

CRITICAL BEHAVIOR OF AN ANHARMONIC NANOSCOPIC SOLID

VICTOR BÂRSAN

“Horia Hulubei” National Institute for Physics and Nuclear Engineering
Str. Reactorului 30, 077125 Magurele, Romania

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Abstract. The paper presents a toy model of phase transition in an anharmonic solid. The starting point of our study is a $2D$ or $3D$ rectangular lattice of on-site quantum quartic oscillators, interacting with their nearest neighbors by elastic forces. The critical equation of the order-disorder transition is obtained using the theory of dielectric susceptibility. To obtain a mathematically tractable model, the quartic potential - a symmetric, two well potential - is replaced by a similar, but more workable one - a rectangular symmetric two well potential. For energies and wave functions corresponding to the lowest states, we obtain accurate analytical approximations, which lead to a simple critical equation. It gives the critical temperature as a function of the “anharmonicity” of potential. Similar toy models can be obtained using other workable, two well potentials. Applications in nanophysics are briefly discussed.

Key words: anharmonic solids, mean-field theory, quantum quartic oscillator, dielectric susceptibility, critical temperature.

1. INTRODUCTION

The anharmonic solid - and, particularly, the solid with ψ^4 anharmonicities - is a system of utmost interest in condensed state physics, both for fundamental and practical reasons. One of the problems investigated in the context of the anharmonic solid is the structural phase transition. It is important not only from the perspective of its applications in ferroelectricity, but from the more general perspective of the theory of phase transitions. Actually, it provides a relatively simple model of phase transition, with real order parameter.

There are at least two approaches of this kind of phase transitions. In one of them, the starting point is the Ginzburg - Landau functional of free energy [1]; in the other one - a polynomial Hamiltonian [2, 3]. The statistical behavior of a n -dimensional solid described by a Ginzburg-Landau functional can be obtained using the transfer matrix theory [4], from the calculation of the energy of the first levels of a Hamiltonian of a quantum $n - 1$ -dimensional system, with quartic anharmonicities. So, a classical system, in n spatial dimensions, is equivalent with a quantum system, in $n - 1$ -dimensions. These two systems, sometimes called dual systems, describe quite similar objects - aggregates of classical, respective quantum oscillators. A well-known example of such aggregates is that studied by Stoeckly and

Scalapino [5, 6], where the evaluation of the partition function of a planar system of coupled chains, composed by quartic oscillators, is reduced to the study of a chain of quantum anharmonic oscillators. If the coupling between quantum oscillators is weak, the 1D Hamiltonian can be transformed in a fermionic Hamiltonian, similar to that obtained by Schultz, Mattis and Lieb, in their study devoted to the Ising model [7], in various variants of the Luttinger model or in other 1D models [8–10], [11]. These 1D systems have interesting theoretical and experimental applications, and it is useful to compare them with other exactly solvable atomic [12] or magnetic models [13–15]. Consequently, the ψ^4 anharmonic solid can be linked to a large class of models intensively studied in the theory of condensed matter, including the Ising model.

After remarkable theoretical progress, which produced, in the '70s, a lot of exact results, the following decades were dominated by numerical investigations, for instance [16–18]. In more recent papers, some authors use both numerical methods, and analytical approximations [19], [20], in order to obtain a better understanding of such systems. A model which extends the Ginzburg-Landau theory beyond the linear chain approximation was proposed for systems where both the nearest neighbor interaction and the near next neighbor interaction is taken into account [21–23]. The transfer matrix theory was applied in the analytic study of thermal or quantum phase transitions in low dimensional systems, with or without external fields [24] - [28]. A critical analysis of these results has been done by Lungu [29].

If the aforementioned analytical results mainly refer to low dimensional systems, the 3D anharmonic systems were investigated with less rigorous theoretical methods, the most frequently used being the mean-field ones; actually, this situation is quite common in solid state theory. As it is well known, the mean field approximations give good results for the structural phase transitions [2, 3]. The model to be discussed in this paper is a d -rectangular lattice of quantum anharmonic (quartic) oscillators, interacting by elastic forces with their nearest neighbors. In principle, the model can be studied for any value of d , but for $d = 1$, it gives incorrect results, including a spurious phase transition. Even if the model is a quantum one, the classical case can be, in general, easily obtained, taking the limit $\hbar \rightarrow 0$.

In this paper, we shall consider only the case of the real order parameter. The physics described by such a model of anharmonic solid is quite simple. In an one-dimensional picture, the particle situated in a lattice point can be placed in one of the two wells of the anharmonic potential, "to the left" or "to the right", if the magnitude of the well - having the dimension of an energy - is large enough, compared to the energy of thermal fluctuations. If one of these position is "preferred" by the particle, the system is in an ordered state; if the positions are equivalent, the state is disordered. For shallow wells, the system can become "polarized", in the sense that the particles can "slip" in the same direction. In this case, a "soft mode transition" occurs, at a

certain temperature. For deep wells, the system undergoes an order-disorder transition, and is equivalent to an Ising model. The interplay between temperature, particle mass, dimensionality and potential strength defines the critical equation.

The main goal of this paper is to obtain an analytical approximation for the critical equation describing the phase transition of a $2D$ or $3D$ anharmonic solid. We shall follow a mean-field approach [30, 31], replacing the N -body Hamiltonian with a sum of N one-site quartic Hamiltonians, placed in an effective field. Technically, our task is to solve a one-particle Schrödinger equation for a quartic potential, with two symmetric wells. Even this much simpler problem has not a simple solution; more than this, the Rayleigh - Schrödinger perturbation series, in the coupling constant of the quartic term, diverges, for any of the bound states [32]; a quite recent review of the results obtained in this domain can be found in [33]. So, looking for an approximate, but reasonably accurate analytic approach, we shall replace the two well quartic potential, with a two well rectangular one. Specifically, this potential will be an infinite square well, with a finite rectangular step, placed symmetrically inside. If the step is sufficiently large, accurate expressions for the energies and wave functions of the first levels of this one-particle problem can be obtained. In this way, we can find a simple expression of the critical equation, describing the phase transition which takes place in the anharmonic solid under consideration.

Finally, our main result will be a toy model for a phase transition in an anharmonic solid, in the mean-field approximation. For this model, we show that a more pronounced anharmonicity generates a higher critical temperature.

The structure of this paper is the following. In Section 2, a model of quantum anharmonic solid is introduced: a $2D$ or $3D$ rectangular lattice of one-site quartic oscillators, interacting with their nearest neighbors by elastic forces. In Section 3, a general formula for the dielectric susceptibility of a system, put in a weak electric external field, is obtained, for $T > 0$, in the second order of the perturbation theory. The expression of the susceptibility, at zero temperature, is also given. These formulas are applied, in the next section, to the calculation of the susceptibility and of the transition temperature, for a specific system, namely for an anharmonic solid, in the mean-field approximation. In order to obtain explicit formulas for the critical behavior, the anharmonic, double well potential, will be replaced with a rectangular, double well one. So, in Section 5 will be worked out a detailed study of a class of double symmetric rectangular wells; specifically, we shall examine a particular case, when accurate analytic approximations can be easily obtained. Section 6 contains a short discussion of applications of rectangular potentials in nanophysics. In Section 7, the susceptibility and the critical temperature of the anharmonic solid are obtained, using the rectangular two well potential studied previously. The last section is devoted to conclusions.

2. A MODEL OF ANHARMONIC SOLIDS

There are, of course, many models of anharmonic solids - actually, as many as anharmonic interatomic potentials can be imagined. One of the most appealing is a simple one, proposed in the pioneering age of the ferroelectricity theory [35–37]. It consists of a rectangular lattice of on-site quartic quantum oscillators, interacting with their nearest neighbors by elastic forces. It is described by the Hamiltonian:

$$H = \sum_n \frac{P_n^2}{2M} - \frac{A}{2} \sum_n X_n^2 + \frac{B}{4} \sum_n X_n^4 + \frac{C}{2} \sum_{n,n'} \sigma_{n,n'} (X_n - X_{n'})^2 \quad (1)$$

where $\sigma_{n,n'} = 1$ for nearest neighbors and 0 otherwise. The model can be used both in the classical, and in the quantum case. We shall study the quantum case; in principle, the classical one can be obtained in the limit $\hbar \rightarrow 0$. In order to avoid physically irrelevant complications, we shall consider the isotropic case; the anisotropy can be easily introduced, if needed. The system displays a phase transition, if its dimensionality is larger than 1, $d > 1$. For $d = 4$, the model gives the exact values of critical indices.

It is convenient to define dimensionless parameters of length, temperature and mass:

$$X = \sqrt{\frac{B}{A}} x, \quad t = \frac{B}{AC} T, \quad m = \frac{CA^2}{\hbar^2 B^2} M \quad (2)$$

as well as a dimensionless parameter characterizing the ratio between the on-site and inter-site potential:

$$a = \frac{A}{C} \quad (3)$$

3. THE DIELECTRIC SUSCEPTIBILITY

In this section, we shall obtain a formula for the dielectric susceptibility of the system, which will allow us to find, in the mean field approximation, the critical temperature of the phase transition underwent by the system described by the Hamiltonian (1) [30, 31].

For the beginning, let us consider that the Hamiltonian describing our system may be written as the sum of an exactly soluble Hamiltonian, \mathcal{H}_0 , and of a perturbation \mathcal{V} :

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V} \quad (4)$$

The eigenvectors and the eigenvalues of \mathcal{H}_0 satisfy the equation:

$$\mathcal{H}_0 |n\rangle = E_n^{(0)} |n\rangle \quad (5)$$

In the second order of the perturbation theory, the energy of an eigenstate of the Hamiltonian \mathcal{H} is:

$$E_n = E_n^{(0)} + \langle n | \mathcal{V} | n \rangle + \sum_{m \neq n} \frac{|\langle n | \mathcal{V} | m \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \quad (6)$$

If

$$\mathcal{V} = -Fx \quad (7)$$

is the potential energy of a particle situated in an external field (which can be an electric field) F , the equation (6) can be put in the form:

$$E_n = E_n^{(0)} - F \langle n | x | n \rangle + F^2 \sum_{m \neq n} \frac{|\langle n | x | m \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \quad (8)$$

and the quantum average of the dipolar momentum will be given by the expression:

$$P_n = -\frac{\partial E_n}{\partial F} \quad (9)$$

The dielectric susceptibility is given by:

$$\chi_n = \frac{\partial P_n}{\partial F} = -\frac{\partial^2 E_n}{\partial F^2} = -\sum_{m \neq n} \frac{2|\langle n | x | m \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \quad (10)$$

Its statistical average is:

$$\chi = \frac{1}{Z_0} \sum_{m \neq n} \exp(-\beta E_n^{(0)}) \frac{2|\langle n | x | m \rangle|^2}{E_m^{(0)} - E_n^{(0)}} \quad (11)$$

where Z_0 is the partition sum corresponding to the Hamiltonian \mathcal{H}_0 :

$$Z_0 = \sum_n \exp(-\beta E_n^{(0)}) \quad (12)$$

At $T = 0$, the formula (11) takes a simpler form:

$$\chi(T=0) = \sum_m \frac{2|\langle 0 | x | m \rangle|^2}{E_m^{(0)} - E_0^{(0)}} \quad (13)$$

It is, as expected, a positive quantity, as $E_m^{(0)} - E_0^{(0)} > 0$ for any $m > 0$.

4. THE SUSCEPTIBILITY AND THE PHASE TRANSITION

Let us consider now, as Hamiltonian describing our anharmonic solid, the dimensionless form of (1), obtained by using (2), (3):

$$\mathcal{H} \rightarrow H = -\frac{1}{2m} \sum_n \nabla_n^2 + \left(2d - \frac{a}{2}\right) \sum_n x_n^2 + \frac{a}{4} \sum_n x_n^4 - \sum_n \left(\sum_m x_n \sigma_{nm} \right) x_n \quad (14)$$

In the mean field approximation, we make the replacement:

$$\left(\sum_m x_n \sigma_{nm} \right) \rightarrow 4d \langle x \rangle \equiv F \quad (15)$$

where F is the effective field, which behaves as an external electric field. So, (14) becomes a sum of non-interacting Hamiltonians:

$$H = \sum_n \left[-\frac{1}{2m} \nabla_n^2 + \left(2d - \frac{a}{2}\right) x_n^2 + \frac{a}{4} x_n^4 - F x_n \right] = H_0 + V \quad (16)$$

with

$$H_0 = \sum_n \left[-\frac{1}{2m} \nabla_n^2 + \left(2d - \frac{a}{2}\right) x_n^2 + \frac{a}{4} x_n^4 \right] \quad (17)$$

and the physics of the system can be obtained from the one-particle Hamiltonian:

$$H_{MF} = -\frac{\nabla^2}{2m} + \left(2d - \frac{a}{2}\right) x^2 + \frac{a}{4} x^4 - Fx \equiv H_{MF}^{(0)} - Fx \quad (18)$$

where we put

$$H_{MF}^{(0)} = -\frac{\nabla^2}{2m} + \left(2d - \frac{a}{2}\right) x^2 + \frac{a}{4} x^4 \quad (19)$$

The average of the reduced coordinate x is given by:

$$\langle x \rangle = \frac{1}{Z} \text{Tr} [-\beta (H_0 - Fx)] = \frac{1}{\beta} \frac{\partial \ln Z}{\partial F} \quad (20)$$

with

$$Z = \sum_n \exp(-\beta E_n) \quad (21)$$

The condition (20) is a self-consistent equation for $\langle x \rangle$, as this quantity enters also in the expression of Z . The phase transition is given by the condition $\langle x \rangle = 0$. It will be put in a more convenient form in the next paragraph.

Taking the derivative with respect to $\langle x \rangle$ in the both sides of equation (20), we get:

$$1 = \frac{1}{\beta_c} \frac{\partial^2 \ln Z}{\partial \langle x \rangle \partial F} \Big|_{\langle x \rangle=0} = \frac{4d}{\beta_c} \frac{\partial^2 \ln Z}{\partial F^2} \Big|_{\langle x \rangle=0} \quad (22)$$

where we put, according to (19),

$$F = 4d \langle x \rangle \quad (23)$$

In the same time:

$$\begin{aligned} \frac{\partial^2 \ln Z}{\partial F^2} \Big|_{\langle x \rangle=0} &= \beta^2 \left\{ \frac{1}{Z} \frac{\partial^2 Z}{\partial F^2} - \left(\frac{1}{Z} \frac{\partial Z}{\partial F} \right)^2 \right\} \Big|_{\langle x \rangle=0} = \\ &= \beta^2 \left[\langle x^2 \rangle - \langle x \rangle^2 \right] \Big|_{\langle x \rangle=0} = \beta^2 \langle x^2 \rangle \Big|_{\langle x \rangle=0} \end{aligned} \quad (24)$$

Consequently, the critical equation (22) can be written as:

$$1 = 4d\beta_c \langle x^2 \rangle \Big|_{\langle x \rangle=0} \quad (25)$$

Coming back now to the factor AC/B , previously omitted for reasons of simplicity, and replacing the reduced coordinate x with the physical one X , we get:

$$1 = \frac{4d}{T_c} C \langle X^2 \rangle \Big|_{\langle X \rangle=0} \quad (26)$$

where T_c is the critical temperature of the phase transition.

The susceptibility of this system can be obtained as derivative of $\langle X \rangle$ with respect to the effective field F . We get from (20):

$$\chi = \frac{\partial \langle X \rangle}{\partial F} \Big|_{F=0} = \beta_c \langle X^2 \rangle \Big|_{F=0} \quad (27)$$

As the condition $F = 0$ is equivalent with $\langle X \rangle = 0$, using (24) and (25), we obtain the condition:

$$4dC\chi = 1 \quad (28)$$

This relation is remarkable, because the phase transition in the system (18) can be obtained using only the simpler, "unperturbed" Hamiltonian, H_0 , defined in the equation (19).

In spite of the simplification produced by the mean field approximation, even the problem of obtaining the eigenfunctions and the eigenvalues of this "simpler" Hamiltonian, necessary for the evaluation of the matrix elements entering in (11), is not very simple. Actually, there are neither exact solutions, nor simple approximations, suitable for thermodynamic applications, as explained in the Introduction. In order to overcome this difficulty, we shall replace the quartic anharmonic potential with a two well rectangular symmetric potential. It maintains the basic physical features of the quartic potential and admits at least one simple approximate solution, useful for obtaining the thermodynamical properties of the system - in particular, of the critical temperature of the phase transition.

5. THE TWO WELL RECTANGULAR SYMMETRIC POTENTIAL

The particular two well rectangular symmetric potential considered here is an one-dimensional infinite square well, of length $2a + b$, with a rectangular step of height V_0 and length b , placed symmetrically at its bottom. We shall study the movement of a particle of mass μ , in the case analyzed by Ter Haar [38], Ch. II, problem 8, when:

$$\frac{2\mu V_0 b^2}{\hbar^2} \gg 1 \quad (29)$$

This means that the step is high, so the ground state energy E^- is close to the bottom of the well and far from the top of the step:

$$E^- \ll V_0 \quad (30)$$

Also, as the two wells of length a are separated by a large step, E can be reasonably approximated by the ground state of a particle of same mass, in an infinite square well of length a :

$$E_0 = \frac{\pi^2 \hbar^2}{2\mu a^2} = \frac{\pi^2 k_0^2}{2\mu}, \quad k_0 = \frac{\pi}{a} \quad (31)$$

This approximation is useful for our problem as only the first two states of the anharmonic potential, or of the two well rectangular potential more or less equivalent to it, are important in the critical behavior. Due to the tunneling, the energy E^+ of the first excited state is very close to E^- , and the energy of the second excited state E_3 is much larger than both E^- and E^+ , so its statistical weight $\exp(-\beta E_3)$ is negligibly small. So, the critical behavior is decided by the first two states of the model Hamiltonian.

In order to conveniently write the wave functions and energies corresponding to the ground state ψ^- , E^- and to the first excited state ψ^+ , E^+ , it is useful to

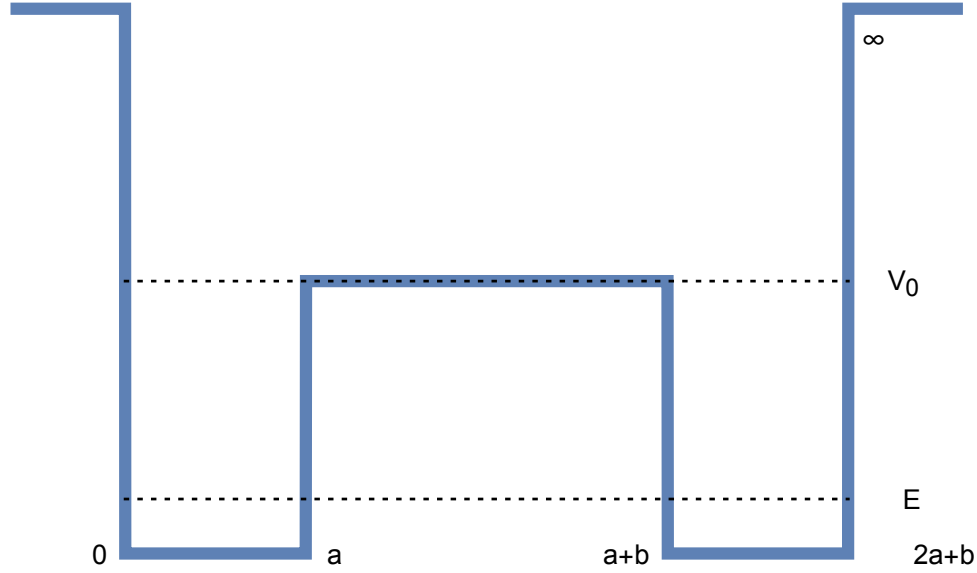


Fig. 1 – The two well rectangular symmetric potential; the lateral branches are infinitely high.

introduce the following notations:

$$q_0 = \frac{\sqrt{2\mu(V_0 - E_0)}}{\hbar} = \sqrt{\left(\frac{2\mu V_0}{\hbar^2} - \frac{\pi^2}{a^2}\right)} \quad (32)$$

or:

$$q_0 = \frac{P_b}{b} \sqrt{1 - \frac{\pi^2}{P_a^2}} \quad (33)$$

where we put

$$P_a^2 = \frac{2\mu V_0}{\hbar^2} a^2, \quad P_b^2 = \frac{2\mu V_0}{\hbar^2} b^2 \quad (34)$$

It is well known, from the study of the finite square well, that the dimensionless quantity, including parameters related both to the particle (μ) and the well (a, V_0), namely the quantity P_a given by the previous equation, is called "strength" of the well. We shall consider that a and b are comparable; so the condition (33) means

$$P_a^2 \gg 1, \quad P_b^2 \gg 1 \quad (35)$$

and $q_0 b$ is a "large" quantity,

$$q_0 b \gg 1 \quad (36)$$

The wave vector and the energies of the ground state and of the first excited one are:

$$k^\pm = \frac{\pi}{a} - \frac{k_0}{aq_0} \mp 2 \frac{k_0}{aq_0} e^{-q_0 b} \quad (37)$$

$$E^\pm = E_0 - \frac{2E_0}{aq_0} \left(1 \mp 2e^{-q_0 b} \right) \quad (38)$$

The wave functions of these states are:

$$\psi^- = \begin{cases} \frac{1}{\sqrt{a}} \sin k^- x, & 0 < x < a \\ \frac{1}{\sqrt{a}} \frac{k_0}{q_0} (e^{-q_0(x-a)} + e^{-q_0(a+b-x)}), & a < x < a+b \\ \frac{1}{\sqrt{a}} \sin k^- (2a+b-x), & a+b < x < 2a+b \end{cases} \quad (39)$$

$$\psi^+ = \begin{cases} \frac{1}{\sqrt{a}} \sin k^+ x, & 0 < x < a \\ \frac{1}{\sqrt{a}} \frac{k_0}{q_0} (e^{-q_0(x-a)} - e^{-q_0(a+b-x)}), & a < x < a+b \\ -\frac{1}{\sqrt{a}} \sin k^+ (2a+b-x), & a+b < x < 2a+b \end{cases} \quad (40)$$

The alternances of sign in (39), (40) are due to the alternances in parity (ψ^- is even, and ψ^+ is odd). For thermodynamic applications, the following relation is important:

$$\langle x\psi^-(x)\psi^+(x) \rangle = \frac{(2a+b)(2ak_0 - \sin 2ak_0)}{4ak_0} - \frac{1}{3}a^2(2a+b)d_0^2 + \mathcal{O}(d_0^4) \quad (41)$$

where

$$d_0 = 2 \frac{k_0}{q_0} e^{-q_0 b} \quad (42)$$

Clearly,

$$\sin 2ak_0 = -\sin \frac{\pi}{a} \frac{1}{aq_0} \simeq -\frac{\pi}{a^2 q_0} \ll 1 \quad (43)$$

so, taking into account (29),

$$\langle x\psi^-(x)\psi^+(x) \rangle = \frac{(2a+b)(2ak_0)}{4ak_0} \simeq a + \frac{b}{2} \quad (44)$$

6. THE SYMMETRIC RECTANGULAR WELL AND THE PHYSICS OF QUANTUM WELLS AND QUANTUM DOTS

We shall discuss now another application of the symmetric rectangular well, which can be developed using the method outlined in the previous subsections. Actually, we shall describe some applications in nanophysics of the simple quantum mechanical problems, where various types of rectangular potentials are involved. The simplest example is provided by the finite rectangular well, which is a useful starting point for understanding the physics of quantum wells and quantum dots. A

physically more interesting is a spherically symmetric potential, its radial part being a step function. Piecewise-defined, locally constant radial functions describe multi-shell spherical quantum dots [39] - [46].

Other examples of quantum dots are cubic - or rectangular - cavities. In spite of the differences between spherical or rectangular cavities, the mathematical methods for obtaining the wave functions and wave vectors are quite similar. The similarity between the 1D cartesian wave equation in a rectangular geometry, and the radial equation in a spherical geometry, are more pronounced for low values of quantum radial number l , and they are almost identical for $l = 0$. So, the results obtained for rectangular wells can be easily transferred to spherical cavities of zero angular momentum.

The double quantum dots are aggregates composed by two quantum dots, used as constitutive components of a large number of electronic or opto-electronic devices. If the shape of each quantum dot can be approximated with a parallelepiped, the "artificial molecule" formed in this way can be studied using the model of the rectangular symmetric two well potential. So, the methods used to get analytical approximations for the particle energy in such potentials have interesting applications in the physics of quantum dots.

7. THE SUSCEPTIBILITY AND THE CRITICAL EQUATION FOR THE RECTANGULAR POTENTIAL

As the energy of first two levels are very close, and much smaller than the next ones,

$$Z_0 \simeq e^{-\beta E^-} + e^{-\beta E^+} \simeq 2e^{-\beta E_0 \left(1 - \frac{2}{aq_0}\right)} \quad (45)$$

we get:

$$\chi \simeq \frac{2}{Z_0} \frac{e^{-\beta E^+}}{E^+ - E^-} |\langle \psi^- | x | \psi^+ \rangle|^2 \quad (46)$$

With (38):

$$E^+ - E^- = 2E_0 \left(1 - \frac{2}{aq_0}\right) \quad (47)$$

and with (44):

$$\chi \simeq \frac{q_0 \mu a^3}{2\pi^2 \hbar^2} e^{q_0 b} e^{-\frac{4\beta E_0}{aq_0}} \left(a + \frac{b}{2}\right)^2 \quad (48)$$

or:

$$q_0 e^{\chi_0 b} \exp\left(-\frac{2\pi^2 \hbar^2}{q_0 a^3 \mu}\right) = \text{const} \quad (49)$$

Defining an effective temperature τ :

$$\tau = \frac{a^3 \mu}{2\pi^2 \hbar^2 b \beta} \quad (50)$$

and an effective V_0 -depending, dimensionless parameter q :

$$q_0 b = q \quad (51)$$

we obtain the following critical equation:

$$q e^{q - \frac{\tau}{q}} = \text{const}, \quad (52)$$

or the following expression of reduced temperature, as function of potential:

$$\tau = q \left(q + \ln \frac{q}{q_0} \right) \quad (53)$$

So, the transition temperature increases with the height of the on-site barrier, which is an intuitive result.

The classical limit, $\hbar \rightarrow 0$, cannot be taken, as, in this case, the first two levels would coincide it can be obtained only if we include in calculation the third energy level.

If $T = 0$, according to (13):

$$\chi(T = 0) \simeq 2 \frac{\mu a^2 (2a + b)}{\pi^2 \hbar^2 \left(1 - \frac{2}{a q_0} \right)} \quad (54)$$

With (33), (34), (35):

$$\frac{1}{\chi(T = 0)} \simeq \frac{\pi^2 \hbar^2}{2\mu a^2 (2a + b)} \left(1 - \frac{2}{a} \frac{\hbar}{\sqrt{2\mu V_0}} \right) \quad (55)$$

If V_0 increases, the zero-temperature limit of the susceptibility decreases - an intuitive result.

For high steps, *i.e.* for large values of V_0 ,

$$q_0 \simeq \frac{\sqrt{2\mu V_0}}{\hbar}, \quad P_b^2 = \frac{2\mu V_0}{\hbar^2} b^2 \quad (56)$$

and the $T = 0$ susceptibility becomes:

$$\chi(T = 0) \simeq 2 \frac{\mu a^2 (2a + b)}{\pi^2 \hbar^2 \left(a \frac{\sqrt{2\mu V_0}}{\hbar} - 2 \right)} a \frac{\sqrt{2\mu V_0}}{\hbar} \quad (57)$$

8. CONCLUSIONS

We studied the phase transitions in a rectangular lattice, with on-site oscillators, interacting by elastic forces with their first order neighbors. We started with quantum quartic oscillators and, using a mean field approach, replaced the exact Hamiltonian with a sum of one particle Hamiltonians, in a weak external field. We obtained the expression of the dielectrical susceptibility of this mean-field Hamiltonian, and a convenient relation for the critical temperature of the phase transition. As this relation is too complicated to obtain an explicit expression of the critical temperature, we replace the two well quartic oscillator with a quite similar one - the two well rectangular potential. It preserves the main features of the quartic one and generates a critical equation of tractable form. In this way, we obtain a simple relation for the critical temperature this quantity increases with height of the step contained by the rectangular well - which corresponds qualitatively to the anharmonicity of the quartic potential.

In this way, we obtain a toy model for phase transitions in anharmonic solids - actually, as many toy models as tractable two well potentials can imagine.

REFERENCES

1. L.D. Landau, E.M. Lifshitz: Physique statistique, Ed. Mir, Moscou, 1972
2. R.A. Cowley, *Adv.Phys.* **29**, 1 (1980)
3. A.D. Bruce, *Adv.Phys.* **29**, 111 (1980)
4. D.J. Scalapino, M. Sears, R.A. Ferrell, *Phys.Rev.* **B6**, 3409 (1972)
5. B. Stoeckly, D.J. Scalapino, *Phys.Rev.* **B11** 205 (1975)
6. B. Stoeckly, *Phys.Rev.* **B14**, 1271 (1976)
7. T.D. Schultz, D.C. Mattis, E.H. Lieb, *Rev.Mod.Phys.* **36**, 856 (1964)
8. G.D. Mahan: Many-particle physics, Plenum Press (1990)
9. V. Bârsan, *Rev.Roum.Phys.* **30**, 775 (1985)
10. V. Bârsan, *J.Phys.:Cond.Matter* **1**, 7961 (1989)
11. V. Bârsan, *J.Phys.:Cond.Matter* **2**, 4815 (1990)
12. V. Bârsan, S.Cojocaru, *Rom.Rep.Phys.* **58**, 123 (2006)
13. S. Cojocaru, V. Bârsan, A.Ceulemans, *physica status solidi B* **243** 1963 (2006)
14. S. Cojocaru, V. Bârsan, A.Ceulemans, *J.Mag.Magn.Mat.* **307**, 62 (2006)
15. S. Cojocaru, V. Bârsan, A.Ceulemans, *Philos.Mag.* **86**, 4983 (2006)
16. R. Toral, A. Chakrabarti, *Phys.Rev.* **B42**, 2445 (1990)
17. W. Janke, T. Sauer, *J.Stat.Phys.* **78**, 759 (1995)
18. W. Loinaz, R.S. Willey, *Phys.Rev.* **D58** 076003 (1998)
19. V.V. Savkin, A.N. Rubtsov, T. Jasen, *Phys.Rev.* **B65**, 214103 (2002)
20. V.V. Savkin, A.N. Rubtsov, *J.Exp.Theor.Phys.* 91, 1204 (2000); arXiv:cond-mat/0112429v2 (2002)
21. V. Bârsan, *J.Phys.:Condensed Matter* **18**, 9275 (2006)
22. V. Bârsan, *J.Phys.:Condensed Matter* **20**, 019701 (2008)
23. V. Bârsan, *The Ramanujan Journal*, **20**, 153 (2009)

24. V. Bârsan, *Philos. Mag.* **87**, 1043 (2007)
25. V. Bârsan, *Philos. Mag.* **88**, 121 (2008)
26. V. Bârsan, *Philos. Mag.* **91**, 477 (2011)
27. V. Bârsan, *Rom.Rep.Phys.* **60**, 205 (2008)
28. V. Bârsan, *Rom.Rep.Phys.* **62**, 219 (2010)
29. R. Lungu, *Optoel. Adv. Mat.-Rapid Comm.* **5**, 1223 (2011)
30. Yu. Ilinskii, L. V. Keldysh: *Electromagnetic response of material media*, Plenum Press (1994)
31. G. Ciobanu: *The dielectric susceptibility* (unpublished)
32. C.M. Bender, T.T. Wu, *Phys.Rev.* **184**, 1231 (1969); *Phys.Rev.* **D7**, 1620 (1973)
33. G. Ciobanu, V. Bârsan, A. T. Mincu, *Rom.J.Phys.* **55**, 539 (2010)
34. E. A. Johnson, H. T. Williams, *Amer.J.Phys.* **50**, 239 (1982)
35. R. Blinc, B. Zeks: *Soft modes in ferroelectrics and antiferroelectrics*, North Holland Publishing Company (1974)
36. A. Strukov, A.P. Levanyuk: *Ferroelectric phenomena in crystals*, Springer (1998)
37. K. Rabe, C. H. Ahn, J.-M. Triscone (Eds.): *Physics of ferroelectrics*, Springer (2007)
38. D. ter Haar: *Selected Problems in Quantum Mechanics*, Infosearch Limited, London (1964)
39. V. Bârsan: *Square wells, quantum wells and ultra-thin metallic films*, *Philos. Mag.* **94**, 190-207 (2014)
40. V. Bârsan, M.-C. Ciornei: *Semiconductor quantum wells with BenDaniel–Duke boundary conditions*, *Eur. J. Phys.* **38**, 015407 (2017)
41. V. Bârsan: *Garrett approximation revisited*, *Eur. J. Phys.* **41** 025404 (2020)
42. V. Bârsan: *Quantum Wells and Ultrathin Metallic Films*, in *Heterojunctions and Nanostructures*, Ed.: V. Stavrou, InTech, (2018)
43. V. Bârsan: *Semiconductor QWs with BenDaniel-Duke boundary conditions*, in: R. Inguanta (Ed.): *Semiconductors*, InTech, (2018)
44. V. Bârsan, *Rom.Rep.Phys.* **64**, 685 (2012)
45. V. Bârsan, R. Dragomir, *Optoel.Adv.Mat. - Rapid Comm.*, **6**, 917 (2012)
46. V.V. Mitin, D. I. Sementsov, N. Z. Vagidov, *Quantum mechanics for nanostructures*, Cambridge University Press (2012)