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Spectral and thermodynamical properties of systems with noncanonical commutation rules: semiclassical approach

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We study different quantum one dimensional systems with noncanonical commutation rule $[x,p]=i\hbar(1+sH),$ where H is the one particle Hamiltonian and s a parameter. This is carried-out using semiclassical arguments and the surmise $\hbar\rightarrow\hbar(1+sE),$ where E is the energy. We compute the spectrum of the potential box, the harmonic oscillator, and a more general power-law potential $|x|^{\nu}$. With the above surmise, and changing the size of the elementary cell in the phase space, we obtain an expression for the partition function of these systems. We calculate the first order correction in s for the internal energy and heat capacity. We apply our technique to the ideal gas, the phonon gas, and to N non-interacting particles with external potential like $|x|^{\nu}$.

Keywords: Quantum statistical mechanics; quantum mechanics; semiclassical theories; thermodynamics.

Estudiamos diferentes sistemas cuánticos en dimensión uno y con relación de conmutación $[x,p]=i\hbar\,(1+sH)$, donde H es el Hamiltoniano de la partícula y s un parámetro. Esto se realiza usando argumentos semi-clásicos y la proposición $\hbar\rightarrow\hbar\,(1+sE)$, donde E es la energía. Calculamos el espectro de la caja de potencial, el oscilador armónico y el caso mas general para la energía potencial $|x|^{\nu}$. Con dicha proposición, y cambiando el tamaño de la celda elemental en el espacio de fase, obtenemos una expresión para la función partición del sistema. Calculamos en primer orden en s la energía interna y capacidad calórica. Aplicamos este método a un gas ideal, gas de fonónes y a N partículas sin interacción en un campo externo del tipo $|x|^{\nu}$.

Descriptores: Mecánica cuántica estadística; mecánica cuántica; teorías semiclásicas; termodinámica.

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1. Introduction

In one dimension, some authors [1-9] have showed that a modification of the usual commutation rule for the momentum and position operators,

$$[x,p]=i\hbar\{1+sH(x,p)\}, \tag{1}$$

with s a parameter and H the Hamiltonian of the system, produces new phenomena which appear, for instance, in high energy physics and mesoscopic systems. In Ref. 1 it was shown that for some commutation relation like (1), space discreteness is compatible with Lorentz transformation. This fact was explicitly related to atomic phenomena. In Refs. 2 and 3 the mass-spectrum for elementary particles was obtained from (1), with H the Hamiltonian of the harmonic oscillator and, applied for energy of the order of GeV-Tev (10^9-10^{12} eV). In Ref. 4 it was shown that, for the free particle Hamiltonian, (1) produces space quantization. This result can be related with quark confinement phenomena. Moreover, in Refs. 5 and 6 mathematical aspects of (1) were studied. In Refs. 7-10 it was found that charge discreteness in mesoscopic circuits can be mathematically formulated with commutation relations similar to (1) between charge and current. This theory becomes related to the descriptions of phenomena like persistent current in a ring of inductance L, Coulomb blockage phenomena in a pure capacitor-design [7], or current magnification [10]. In these cases the parameter s becomes related to the elementary charge q_e by the relationship $s=Lq_e^2/\hbar^2$. The analogy between Refs. 4 and 7 becomes from charge and space quantization. We remark that in Ref. 2 the general case $[x,p]=i\hbar f(H)$ was considered. The particular case $f=e^{sH}$ deserves some attention in our paper. In fact, thermodynamical properties are easily found in this case.

In this article we propose a method, supported with semiclassical arguments, which permits to calculate the spectrum of systems with canonical commutation relations like (1). In fact, (1) suggests a formal energy dependence of the Planck constant $\hbar$ given by

$$\hbar\rightarrow\hbar\{1+sE\}. \tag{2}$$

With this surmise we reproduce the spectrum of the systems treated in [2-4] such as the harmonic oscillator, the free particle and the particle in a quantum box. Moreover, we characterize the spectrum for the power-law potential given by $U(x)=k|x|^{\nu}$.

On the other hand, we compute the thermodynamical properties of systems with noncanonical commutation rule (1). The surmise (2) introduces a new size for the elementary cell in the corresponding phase-space, and then for the number of microstates. We calculate the internal energy and the heat capacity for the ideal gas, for particles in a general potential $U \sim\mid x \mid^{\nu}$ and, finally, the phonon gas. We remark that thermodynamical properties of a mesoscopic circuit, with charge discreteness [7-10], could be studied by analogy with the mechanical case.

The paper is structured as follows: in Sec. II, we compute the spectrum of the harmonic oscillator and the potential box, in accordance with the results found in the literature. Moreover, we consider systems with potentials of the form $U \sim |x|^{\nu},\ \nu > 0$ and noncanonical commutation rule (1). In Sec. III, we study the thermodynamical properties of these systems. We calculate the density of states and, at first order in s, the internal energy and heat capacity. Finally, in Sec. IV, we give some conclusions and discussion.

2. Spectral properties: semiclassical approach

The old quantum theory (Bohr-Wilson-Sommerfeld) provides a general method for calculating spectra for some regular systems using simple rules. It works for different systems like the harmonic oscillator, the hydrogen atom, and others. In one dimension, the correspondence between classical and quantum theory is established by the non linear differential equation [11,12]

$$\frac{dE}{dn} = \hbar\omega_{cl}(E), \tag{3}$$

where $\omega_{cl}(E)$ denotes the classical frequency of a given system with energy E. In (3), $\hbar$ is the Planck's constant, and n will correspond to the quantum number. The quantization of energy results from the fact that n can take only integer values in the solution of (3). The initial condition $E(n = 0) = E_o$ corresponds to the fundamental level of energy. The deduction of (3) comes from the classical relation between the action variable I and the period of the classical orbit T_{cl} where $dI/dE = T_{cl}$ and the quantization rule $I = n2\pi\hbar$.

Our hypothesis is that, for systems with noncanonical commutation rules (1), the Eq. (3) must be modified by considering the surmise (2), namely

$$\frac{dE}{dn} = \hbar(1 + sE)\omega_{cl}(E). \tag{4}$$

Hereafter, we assume that $(1 + sE) \geq 0$. Note that (4) introduces a new fixed-point $E_f = -1/s$ which modifies the spectral structure of the system. Since $\omega_{cl} > 0$, the stability of this new fixed-point, with respect to variations of n, depends only on the sign of the parameter s.

As a first application of the semiclassical Eq. (4), we consider a particle of mass m in a quantum box potential defined by

$$U(x) = \left\{ \begin{array}{cc} 0 & \text{if } 0 < x < a \\ \infty & \text{otherwise .} \end{array} \right. \tag{5}$$

The classical frequency is given by $\omega_{cl} = (\pi/a)\sqrt{(2E/m)}$ and the Eq. (4) becomes

$$\frac{dE}{dn} = \hbar\{1 + sE\}\frac{\pi}{a}\sqrt{\frac{2E}{m}}. \tag{6}$$

For $s > 0$ the solution of (6) is given by

$$E_n = \frac{1}{s}\tan^2(\gamma n\sqrt{s}), \tag{7}$$

where $\gamma = (\pi\hbar)/(\sqrt{2m}a)$, in accordance with the result of Ref. 4. The above result shows the power of our method because the quantum calculation [4] is hard. Moreover (7) corresponds to one case of finite number of states (when $\gamma\sqrt{s} = \pi/m$, m integer). Namely, our method also applies to these cases.

As a second application we consider the harmonic oscillator $U(x) = (1/2)\omega_o^2 x^2$, where ω_o is the classical frequency. The Eq. 4 for the spectrum becomes

$$\frac{dE}{dn} = \hbar\{1 + sE\}\omega_o. \tag{8}$$

The solution of this equation is

$$E_n = (E_o + \frac{1}{s})e^{s\hbar\omega_o n} - \frac{1}{s}, \tag{9}$$

where the fundamental level $E_o = \hbar\omega_o/2$. This result is in agreement, to first order in $s\hbar\omega_o$, with Ref. 3. Note that the spectrum is unbounded when $s > 0$. Besides, if $-1/E_o < s < 0$, then in the limit $n \to \infty$ we have $E_n \to -1/s$ that corresponds to the stable fixed point of Eq. 8.

Now, we consider the general case of a particle in the potential energy

$$U(x) = k \mid x \mid^{\nu}, \tag{10}$$

where ν and k are arbitrary positive constants. In this case the system admits always classically bounded trajectories and the classical frequency is [13]

$$\omega_{cl}(E) = \alpha(k,\nu)E^{\frac{1}{2}-\frac{1}{\nu}};$$

$$\text{where} \quad \alpha(k,\nu) = \frac{\sqrt{2\pi}\nu k^{1/\nu}\Gamma(1/2 + 1/\nu)}{2\sqrt{m}\Gamma(1/\nu)}, \tag{11}$$

with Γ the Gamma function. The differential equation (4) becomes

$$\frac{dE}{dn} = \hbar\alpha(k,\nu)\{1 + sE\}E^{\frac{1}{2}-\frac{1}{\nu}}, \tag{12}$$

which could be analytically solved in some cases. Notice that (12) defines in a direct way the density of states dn/dE of these systems. This expression will be re-obtained in the next section by an adequate definition of the elementary cell volume in phase space and its thermodynamical properties.

3. Thermodynamical properties

In this section we compute thermodynamical properties of systems with noncanonical commutation rules like (1). The change in $\hbar$ (2) introduces a modification of the size of the elementary cell in the phase space and then in the number of microstates. From the number of microstates, we obtain the density of states and the partition function. As usual, the knowledge of the partition function allows us to compute the thermodynamical properties of the system. In particularly, we study the ideal gas, the phonon gas, and then we generalize these results to the case with potential (10).

In statistical mechanics [14], the number of microstates Δn with energies between E and $E+\Delta E$ is given by a semiclassical expression related to the volume in phase-space (see (13) below with $s=0$). The factor h, the size of the elementary cell in this semiclassical approach, is chosen to contact with quantum theory. Thus (2) suggests to consider for the number of microstates Δn the expression

$$\Delta n = \frac{1}{h(1+sE)} \int\limits_{E<H<E+\Delta E} dxdp. \tag{13}$$

Note that the integral in (13) coincides with the usual one ($s=0$) because the functional form of the Hamiltonian H does not change as a function of the variables x and p. The density of states $\rho = \Delta n/\Delta E$ becomes

$$\rho = \frac{\rho^{(o)}}{1+sE}, \tag{14}$$

$\rho^{(o)}$ being the usual density function. The partition function for the Boltzmann distribution is given by

$$Z = \int \frac{e^{-E/T}\rho^{(o)}}{1+sE} dE, \tag{15}$$

where we consider units so that the Boltzman's constant $k=1$. From (15) we can obtain the thermodynamical quantities. For instance, the internal energy $U = T^2 \partial \ln Z/\partial T$ becomes

$$sU = \frac{Z^{(o)}}{Z} - 1, \tag{16}$$

where $Z^{(o)}$ stands for the usual function partition ($s=0$). From (15-16), we have the first correction in the parameter s for the internal energy:

$$U = U^{(o)} - sT^2 \frac{\partial U^{(o)}}{\partial T} + O(s^2). \tag{17}$$

From (17), the heat capacity could be computed from the usual definition $C_V = \partial U/\partial T$. Note that the use of (17) is easy since one only needs to know the energy of the unperturbed system.

Recall that Eq. (17) allows us to compute the first order correction to the internal energy from the usual expression for the internal energy $U^{(o)}$. Moreover, when $U^{(o)}$ increases with temperature, for $s>0$, the new internal energy is smaller than the usual one.

For the ideal gas, where $U^{(o)} = (1/2)NT$, we have $U \approx (1/2)NT(1-sT)$ and the correction to the heat capacity is $C = (1/2)N\,(1-2sT)$. These results agree with Ref. 4.

Now we shall consider N non interacting particles in an external energy potential like (10). When $s=0$ it is direct to show that

$$Z^{(o)}{=}T^{\frac{1}{\nu}+\frac{1}{2}} \int e^{-x} x^{\frac{1}{\nu}-\frac{1}{2}} dx;\ U^{(o)}{=}\left(\frac{1}{\nu}{+}\frac{1}{2}\right) NT. \tag{18}$$

We note that the density of states can be evaluated directly from (12). Using (17) and (18) we obtain the internal energy to first order in s:

$$U = \left(\frac{1}{\nu} + \frac{1}{2}\right) NT\{1-sT\}. \tag{19}$$

While the heat capacity, to this order becomes

$$C = \left(\frac{1}{\nu} + \frac{1}{2}\right) N\,(1-2sT)\,. \tag{20}$$

where the usual harmonic oscillator corresponds to the case $\nu = 2$.

For the phonon gas at the regime of low temperature with internal energy $U^{(o)} = AT^4$, where A is a constant [14], we obtain $U \approx AT^4(1-4sT)$. The corresponding correction to the heat capacity is $C = A\left(4T - 20sT^4\right)$.

4. Conclusions and discussion

We have studied some systems with noncanonical commutation rules like (1). This was carried-out using a semiclassical method and the surmise $\hbar \to \hbar\{1+sE\}$. With this method we have reproduced the spectrum of the particle in a quantum well [4] and the harmonic oscillator [2,3]. Moreover, we have given an explicit equation to determine the spectrum of a particle in an external energy potential like $|x|^\nu$ with ν a positive constant (12).

Thermodynamical properties of a system with noncanonical commutation rules can be directly calculated, if we note that our surmise implies a change in the size of the elementary cell in phase space. We have obtained the general expression for the density of states (14) and the partition function (15). to first order in the parameter s, we have found an expression for the internal energy U as a function of the usual one $U^{(o)}$. We have applied this method to study the ideal gas, the phonon gas and the noninteracting particle in a potential like $|x|^\nu$. Thermodynamical properties were calculated using the Boltzman distribution. Since we have the density of states (14) in principle we can calculate the partition function with the Fermi-Dirac or Bose-Einstein distribution.

As mentioned in the introduction, charge quantization for mesoscopic circuits can be considered by noncanonical quantization rules like (1) [7-10]. These physical systems are today the object of research because of eventual technological applications. Our semiclassical calculation of energy spectra and thermodynamical properties is useful as a first approach to these mesoscopic systems. For instance, from the analogy between an electric circuit and the harmonic oscillator, the spectrum (9) could be related to the LC quantum circuit with charge discreteness.

As a curiosity, we remark that several experiments in particle physics show that the fine structure fine $\alpha = e^2/c\hbar$ depends on the energy [15,16]. This is usually interpreted as the change of the electron charge with the energy parameter. It seems to us that this presents an analogy with our results, namely, an energy dependence of the constant $\hbar$. This subject will be studied elsewhere.

Finally, as mentioned in the introduction, the case $\hbar \to \hbar e^{sE}$ in (2) is soluble in many cases since here

$$Z = \int e^{-E/T-sE} \rho^{(o)} dE$$

and defining the effective temperature

$$\frac{1}{*T^*} = \frac{1}{T} + s$$

then we can operate with the formal change $T \to T^*$ in any solvable thermodynamical system.

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1. H.S. Snyder, *Phys.Rev.* **71** (1947) 38.
2. I. Saavedra, *Quantum Theory And The Structure Of Time And Space*, Vol. IV, Eds.L. Castel, M. Drieshner, and C. F. von Weissacher (Carl Hausser Munich, 1981).
3. I. Saavedra and C. Utreras, *Phys. Lett. B* **98** (1981) 74.
4. S. Montecinos, I. Saavedra, and O. Kunstmann, *Phys. Lett. A* **109** (1985) 131.
5. K. Kempf, *J. Math. Phys.* **35** (1994) 4483.
6. A. Kempf, G. Mangano, and R.P. Mann, *Phys. Rev. D* **52** (1995) 1108.
7. You-Quan Li and Bin Chen, *Phys. Rev. B* **53** (1996) 4027.
8. You-Quan Li, *AIP Conference Proceeding* **545** (2000) 85.
9. You-Quan Li, “Commutation Relation In Mesoscopic Electric Circuits.” cond-mat/0009352 (unpublished).
10. J.C. Flores, *Phys. Rev. B* **64** (2001) 235309; J.C. Flores and C.A. Utreras, *Phys. Rev. B* **66** (2002) 153410.
11. A. Messiah, *Quantum Mechanics* Vol.I (North-Holland, 1975).
12. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics* (Oxford Pergamon Press, 1980).
13. L.D. Landau and E.M. Lifshitz, *Classical Mechanics* (Oxford Pergamon Press, 1980).
14. K. Huang, *Statistical Mechanics* (Wiley, 1987).
15. I. Levine *et al.*, *Phys. Rev. Lett.* **78** (1997) 424.
16. Y. Ohnishi *et al.*, *Phys. Lett. B* **313** (1993) 475.