitary way as:

$$\omega^3-\sigma_a\omega-6\lambda=0. \tag{48}$$

Noting that

$$\frac{\xi_0}{\beta}\sqrt{\frac{|a|}{c}}=\epsilon_{MF}\cdot t\cdot\sqrt{|1-t|}$$

the ground state energy of (3) can be written in a compact form as:

$$E^0=\epsilon_{MF}\cdot t\cdot\sqrt{|1-t|}E_0=\epsilon_{MF}\cdot t\cdot\sqrt{|1-t|}\frac{3\omega^2+\sigma_a}{8\omega} \tag{49}$$

For the evaluation of $\langle\psi^2\rangle$, we shall need the derivative:

$$\frac{\partial E^0}{\partial a}=\sigma_a\frac{\xi_0}{8\beta\sqrt{|a|c}}\left[\frac{1}{2}\left(3\omega+\frac{\sigma_a}{\omega}\right)+\left(3\omega-\frac{\sigma_a}{\omega}\right)\frac{a}{\omega}\frac{\partial\omega}{\partial a}\right]. \tag{50}$$

It is more convenient to express $\frac{\partial\omega}{\partial a}$ through $\frac{\partial\omega}{\partial\lambda}$, which can be evaluated using the cubic equation. We have:

$$\frac{\partial\lambda}{\partial a}=-\frac{3}{2}\frac{\lambda}{a};\quad \frac{\partial E_0}{\partial a}=-\frac{9}{8}\frac{\lambda}{a}\frac{1}{\omega^2};\quad \frac{\partial\omega}{\partial\lambda}=\frac{6}{3\omega^2-\sigma_a}, \tag{51}$$

so (57) becomes:

$$\frac{\partial E^0}{\partial a}=\frac{\xi_0}{16\beta\sqrt{|a|c}}\left[\frac{1}{\omega}+3\sigma_a\omega-18\sigma_a\frac{\lambda}{\omega^2}\right] \tag{52}$$

or, using again the cubic equation satisfied by ω,

$$\langle\psi^2\rangle=\frac{\partial E^0}{\partial a}=\frac{\xi_0}{4\beta\sqrt{|a|c}}\frac{1}{\omega}=\frac{1}{4}\frac{\epsilon_{MF}}{a'}\frac{t}{\sqrt{|1-t|}}\frac{1}{\omega}. \tag{53}$$

3.1. THE SOLUTIONS OF THE CUBIC EQUATION

3.1.1. Preliminary discussion of limiting cases

Let us firstly discuss two limiting cases, $\lambda \to 0$ and $\lambda \to \infty$, of the cubic equation. For $\lambda = 0$, it becomes:

$$\omega^3 - \sigma_a \omega = 0 \tag{54}$$

so its roots are:

$$\omega = 0, \tag{55}$$

and

$$\omega^2 = \sigma_a. \tag{56}$$

The second relation gives real roots only for $\sigma_a = 1$ (the "supra-critical" case). The result $\omega = 0$ can by interpreted as follows: the equation has a root which tends to 0 when λ tends to 0.

If $\lambda \to \infty$,

$$\omega^3 = 6\lambda \tag{57}$$

so the only real root of (45) behaves as

$$\omega \sim (6\lambda)^{1/3}. \tag{58}$$

3.2.2. The roots of the equation

We shall use the notations from [11] for the discriminant of the cubic equation (45):

$$\Delta = q^3 + r^2 = -\frac{\sigma_a}{27} + 9\lambda^2 \tag{59}$$

In Fig. 2 we can see the domain where the discriminant is positive, so the equation has one real root, or negative, so the equation has three real roots (however, only one root will be positive). These domains are separated by the zero of the function Δ, let us call it t_Δ. The values of the root t_Δ, for $\Delta t = 0.2; 0.1; 0.05$ are 1.2941; 1.1347; 1.0645, respectively. The point $t = 1$, where the discriminant is singular, is also important. In fact, we can identify a "subcritical" domain, $0 < t < 1$; a "near-supercritical", $1 < t < t_\Delta$; and a "far-supercritical" one, $t > t_\Delta$. In the "subcritical" and "near-supercritical" domains, the roots are given by

$$\omega = \left(3\lambda + \sqrt{-\frac{\sigma_a}{27} + 9\lambda^2}\right)^{1/3} + \left(3\lambda - \sqrt{-\frac{\sigma_a}{27} + 9\lambda^2}\right)^{1/3}, \tag{60}$$

and in the "far-supercritical" one, by

$$\omega = \frac{2}{\sqrt{3}} \cos\left(\frac{1}{3}\left(\arccos 9\sqrt{3}\lambda\right)\right). \tag{61}$$

Our main interest will be focused on "critical" $(t \sim 1)$ or low $(t \sim 0)$ temperatures, so we shall pay little attention to the "far-supercritical" regime. However, it can be important in the study of quantum phase transitions of the Hamiltonian (4).

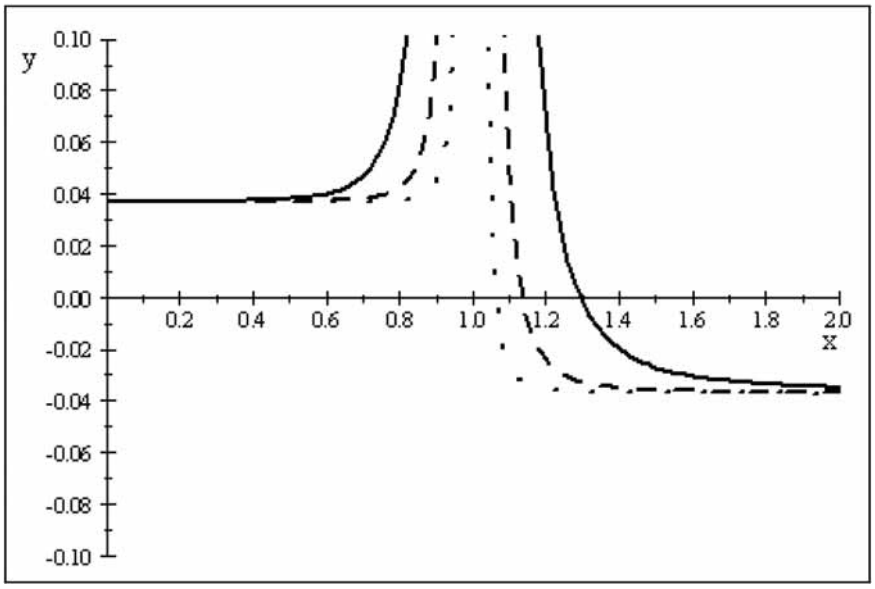

Fig. 2 – The discriminant of the eq. (45), for various values of Δt. $\Delta(t, \Delta t)$, $\Delta t = 0.2$ line; 0.1 dash; 0.05; dots.

We shall discuss now, in detail, the form of the roots, for the "subcritical" $(\sigma_a = -1)$ and "near-supercritical" $(\sigma_a = 1)$ regimes. For large values of λ, which correspond to "critical" $(t \sim 1)$ temperatures, it is possible to discuss together the both cases $\sigma_a = \pm 1$.

3.1.3. The case of "critical" temperatures

For $t \sim 1$, λ is large, and the discriminant

$$\sqrt{\Delta} = \sqrt{-\frac{\sigma_a}{27} + 9\lambda^2} = 3\lambda\sqrt{1 - \frac{\sigma_a}{27 \cdot 9\lambda^2}} = 3\lambda\sqrt{1 - \frac{\sigma_a}{3 \cdot (9\lambda)^2}} \tag{62}$$

is real, irrespective of the value of σ_a. Therefore, the only real root,

$$\omega=(3\lambda)^{1/3}\left(\left(1+\sqrt{1-\frac{\sigma_a}{3\cdot(9\lambda)^2}}\right)^{1/3}+\left(1-\sqrt{1-\frac{\sigma_a}{3\cdot(9\lambda)^2}}\right)^{1/3}\right) \tag{63}$$

can be written as a series expansion:

$$\omega=(6\lambda)^{1/3}\left(1+\frac{\sigma_a}{3}(6\lambda)^{-2/3}-\sigma_a\frac{1}{81}(6\lambda)^{-2}+\frac{1}{3^5}(6\lambda)^{-8/3}-\frac{2^2}{3^8}(6\lambda)^{-4}+\ldots\right) \tag{64}$$

$$\begin{aligned}\frac{1}{\omega}=(6\lambda)^{-1/3}\Big(1-\sigma_a\frac{1}{3}(6\lambda)^{-2/3}+\frac{1}{9}(6\lambda)^{-4/3}-\sigma_a\frac{2}{3^4}(6\lambda)^{-2}+\\ +\sigma_a\frac{2}{3^6}(6\lambda)^{-10/3}-\frac{7}{3^8}(6\lambda)^{-4}+\ldots\Big).\end{aligned} \tag{65}$$

For the evaluation of the validity of the two level approximation (see further on), the following function is important:

$$\begin{aligned}\frac{3\lambda}{\omega^3}=\frac{1}{2}\times\Bigg(1+\frac{1}{3}\left(\frac{3}{2}\left(\frac{\Delta t}{2}\right)^{3/2}\frac{t}{|1-t|^{3/2}}\right)^{-2/3}+\frac{1}{9}\left(\frac{3}{2}\left(\frac{\Delta t}{2}\right)^{3/2}\frac{t}{|1-t|^{3/2}}\right)^{-4/3}+\\ +\frac{2}{3^4}\left(\frac{3}{2}\left(\frac{\Delta t}{2}\right)^{3/2}\frac{t}{|1-t|^{3/2}}\right)^{-2}-\frac{2}{3^6}\left(\frac{3}{2}\left(\frac{\Delta t}{2}\right)^{3/2}\frac{t}{|1-t|^{3/2}}\right)^{-10/3}-\\ -\frac{7}{3^8}\left(\frac{3}{2}\left(\frac{\Delta t}{2}\right)^{3/2}\frac{t}{|1-t|^{3/2}}\right)^{-4}+\ldots\Bigg).\end{aligned} \tag{66}$$

3.1.4. The case of small temperatures

This means that $\sigma_a<0$, so

$$\omega=\left(3\lambda+\sqrt{\frac{1}{27}+9\lambda^2}\right)^{1/3}+\left(3\lambda-\sqrt{\frac{1}{27}+9\lambda^2}\right)^{1/3}, \tag{67}$$

and we have the following series expansions:

$$\omega=6\lambda\left(1-4(3\lambda)^2+48(3\lambda)^4+\ldots\right) \tag{68}$$

$$\frac{1}{\omega}=\frac{1}{6\lambda}\left(1+4(3\lambda)^2-32(3\lambda)^4-320(3\lambda)^6+\ldots\right) \tag{69}$$

3.2. THE GROUND STATE ENERGY OF THE REDUCED HAMILTONIAN

We can compute now the ground state energy of the reduced Hamiltonian:

$$\mathcal{E}_0 = \frac{3\omega^2 + \sigma_a}{8\omega} = \frac{3}{8}\omega + \frac{\sigma_a}{8}\frac{1}{\omega}. \tag{70}$$

At small temperatures, therefore when $\sigma_a = -1$:

$$\mathcal{E}_0 = \frac{1}{4}\left(-\frac{1}{12\lambda} + 6\lambda - 4(3\lambda)^3 + 224(3\lambda)^5 + ...\right). \tag{71}$$

It is easy to verify that the terms explicitly written in (71) provides an excellent approximation, with an error less than 10^{-3} for $t \sim 0.9$, $\Delta t = 0.1$.

At "critical" temperatures, λ is large, and we have, in both cases $\sigma_a = \pm 1$:

$$\begin{aligned}\mathcal{E}_0 = {} & \frac{1}{8}(6\lambda)^{1/3} \cdot \\ & \cdot\left(3 + 2\sigma_a(6\lambda)^{-2/3} - \frac{1}{3}(6\lambda)^{-4/3} + \sigma_a\frac{2}{27}(6\lambda)^{-2} - \right. \\ & \left. - \frac{1}{3^4}(6\lambda)^{-8/3} + \frac{2}{3^7}(6\lambda)^{-4} - \sigma_a\frac{7}{3^8}(6\lambda)^{-14/3} + ...\right)\end{aligned} \tag{72}$$

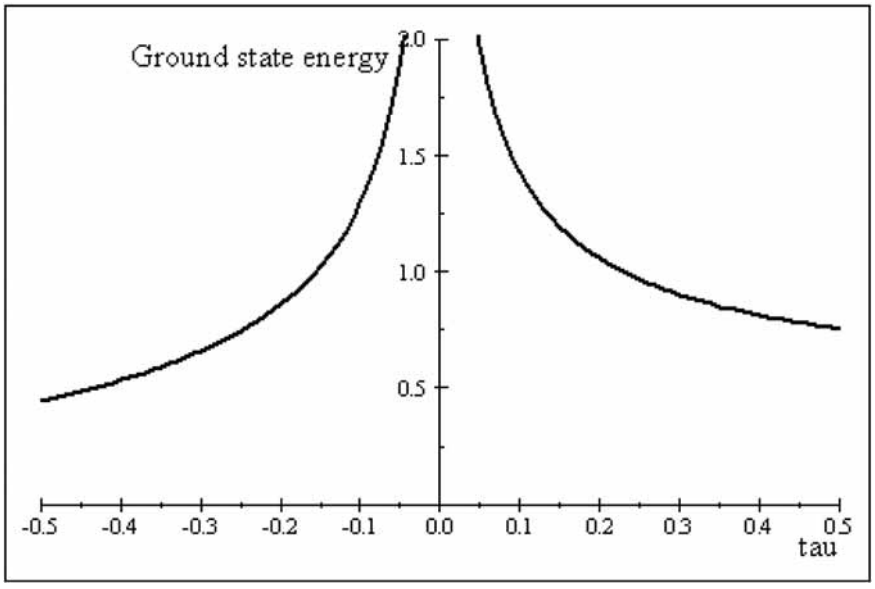

Fig. 3 – The ground state energy of the anharmonic oscillator in function of the "reduced temperature" τ.

With the notation:

$$\tau = \frac{2}{\Delta t}\frac{t-1}{t^{2/3}} \tag{73}$$

which can be interpreted as a "reduced temperature", we have:

$$\mathcal{E}_0 = \frac{3}{8}\left(\frac{3}{2}\right)^{1/3}|\tau|^{-1/2}\cdot\left(1+\frac{2}{3}\left(\frac{2}{3}\right)^{2/3}\tau-\frac{2}{3^3}\left(\frac{2}{3}\right)^{1/3}\tau^2+\frac{2^3}{3^6}\tau^3-\frac{2^2}{3^7}\left(\frac{2}{3}\right)^{2/3}\tau^4+\right.$$
$$\left.+6.0214\times10^{-5}\times\tau^6-7\frac{2^4}{3^{13}}\left(\frac{2}{3}\right)^{2/3}\tau^7+\ldots\right). \tag{74}$$

3.3. THE ENERGY OF FIRST EXCITED LEVELS

The energy of first excited levels is given by [12]:

$$\mathcal{E}_n = \mathcal{E}_0 + n\omega + \frac{3\lambda}{2\omega^2}n(n-1). \tag{75}$$

The spacing of these levels is important for the validity of the two level approximation; it works if the levels $\mathcal{E}_0$, $\mathcal{E}_1$ are close together, and $\mathcal{E}_2$ is more distant. So, the ratio

$$\frac{\mathcal{E}_1-\mathcal{E}_0}{\mathcal{E}_2-\mathcal{E}_1} = \frac{\omega^3}{3\lambda} \tag{76}$$

is relevant for the accuracy of the "two-level approximation".

4. THE VALIDITY OF THE TWO-LEVEL APPROXIMATION

The two-level approximation is largely used in the study of anharmonic oscillators. It consists, essentially, in the fact that, if the first two energy levels are close together, and the third one is quite distant, the physics of the system is governed by the first two levels. The Hsue-Chern solution allows one to obtain analytical formulae for the evaluation of the validity of this approximation.

First of all, let us see where is placed the level $\mathcal{E}_0$ in the well. For small values of λ (or of t), $\mathcal{E}_0 < 0$, so the level is "inside the well". It is easy to see that

$$\lim_{t\to 0}\frac{|\mathcal{E}_0|}{V_m} = \frac{1}{3}. \tag{77}$$

In the same limit, $\mathcal{E}_0 \simeq -\frac{1}{8\omega}\to\infty$, $\mathcal{E}_1-\mathcal{E}_0=\omega\to 0$, $\mathcal{E}_2-\mathcal{E}_1\simeq\frac{3\lambda}{\omega^2}\sim\frac{1}{t}\to\infty$,

so the two level approximation becomes an exact approach. The level $\mathcal{E}_0$ goes up in the well ($|\mathcal{E}_0|$ decreases) and it reaches the top of the well when $\mathcal{E}_0 = 0$, or $\omega = \frac{1}{\sqrt{3}}$. Using the cubic equation, this corresponds to:

$$t \simeq 1 - \left(\frac{1}{3}\right)^{1/3} \frac{\Delta t}{2} \tag{78}$$

So, when the statistical system enters into the critical region, the ground state of the matrix transfer Hamiltonian tends to "get out of the well".

As already mentioned, the ratio

$$\frac{\mathcal{E}_1 - \mathcal{E}_0}{\mathcal{E}_2 - \mathcal{E}_1} = \frac{1}{1 + \frac{3\lambda}{\omega^3}}$$

must be small in order to be able to apply properly the aforementioned approximation.

At low temperatures – or, equivalently, at small values of λ – we have $\omega \simeq 6\lambda$, so $\frac{3\lambda}{\omega^3} \simeq \frac{1}{108\lambda^2}$ and

$$\frac{\mathcal{E}_1 - \mathcal{E}_0}{\mathcal{E}_2 - \mathcal{E}_1} \simeq 108\lambda^2 \sim t^2 \tag{79}$$

At "critical" temperatures, or large values of λ, $\frac{3\lambda}{\omega^3} \simeq \frac{1}{2}$ and

$$\frac{\mathcal{E}_1 - \mathcal{E}_0}{\mathcal{E}_2 - \mathcal{E}_1} \simeq \frac{2}{3}, \tag{80}$$

so the approximation is poor, but still not unusable.

For instance, let us ask that

$$\frac{\mathcal{E}_1 - \mathcal{E}_0}{\mathcal{E}_2 - \mathcal{E}_1} = \frac{1}{1 + \frac{3\lambda}{\omega^3}} = \frac{1}{10} \tag{81}$$

Using again the cubic equation, we find that the condition (81) corresponds to the following value of *t*:

$$t \simeq 1 - \frac{\Delta t}{2} \tag{82}$$

So, when *t* is in the middle of the "pre-critical" domain, the two level approximation is still good.

5. APPLICATIONS TO THE STATISTICAL PHYSICS OF 1D SYSTEMS

5.1. CORRELATION LENGTHS

With the definitions of [2], the correlation lengths ξ_1, ξ_2 of the order parameter-order parameter and, respectively, intensity-intensity correlation functions are

$$\frac{1}{\xi_{1,2}} = \frac{1}{\xi_0}\frac{1}{k_B T}\left(E_{1,2} - E_0\right). \tag{83}$$

With (46, 47, 75), we get for the order parameter-order parameter correlation length:

$$\frac{1}{\xi_1} = \frac{1}{\xi_0}\sqrt{|1-t|}\,\omega. \tag{84}$$

At small t,

$$\omega \simeq 6\lambda = \frac{3}{2}\left(\frac{\Delta t}{2}\right)^3 \frac{t}{(1-t)^{3/2}}, \tag{85}$$

consequently:

$$\frac{1}{\xi_1} = \frac{3}{2}\left(\frac{\Delta t}{2}\right)^3 \frac{1}{\xi_0}\frac{t}{(1-t)} \sim t, \qquad t \to 0. \tag{86}$$

At $t \sim 1$,

$$\omega = (6\lambda)^{1/3} \simeq \left(\frac{3}{2}\right)^{1/2}\left(\frac{\Delta t}{2}\right)^{1/2}\frac{t^{1/3}}{\sqrt{|1-t|}} \tag{87}$$

so:

$$\frac{1}{\xi_1} = \left(\frac{3}{2}\right)^{1/2}\left(\frac{\Delta t}{2}\right)^{1/2}\frac{1}{\xi_0}t^{1/3}. \tag{88}$$

$\frac{1}{\xi_1}$ remains non-zero at any finite temperature, as expected for a 1D system. At $t = 1$, $\frac{1}{\xi_1}$ has just an inflexion point; it separates an interval ($t > 1$) with a slow decrease of $\frac{1}{\xi_1}$, from an interval ($t < 1$) with a more pronounced decrease of $\frac{1}{\xi_1}$, when t descreases; at the end of this latter interval, $\frac{1}{\xi_1} = 0$.

The intensity-intensity correlation length is:

$$\frac{1}{\xi_2} = \frac{2}{\xi_1}\left(1 + \frac{3\lambda}{\omega^3}\right) = \frac{2}{\xi_0}\sqrt{1-t}\,\omega\left(1 + \frac{3\lambda}{\omega^3}\right) \tag{89}$$

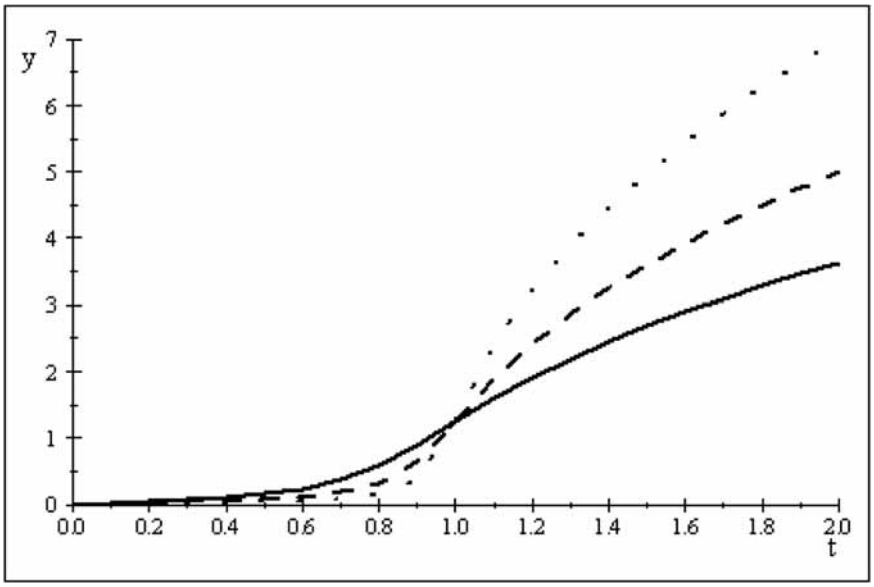

Fig. 4 – The inverse correlation length for the order parameter – order parameter correlation function, eq. (84). $y = \frac{\xi_0}{\xi_1}(t, \Delta t) \times (\Delta t)^{-1/2} \times 1.5565$; Δt =0.2 line; 0.1 dash; 0.05 dots.

or

$$\frac{1}{\xi_2} = \frac{2}{\xi_0}\sqrt{1-t}\,\omega\left(1+\frac{3\lambda}{\omega^3}\right) \tag{90}$$

At small t,

$$\omega\left(1+\frac{3\lambda}{\omega^3}\right) = \omega + \frac{3\lambda}{\omega^2} \simeq 6\lambda + \frac{3\lambda}{36\lambda^2} = 6\lambda + \frac{1}{12\lambda} \tag{91}$$

and because $\lambda \sim t$, the inverse of the correlation length diverges at $t = 0$ like $1/t$.

At $t \simeq 1$,

$$\frac{3\lambda}{\omega^3} \sim \frac{1}{2} \tag{92}$$

so ξ_2 behaves similar to ξ_1. However, at t slightly smaller than 1, ξ_2 has a maximum, which could be interpreted as the only indication of the fact that $t = 1$ is the mean field critical point.

We obtain, at least qualitatively, the results of [2]. Quantitatively, it should be a difference about our results and [2], due to the fact that the temperature dependence of the parameters in (1) differs slightly of that usen in [2].

5.2. AVERAGE VALUE OF THE SQUARED ORDER PARAMETER

It is easy to see, from (54), that the expectation value of the field intensity can be written as:

$$\left\langle \psi^2 \right\rangle \sim t\xi_1. \tag{93}$$

At "critical" temperatures:

$$\left\langle \psi^2 \right\rangle = \frac{1}{4}\frac{\epsilon_{MF}}{a'}\left(\frac{2}{3}\right)^{1/3}\left(\frac{2}{\Delta t}\right)^{1/2} t^{2/3}\times\left(1-\sigma_a\frac{1}{3}(6\lambda)^{-2/3}+\right.$$
$$\left.+\frac{1}{9}(6\lambda)^{-4/3}-\sigma_a\frac{2}{3^4}(6\lambda)^{-2}+\sigma_a\frac{2}{3^6}(6\lambda)^{-10/3}-\frac{7}{3^8}(6\lambda)^{-4}+\ldots\right), \tag{94}$$

or

$$\left\langle \psi^2 \right\rangle\times 4\left(\frac{3}{2}\right)^{1/3}\left(\frac{\Delta t}{2}\right)^{1/2}\frac{a'}{\epsilon_{MF}} = t^{2/3}\times$$
$$\times\left(1-0.25438\frac{2}{\Delta t}\frac{t-1}{t^{2/3}}+6.4710\times10^{-2}\left(\frac{2}{\Delta t}\frac{t-1}{t^{2/3}}\right)^2-1.0974\times10^{-2}\left(\frac{2}{\Delta t}\frac{t-1}{t^{2/3}}\right)^3+\right. \tag{95}$$
$$\left.+7.1012\times10^{-4}\left(\frac{2}{\Delta t}\frac{t-1}{t^{2/3}}\right)^5-2.1075\times10^{-4}\left(\frac{2}{\Delta t}\frac{t-1}{t^{2/3}}\right)^6+\ldots\right).$$

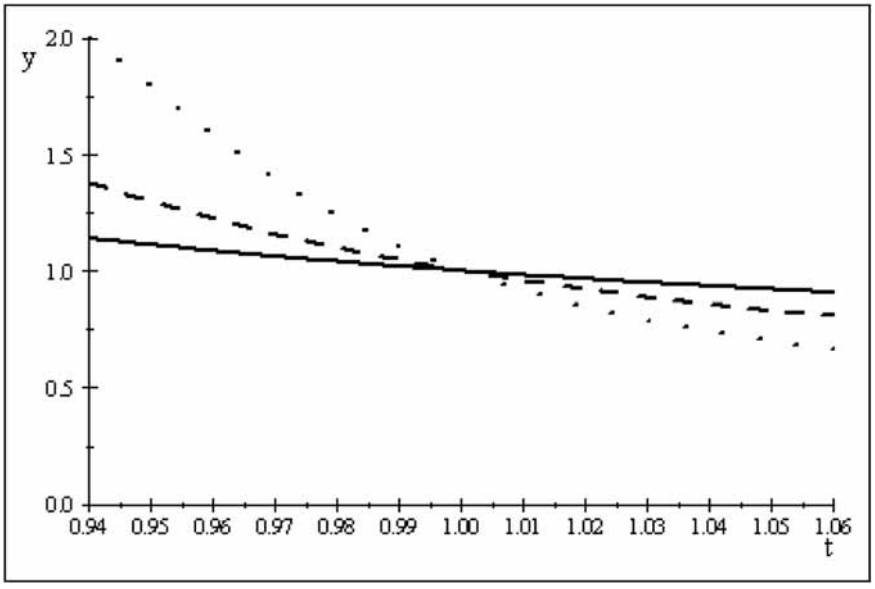

Fig. 5 – The "normalized" average field intensity in the "critical" region, for various values of Δt. $y = \left\langle \psi^2 \right\rangle \times 4(3/2)^{1/3}(\Delta t/2)^{1/2}(a'/\epsilon_{MF})$, Δt =0.2 line; 0.1 dash; 0.05 dots.

The behavior of the squared order parameter is specially relevant for what happens in a 1D material, near the mean field transition temperature: instead of a neat phase transition, a smooth passage from a regime where the order parameter is sensibly non-zero and is growing while lowering of temperature, to a regime where it is small and becomes smaller for larger temperatures. This behavior is more pronounced for smaller values of Δt.

Contrary to E_0, ω, ξ_1 and ξ_2, which can be expressed as functions of λ, or of the "reduced temperature" τ, $\left\langle \psi^2 \right\rangle$ does not enjoy this property: it depends on both t and Δt. However, it can be put in a form somewhat simpler than (95), *i.e.*

$$\left\langle \psi^2 \right\rangle = \frac{1}{4}\frac{\epsilon_{MF}}{a'}\left(\frac{2}{3}\right)^{1/3}\left(\frac{2}{\Delta t}\right)^{1/2} t^{2/3} \times \left(1 - \frac{1}{3}\left(\frac{2}{3}\right)^{2/3}\tau + \frac{1}{9}\left(\frac{2}{3}\right)^{4/3}\tau^2 - \right.$$
$$\left. - \frac{2}{3^4}\left(\frac{2}{3}\right)^2 \tau^3 + \frac{2}{3^6}\left(\frac{2}{3}\right)^{10/3}\tau^5 - \frac{7}{3^8}\left(\frac{2}{3}\right)^4 \tau^6 + \ldots\right). \tag{96}$$

5.3. CHOICES OF THE TRANSFER HAMILTONIAN PARAMETERS USED IN LITERATURE

In the physical applications of the transfer matrix operators, as developed by Scalapino and co-workers [13, 14], there are several choices of the Ginzburg-Landau functional. It is useful to take in account these differences in order to be able to compare properly the results of various theories. We shall shortly discuss this issue here.

In [2], "the natural length unit" ξ_0 is used, but in [13], the authors put $\xi_0 = 1$. In [2], the temperature dependence of the mass of the anharmonic oscillator is neglected, making the choice $T = T_c$. This choice is based on the fact that the "Landau form" of the coefficient a, (2), can be used only the point $t = 1$. An advantage of this convention is the fact that the "reduced temperature" has a very simple form. In [13], the transfer matrix Hamiltonian has an extra factor β. In all these papers, a has the "Landau form", eq. (2), but in the standard statistical mechanics approach [3, 4], a is just a number. Of course, a defined by (2) and $a = \text{const}$ will give different physical behaviors. To the contrary, all the other choices produce essentially the same physics. The results obtained in this paper can be easily adapted to any of the aforementioned situations.

6. CONCLUSIONS

The present paper provides a detailed analysis of a quite accurate analytical approximation of the quantum quartic oscillator. These results are applied to the

statistical mechanics of a 1D Ginzburg-Landau system. Simple and compact expressions for several physical quantities, like correlation lengths, or average field intensity, are obtained. Their behavior is analyzed in detail in the "critical" region, *i.e.*, near the zero of the Ginzburg-Landau coefficient a. In fact, no phase transition occurs, as expected for a 1D system, but the averaged field intensity strongly decreases, remaining however at a non-zero value, while temperature increases. The validity of the two-level approximation is analyzed quantitatively. Our formulae give an analytic form to the numeric results obtained in the well-known paper of Scalapino, Sears and Ferrell [2].

As the spectrum of the single anharmonic oscillator is of central importance for the statistical mechanics of the higher-dimensional Ginzburg-Landau systems, our results are relevant for the 2- and 3D physics too; the same remark is valid for the standard statistical mechanical approach of structural phase transitions, where the starting point is the atomic Hamiltonian, rather than a Ginzburg-Landau functional, obtained, in principle, by coarse-graining this Hamiltonian. Our results are also relevant for the study of quantum phase transitions in low dimensional systems of quantum anharmonic oscillators.

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