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Remarks on the Choice of Trial Hamiltonians for the Quantum Statistical Treatment of Anharmonic Systems

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The use of the Variational Method to discuss Quantum Statistical Mechanics of anharmonic systems requires, in order to be able to obtain the correct classical limit, the allowance for renormalization of every operator whose definition depends of the harmonic coefficients. The point is exhibited for a single anharmonic oscillator. In this particular case there is no need for mass renormalization.

A utilização do Método Variacional no estudo estatístico de sistemas anarmônicos exige, para poder obter o limite clássico correto, a renormalização de todos os operadores cuja definição depende dos coeficientes anarmônicos. Este ponto é ilustrado com um oscilador anarmônico. Neste caso particular é desnecessário renormalizar a massa.

1. INTRODUCTION

The Variational Method in Statistical Mechanics[1,2] is widely used to study a great number of anharmonic classical or quantum systems, assemblies of interacting fermions or bosons, etc (see, for example, Refs. |3| to |7|). If it is true that in Classical Statistics the use of this method presents no particular problems, this is not the case in Quantum Statistics, where some care is needed to avoid a subtle - but severe - error, which is unfortunately commited from time to time in the general literature in Physics. The problem appears in Hamiltonians of the type* $\sum_q \omega_q a_q^+ a_q$ + anharmonic terms, *every time that the frequency* ω_q *enters in the definition of the creation and annihilation operators* - as it is namely the case of quantum oscillators -. If we want to treat the Statistics of this problem by proposing a trial harmonic Hamiltonian, we might hesitate between $\sum_q \Omega_q a_q^+ a_q$ (where the operators are defined with the frequency ω_q) and $\sum_q \Omega_q A_q^+ A_q$ (where the operators are defined with the renormalized frequency Ω_q), or even some other choice. It is the aim of this paper to prove that the second possibility is the only coherent choice to be done. This care must be indistinctly taken for fermions (electrons, holes, etc) or bosons (phonons, magnons, plasmons, etc), however the point is exhibited here only for a single anharmonic oscillator. Furthermore it is also shown (Section 4) that in this case there is no need to renormalize the mass of the oscillator. Let us finally emphasize that the point we are dealing with in the present work, must be correctly taken into account in any renormalized - phonon - theory (as those leading, for example, to the calculation of the Debye-Waller factor in crystals). In Section 2 we solve, within the Variational Approximation, the single anharmonic oscillator in Classical Statistics; and in Section 3 we present the wrong and right uses of the Variational Method in Quantum Statistics.

2. CLASSICAL STATISTICS

Let us assume we have a one dimensional anharmonic oscillator whose Hamiltonian is given by**

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + bx^4 \tag{1}$$

* For the general form of the harmonic part, see for example, Ref.8.

**In order to make our discussion as clear as possible, we shall not include terms in x^3.

where m, ω and b are real positive constants, and let the oscillator be in thermal equilibrium at temperature T. We intend to solve this problem within the framework of the Variational Method in Classical Statistical Mechanics, by using the trial Hamiltonian

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\Omega^2 x^2 \qquad (2)$$

where $\Omega \equiv \omega\nu$ is to be found as a function of temperature. The variational free energy is given by

$$\tilde{F} = F_0 + \langle H-H_0\rangle_0 = F_0 + \frac{1}{2} m\omega^2(1-\nu^2)\langle x^2\rangle_0 + 3b\langle x^2\rangle_0^2$$

where F_0 is the free energy associated to H_0, $\langle\ldots\rangle_0$ denotes a mean value calculated with a Gaussian law proportional to e^{-H_0/k_BT}, and where we have used the well known Gaussian property $\langle x^4\rangle_0 = 3\langle x^2\rangle_0^2$. The minimization condition leads to

$$\nu^2 - 1 - \frac{12b\langle x^2\rangle_0}{m\omega^2} = 0$$

where we have used that $\partial F_0/\partial\nu = m\omega^2\nu\langle x^2\rangle_0$. By using the equipartition principle (which, in this case, states $\frac{1}{2} m\omega^2\nu^2\langle x^2\rangle_0 = \frac{1}{2} k_BT$, this equation may be rewritten as follows

$$\nu^4 - \nu^2 - \frac{12bk_BT}{m^2\omega^4} = 0 \quad \text{(See Fig.1)} \qquad (3)$$

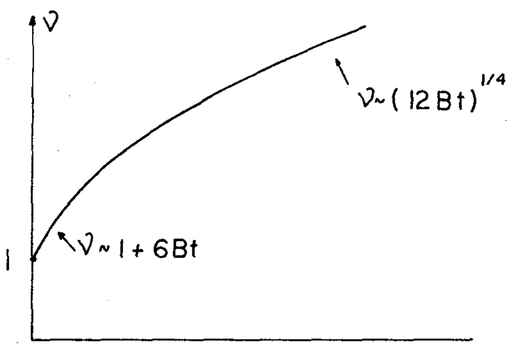

Fig.1 - The classical thermal behaviour of the reduced frequency $\nu \equiv \Omega/\omega$ ($t \equiv k_BT/\hbar\omega$ and $B \equiv \hbar b/m^2\omega^3$).

3. QUANTUM STATISTICS

We pretend to study here the Quantum Statistics of the same system as before (Hamiltonian given by (1)) within the same variational framework. If we entend to work in the (x,p) representation [1] there is no doubt that the trial Hamiltonian to be considered is the one given by (2). But if we entend to work in the creation and annihilation operators - representation, the problem appears of how to define these operators (by using the old or the renormalized frequency?). In order to make the point clear, we hsall perform the calculation in both possibilities, and it will become evident that we must necessarily choose the second one.

3a. The Wrong Choice

Let us assume a trial Hamiltonian

$$H_0 = \hbar\Omega(a^+a + \frac{1}{2}) \tag{4}$$

where $\Omega \equiv \omega\nu$ is to be found, and

$$x = (\hbar/2m\omega)^{1/2} (a^+ + a)$$

$$p = i(\hbar m\omega/2)^{1/2} (a^+ - a)$$

$$[a,a^+] = 1$$

It follows easily that

$$<H>_0 = \hbar\omega \{(<a^+a>_0 + \frac{1}{2}) + 3B(<a^+ a>_0 + \frac{1}{2})^2\}$$

where $B \equiv \hbar b/m^2\omega^3$ and $<...>_0$ denotes the canonical mean value taken with e^{-H_0/k_BT}. The variational free energy is given by

$$\bar{F} = F_0 + \hbar\omega \{(1-\nu)z + 3Bz^2\}$$

where

$$r_0 = k_B T \ \ell n \ (2 \ \mathrm{sh} \ \frac{\nu}{2t}) \quad ,$$

$$z \equiv \langle a^+ a \rangle_0 + \frac{1}{2} = \frac{1}{2} \coth \frac{\nu}{2t} \quad ,$$

and

$$t \equiv k_B T/\hbar \omega$$

The minimization condition $\partial\bar{F}/\partial\nu = 0$ leads to

$$\nu - 1 - 3B \coth \frac{\nu}{2t} = 0$$

In the classical limit $t \to \infty$, this expression assymptotically becomes

$$\nu^2 - \nu - 6Bt = 0$$

which is different from (3), thus the trial Hamiltonian (4) is unacceptable.

3b. The Right Choice

Let us now assume a trial Hamiltonian

$$H_0 = \hbar\Omega(A^+A + \frac{1}{2}) \qquad (5)$$

where $\Omega \equiv \omega\nu$ is to be found, and

$$x = (\hbar/2m\omega\nu)^{1/2} \ (A^+ + A) \ ,$$

$$p = i(\hbar m\omega\nu/2)^{1/2} \ (A^+ - A) \ ,$$

$$[A, A^+] = 1$$

It follows now that

$$\langle H \rangle_0 = \hbar\omega \ \{\frac{1}{2} \ (\nu + \frac{1}{\nu})(\langle A^+A \rangle_0 + \frac{1}{2}) + \frac{3B}{\nu^2} \ (\langle A^+A \rangle_0 + \frac{1}{2})^2\}$$

The variational free energy is given by

$$\bar{F} = F_0 + \hbar\omega \ \{\frac{1}{2} \ (\frac{1}{\nu} - \nu)z + \frac{3B}{\nu^2} \ z^2\}$$

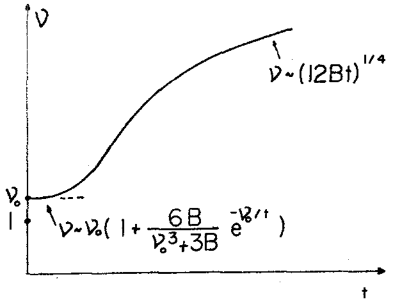

FIG. 2

Fig.2 - The quantum thermal behaviour of the reduced frequency $\nu \equiv \Omega/\omega$ ($t \equiv k_B T/\hbar\omega$, $B \equiv \hbar b/m^2\omega^3$ and $\nu_0^3 - \nu_0 = 6B$).

where

$$F_0 = k_B T \ \ell n \ (2 \ \mathrm{sh} \ \frac{\nu}{2t})$$

and

$$z \equiv \langle A^+ A\rangle_0 + \frac{1}{2} = \frac{1}{2} \coth \frac{\nu}{2t}$$

The minimization condition $\partial\bar{F}/\partial\nu = 0$ leads now to

$$[\nu^4 - \nu^2 - 12B\nu z]\left[1 + \frac{\nu}{zt}\left(z^2 - \frac{1}{4}\right)\right] = 0$$

hence (after elimination of the spurious solution)

$$\nu^3 - \nu - 6B \coth \frac{\nu}{2t} = 0 \qquad \text{(See Fig.2)} \qquad (6)$$

In the classical limit $t \to \infty$ this expression exactly becomes expression (3), *as it should*. It is now clear that, for being consistent, we must *renormalize the creation and annihilation operators* as well as the frequency.

In the limit $t \to 0$ we obtain

$$\nu \sim \nu_0 \left(1 + \frac{6B}{\nu_0^3 + 3B} e^{-\nu_0/t}\right)$$

where $\nu_0^3 - \nu_0 - 6B = 0$ (hence* $\nu_0 > 1$ if $B > 0$).

* The fact that $T = 0$ leads to $\Omega > \omega$ is a quantum effect related to the energy $\hbar\Omega/2$ of the fundamental state.

4. MASS RENORMALIZATION

Let us now examine another aspect: is it necessary or convenient (in the sence of achieving a better minimization of $\bar{F}$) to renormalize the mass? In Classical Statistics the answer is obviously *no*, as the commutation between x and p leads to a complete factorization of the probability law. However in Quantum Statistics the point must be more carefully analysed. Our Hamiltonian is still given by (1) but we propose now the following trial Hamiltonian

$$H_0 = \frac{p^2}{2M} + \frac{1}{2} M\Omega^2 x^2 = \hbar\Omega(A^+A + \frac{1}{2})$$

where $\Omega \equiv \omega\nu$ and $M \equiv m\mu$ are to be found as functions of temperature, and where

$$x = (\hbar/2m\omega\mu\nu)^{1/2} (A^+ + A) ,$$

$$p = i(\hbar m\omega\mu\nu/2)^{1/2} (A^+ - A) ,$$

$$[A, A^+] = 1$$

It follows that*

$$\langle H\rangle_0 = \hbar\omega \{\frac{1}{2} (\mu\nu + \frac{1}{\mu\nu}) (\langle A^+A\rangle_0 + \frac{1}{2}) + \frac{3B}{\mu^2\nu^2} (\langle A^+A\rangle_0 + \frac{1}{2})^2\}$$

and

$$\langle H_0\rangle_0 = \hbar\omega\nu (\langle A^+A\rangle_0 + \frac{1}{2})$$

hence

$$\bar{F} = F_0 + \hbar\omega \{[\frac{1}{2} (\mu\nu + \frac{1}{\mu\nu}) - \nu]z + \frac{3B}{\mu^2\nu^2} z^2\}$$

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* Looking at the expression of $\langle H\rangle_0$ (where μ appears everywhere in the form $\mu\nu$), one might be tempted to think that any eventual mass renormalization could be absorbed into the frequency renormalization: this is not necessarily so as it becomes clear looking, for example, at the expression of $\langle H_0\rangle_0$.

where

$$F_0 = k_B T \ \ln \left(2 \ \ \mathrm{sh} \ \frac{\nu}{2t}\right)$$

and

$$z \equiv \langle A^+ A \rangle_0 + \frac{1}{2} = \frac{1}{2} \ \coth \ \frac{\nu}{2t}$$

The minimization conditions $\partial\bar{F}/\partial\nu = 0$ and $\partial\bar{F}/\partial\mu = 0$ lead quite straightforwardly to expression (6) and $\mu = 1$. So in spite of the non-commutativity of x and p, the mass need not to be renormalized.

5. CONCLUSION

Let us conclude by saying that if we intend to use the Variational Method for studying the Statistics of an assembly of interacting bosons or fermions, we *must* allow (besides the obvious renormalization of the frequencies) for the renormalization of all the operators whose definitions includes those frequencies, otherwise the quantum results will not reproduce the classical ones in the limit $\hbar \to 0$. Put in this way this statement might sound trivial, however experience proves that, within renormalized self-consistent statistical treatments of complicate anharmonic systems, this point can dangerously be overlooked. Let us also recall that we have conclude that in the particular case of a single anharmonic oscillator there is no need for renormalization of its mass.

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