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About Statistical Mechanics in the Configuration Space (*x*, *v*)

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Abstract

The classical and quantum Statistical Mechanics is straightforwardly formulated in the configuration space (***x***, ***v***), and an example of a system is given to make the comparison with the formulation of the Statistical Mechanics in the phase space (***x***, ***p***). It is shown that the advantage of using configuration space for system with their interaction force depends explicitly on the velocity of the bodies. In addition, for these types of systems it is shown that their partition function can be well defined in the configuration space but it is not defined in the phase space, or they can bring about different results, bringing the possibility of experimental verification of the formulation of Statistical Mechanics in the configuration space.

Keywords

Classical Statistical Mechanics, Constant of Motion, Quantum Statistical Mechanics

1. Introduction

It is well known that the formulation of the Statistical Mechanics for conservative systems in the phase space $(\mathbf{x},\mathbf{p})$ [1]-[7]. As we know, this formulation is based mainly on a scalar function $H = H(\mathbf{x},\mathbf{p})$, where $\mathbf{x},\mathbf{p} \in \Re^{3N}$ and N the number of identical particles. This function is called the Hamiltonian of the system. However, as it is also well known, the Hamiltonian and Lagrangian formulations of Classical Mechanics are not free of mathematical ambiguities [8]-[12]. For example: Lagrangian and Hamiltonian are not unique since for any conservative system one can add an arbitrary time depending function, having the same equations for the conservative dynamical system. Therefore, exists a no numerable set Lagrangian and Hamiltonian associated to the same conservative system, and one has always the same trivial relation between the generalized linear momentum and the Lagrangian, $\mathbf{p} = \partial L/\partial \mathbf{v} = m\mathbf{v}$. For explicitly velocity dependence dynamical system, but time explicitly independence (what is called an autonomous dynamical system), the situation is more complicated since one does not have the above trivial relation between the coordinate $\mathbf{p}$ and the coordinate $\mathbf{v}$, but one has a relation of the form $\mathbf{p} = \mathbf{p}(\mathbf{x}, \mathbf{v})$ where the inverse relation $\mathbf{v} = \mathbf{v}(\mathbf{x}, \mathbf{p})$ not necessarily can be obtain, and the Hamiltonian can no be found explicitly. In addition for these type of autonomous system, one can find two functionally different Hamiltonian for the same autonomous system which will bring about two different Quantum and Statistical dynamics. Even worse, the Lagrangian (therefore, the Hamiltonian) may not exist for higher than one-dimensional dynamical systems [13] [14]. In other words, these ambiguities may affect the theoretical results of Statistical Mechanics, Quantum Mechanics, or Field Theory [15]-[18] since the theoretical basis of these theories are the Lagrangian or the Hamiltonian formulation of the dynamical system. That is why one would like to have an approach free of these ambiguities for these type of dynamical system, and which can also be compared with experiments and the usual formulation on the phase space $(\mathbf{x}, \mathbf{p})$. For this reason, I want to present on the following sections the formulation of the Statistical Mechanics defined in the configuration space $(\mathbf{x}, \mathbf{v})$. It is necessary to point out that for conservative dynamical systems (where the trivial relation $\mathbf{p} = m\mathbf{v}$ is always stablished) both formulation are totally identical. To do this, I will point out some elements of Quantum Mechanics which help to have a correct formulation of Statistical Mechanics for non conservative autonomous systems.

Contribution-1 from the Quantum Mechanics

Quantum Mechanics formulation in the phase space $(\mathbf{x}, \mathbf{p})$ is based [19]-[23] on the assignation of linear operators to the classical variables $\mathbf{x}$ and $\mathbf{p}$ (considering here that $\mathbf{x}, \mathbf{p} \in \Re^3$) and the Hamiltonian scalar function $H = H(\mathbf{x}, \mathbf{p}, t)$ (the variable "t" represents the time evolution of the system) such that

$$\hat{\mathbf{x}} = \mathbf{x} \text{ and } \hat{\mathbf{p}} = -i\hbar\nabla, \tag{1}$$

satisfying the following commutation relation between their components

$$[x_l, \hat{p}_k] = i\hbar\delta_{lk} I, \tag{2}$$

where "I" is the identity operator and $h = \hbar/2\pi$ is the Plank's constant. The linear Hamiltonian operator $\hat{H}(\mathbf{x}, \hat{\mathbf{p}}, t)$ is used to form a linear partial differential equation, the so called Schrödinger's equation

$$i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}(\mathbf{x}, \hat{\mathbf{p}}, t)\Psi, \tag{3}$$

where $\Psi = \Psi(\mathbf{x}, t)$ is the wave function which is used to calculate the expected value of the dynamical variables or probabilities. This equation can also be written in the Fourier space as

$$i\hbar\frac{\partial\hat{\Psi}}{\partial t}=\hat{H}\left(\hat{\mathbf{x}},\mathbf{p},t\right)\hat{\Psi},\tag{4}$$

where $\hat{\Psi}=\hat{\Psi}\left(\mathbf{p},t\right)$ is the scalar function defined by the Fourier transformation

$$\hat{\Psi}\left(\mathbf{p},t\right)=\mathcal{F}\left[\Psi\left(\mathbf{x},t\right)\right]=\frac{1}{\left(2\pi\right)^{3/2}}\int_{\Re^3}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}\Psi\left(\mathbf{x},t\right)\mathrm{d}^3\mathbf{x},\tag{5}$$

where $\mathbf{k}=\mathbf{p}/\hbar$ is the D'Broglie wave number, and the operator $\hat{\mathbf{x}}$ is now given by $\hat{\mathbf{x}}=-i\nabla_{\mathbf{k}}=-i\hbar\nabla_{\mathbf{p}}$.

So, for a 1-D Gaussian wave function, centered at the origin with a dispersion σ_x. on its values, its Fourier transformation is

$$\mathcal{F}\left[\frac{1}{\sqrt{2\pi\sigma_x^2}}\mathrm{e}^{-x^2/2\sigma_x}\right]\sim\mathrm{e}^{-k^2/2\sigma_k^2},\tag{6}$$

where one has that

$$\sigma_x\sigma_k=1.\tag{7}$$

That is, the dispersion of the expected values of x and the expected values of k are such that $\Delta x\cdot\Delta k=1$, or $\Delta x\cdot\frac{\Delta p}{\hbar}=1$,or

$$\Delta x\cdot\Delta v=\hbar/m,\tag{8}$$

where m is the mass of the particle. Therefore, the minimum dispersion area of the expected values on the configuration space $\left(x,v\right)$ that one can have is about $\hbar/m$ or

$$\text{minimum dispersion area}=\frac{2\pi\hbar}{m}.\tag{9}$$

Of course, considering the time depending functions, the Fourier transformation would bring a frequency (or Energy through the relation $\omega=E/\hbar$) dependent function,

$$\hat{\psi}\left(\mathbf{x},\omega\right)=\mathcal{F}\left[\Psi\left(\mathbf{x},t\right)\right]=\frac{1}{\sqrt{2\pi}}\int_{\Re}\mathrm{e}^{-i\omega t}\Psi\left(\mathbf{x},t\right)\mathrm{d}t,\tag{10}$$

which, in turns, for a Gaussian distribution in time with dispersion σ_t, one will obtain a Gaussian distribution in the frequency Fourier space with dispersion σ_ω, satisfying

$$\sigma_t\sigma_\omega=1,\tag{11}$$

The dispersion of the expected values of "t" and $\omega=E/\hbar$ are such that $\Delta t\cdot\Delta E=\hbar$, and it represents the minimum dispersion area in the space $\left(t,E\right)$ of the expected values of these variables.

It is important to emphasize that these uncertainty relations appear intrinsically within the mathematical formalism of Quantum Mechanics and they do not depend on any particular physical phenomenon. That is why Quantum Mechanics is a nondeterministic theory (do not confuse this with the fact that the Schrödimger equation is a linear well-behaved equation whose solutions are well defined), in contrast to Classical Mechanics where position, velocity, time and energy are are well determined (if there is not random process in consideration).

Another contribution of Quantum Mechanics is that N identical particles' wave functions must have a normalized factor of $N!$ because they are indispensable under any permutation of particles. So, this factor must be considered when dealing with identical particles in Statistical Mechanics.

In addition, one must point out that the relationship between the phase space (x, p) and the configuration space (x, v) for autonomous systems is given by the classical relation defined by a Lagrangia $L(x, v)$ of the system as

$$p(x, v) = \frac{\partial L}{\partial v}. \tag{12}$$

2. Classical Statistical Mechanics in the Configuration Space (*x*, *v*)

Classical Statistical Mechanics pretends to determine the thermodynamic characteristics of a system (pressure, internal energy, entropy, potential energies) in thermodynamic equilibrium with just a few parameters of the system, like temperature T and the volume V of the system, and the type of interaction among the elements of the system. Because we are dealing with the thermodynamic equilibrium of the system, this interaction must be related to an autonomous system (interaction must not depend explicitly on time). The thermodynamic characteristics of the system are then calculated with the so called partition function associated with some particular ensemble (all possible replicas of the system defined on the phase space (x, p)), where one has to assume the ergodic theorem [24], that is, the average over time is the same as the average over the ensemble, and the thermodynamic characteristics are determined by the partition function (canonical ensemble)

$$Z = \frac{1}{N!}\left(\frac{1}{2\pi\hbar}\right)^N \int_{\Re^{3N}} \mathrm{e}^{-\beta H(\mathbf{x},\mathbf{p})} \mathrm{d}^{3N}x \mathrm{d}^{3N}p, \quad x, p \in \Re, \tag{13}$$

where $\beta = 1/k_B T$, being k_B the Boltzmann's constant ($k_B = 1.38 \times 10^{-23}$ J/K), T the temperature, N the number of identical particles, the number $N!$ comes from quantum mechanics considerations. The idea of using the configuration space $(\boldsymbol{x}, \boldsymbol{v})$ to determine the thermodynamic characteristics of a system comes from the Maxwell distribution of molecular speeds [25]. In general, it is possible to define a partition function in the configuration space $(\boldsymbol{x}, \boldsymbol{v})$, for example, for the so called Canonical Ensemble (the same idea can be applied to any other ensemble, like Microcanonical or Gran Canonical Ensembles), where the system interchanges energy with its surrender, and using the quantum mechanical information given above, the canonical partition function (without units) can be written in the configuration space $(\boldsymbol{x}, \boldsymbol{v})$ as

$$Z = \frac{1}{N!}\left(\frac{m}{2\pi\hbar}\right)^N \int_{\Re^{3N}} \mathrm{e}^{-\beta K(\mathbf{x},\mathbf{v})} \mathrm{d}^{3N}x \mathrm{d}^{3N}v, \quad x, v \in \Re \tag{14}$$

where m represents the mass of each particle, ($m/2\pi\hbar$) represents the minimum uncertainty on the state of each element of the ensemble we can have in the configuration space ($\boldsymbol{x},\boldsymbol{v}$), and the scalar function $K(\mathbf{x},\mathbf{v})$ can be chosen as a constant of motion of the autonomous dynamical system. It is known that the factor $N!$ is required to solve the Gibbs paradox [26] [27] to make the entropy an extensive quantity [28], and the factor ($m/2\pi\hbar$) is required to make the partition function an dimensionless function. The thermodynamics characteristics like Energy E, pressure P, entropy S, and Helmoholtz's free energy F are determined by the following expressions

$$E=-\frac{\partial \ln Z}{\partial \beta}, \tag{15}$$

$$P=k_B\frac{\partial \ln z}{\partial V}, \tag{16}$$

$$S=k_B\beta E+k_B\ln Z, \tag{17}$$

and

$$F=-k_BT\ln Z. \tag{18}$$

Now, if the dynamical system associated is given by

$$\frac{\mathrm{d}\mathbf{x}_i}{\mathrm{d}t}=\mathbf{v}_i,\ \frac{\mathrm{d}(\gamma_i\mathbf{v}_i)}{\mathrm{d}t}=\mathbf{F}_i(\mathbf{x},\mathbf{v})/m,\ i=1,\cdots,N, \tag{19}$$

where $\mathbf{x}_i,\mathbf{v}_i\in\Re^3$ represent the position and velocity of the ith-particle, $\mathbf{F}_i(\mathbf{x},\mathbf{v})$ represents the total force acting on the ith-particle, and $\gamma_i=\left(1-v_i^2/c^2\right)^{-1/2}$ being the relativistic factor with $v_i^2=v_{ix}^2+v_{iy}^2+v_{iz}^2$ and c being the speed of light (the mass of the particles are considered constants and for the no-relativistic case one defines $\gamma_i=1$). On the other hand, $\mathbf{x}=(\mathbf{x}_1,\cdots,\mathbf{x}_N)$ and $\mathbf{v}=(\mathbf{v}_1,\cdots,\mathbf{v}_N)\in\Re^{3N}$. The scalar function $K(\mathbf{x},\mathbf{v})$ is a constant of motion of this dynamical system, that is, $\mathrm{d}K/\mathrm{d}t=0$. Therefore, it satisfies the following linear partial differential equation of first order [29] [30]

$$\sum_{i=1}^N\sum_{j=1}^3\left(v_{ij}\frac{\partial K}{\partial x_{ij}}+\frac{F_{ij}(\mathbf{x},\mathbf{v})}{m}\frac{\partial K}{\partial v_{ij}}\right)=0. \tag{20}$$

If the system is separable, that is, the total force acting on the ith-particle depends only on its coordinates and its velocity ($\mathbf{F}_i=\mathbf{F}_i(\mathbf{x}_i,\mathbf{v}_i)$), the constant of motion would be of the form

$$K(\mathbf{x},\mathbf{v})=\sum_{i=1}^N\sum K_i(\mathbf{x}_i,\mathbf{v}_i), \tag{21}$$

where the scalar functions K_i would be the solution of the equation

$$\sum_{j=1}^3\left(v_j\frac{\partial K_i}{\partial x_j}+\frac{F_i(\mathbf{x}_i,\mathbf{v}_i)}{m}\frac{\partial K_i}{\partial v_j}\right)=0,\ i=1,\cdots,N. \tag{22}$$

Thus, the partition function would of the form

$$Z=\frac{1}{N!}\prod_{i=1}^N Z_i,\ \text{with } Z_i=\left(\frac{m}{2\pi\hbar}\right)\int_{\Re^3}\mathrm{e}^{-\beta K_i(\mathbf{x}_i,\mathbf{v}_i)}\mathrm{d}^3x_i\mathrm{d}^3v_i,\ x_i,v_i\in\Re \tag{23}$$

In the next section, some examples are given of constants of motion which can or can nor have their equivalent in the Hamiltonian formulation.

3. Example of Constant of Motion of Several Systems

Several cases will be considered here, pointing out the use of (19), (20), and (22). One must remember that, generally, when dealing with dissipation systems in classical mechanics, this dissipation arises from the interaction (or collision) with the particles forming the medium where the particles of our analysis are moving. The velocity depending force on the particle's motion can be considered as the average of these interactions. In the following examples, $\gamma = 1$ will means $\lim_{c\to\infty}\gamma$.

(a1) $\gamma_i = 1$ and $\mathbf{F}_i = \mathbf{0}$, corresponding a nonrelativistic free (non interacting) particles (ideal gas)

$$K(\mathbf{x},\mathbf{v}) = \sum_{i=1}^{N}\frac{m}{2}v_i^2, \quad v_i^2 = v_{ix}^2 + v_{iy}^2 + v_{iz}^2 \tag{24}$$

(a2) $\gamma_i = 1$ and $\mathbf{F}_i = \mathbf{F}$, nonrelativistic particles under the same constant force (examples: gravity or electric field on ions)

$$K(\mathbf{x},\mathbf{v}) = \sum_{i=1}^{N}\left(\frac{m}{2}v_i^2 - \mathbf{F}\cdot\mathbf{x}_i\right) \tag{25}$$

(a3) $\gamma_i = 1$ and $\mathbf{F}_i = -k_i\mathbf{x}_i$, nonrelativistic particles under the Hook's law, representing a bounded system where the particles oscillate with an angular frequency $\omega_i = \sqrt{k_i/m}$.

$$K(\mathbf{x},\mathbf{v}) = \sum_{i=1}^{N}\left(\frac{m}{2}v_i^2 + \frac{m\omega_i^2}{2}\mathbf{x}_i^2\right), \quad \mathbf{x}_i^2 = x_i^2 + y_i^2 + z_i^2. \tag{26}$$

(a4) $\gamma_i = 1$, $\mathbf{F}_i = -k_i\mathbf{x}_i - \alpha\mathbf{v}_i, i = 1,\cdots,N_1$, and $\mathbf{F}_l = \mathbf{0}, l = 1,\cdots,N_2$ with $N = N_1 + N_2$, corresponding to N_1 nonrelativistic particles of mass m are inside a linear dissipative medium formed by N_2 non interacting particles of mass $\tilde{m}$ [32].

$$K(\mathbf{x},\mathbf{v}) = \sum_{j=1}^{3}\sum_{i=1}^{N_1}\left(\frac{m}{2}v_{ij}^2 + \frac{m\omega_i}{2}x_{ij}^2 + \frac{\alpha}{2}x_{ij}v_{ij}\right)\mathrm{e}^{-2\omega_\alpha G_\alpha\left(v_{ij}/x_{ij},\omega_\alpha\right)} + \sum_{l=1}^{N_2}\frac{\tilde{m}}{2}v_l^2 \tag{27}$$

where $\omega_\alpha = \alpha/2m$, and the function G_α is defined as

$$G_\alpha = \begin{cases} \dfrac{1}{\sqrt{\omega_\alpha^2 - \omega_i^2}}\ln\left(\dfrac{\omega_\alpha + v_{ij}/x_{ij} - \sqrt{\omega_\alpha^2 - \omega_i^2}}{\omega_\alpha + v_{ij}/x_{ij} + \sqrt{\omega_\alpha^2 - \omega_i^2}}\right) & \text{if } \omega_i^2 < \omega_\alpha^2 \\ \dfrac{1}{\omega_i + v_{ij}/x_{ij}} & \text{if } \omega_i^2 = \omega_\alpha^2 \\ \dfrac{1}{\sqrt{\omega_i^2 - \omega_\alpha^2}}\arctan\left(\dfrac{\omega_\alpha + v_{ij}/x_{ij}}{\sqrt{\omega_i^2 - \omega_\alpha^2}}\right) & \text{if } \omega_i^2 > \omega_\alpha^2 \end{cases} \tag{28}$$

At first order in the dissipation parameter α one can write this constant of motion as

$$K(\mathbf{x},\mathbf{v}) = \sum_{j=1}^{3}\sum_{i=1}^{N_1}\left(\frac{m}{2}v_{ij}^2 + \frac{m\omega_i}{2}x_{ij}^2 + \frac{\alpha}{2}x_{ij}v_{ij}\right) + \sum_{l=1}^{N_2}\frac{\tilde{m}}{2}v_l^2, \tag{29}$$

in the region where $\left|\frac{1}{\omega_i x_{ij} v_{ij}} \arctan\left(\frac{\omega_\alpha + v_{ij}/x_{ij}}{\omega_i}\right)\right| \ll 1$.

(a5) $\gamma_i = 1$, $F_{ij} = -\alpha v_i^2/m, i = 1,\cdots,N_1; j = 1,2,3$ $(v_{ij} > 0)$, and $\mathbf{F}_l = \mathbf{0}, l = 1,\cdots,N_2$ with $N = N_1 + N_2$, corresponding to N_1 nonrelativistic particles of mass m inside a quadratic dissipative medium formed by N_2 non interacting particles of mas $\tilde{m}$ [33],

$$K(\mathbf{x},\mathbf{v}) = \sum_{j=1}^{3}\sum_{i=1}^{N_1}\frac{1}{2}mv_{ij}^2 e^{2\alpha x_{ij}/m} + \sum_{l=1}^{N_2}\frac{1}{2}\tilde{m}v_l^2. \tag{30}$$

(a6) $\gamma = 1$ and $\mathbf{F}_i = \sum_{l=1}^{N-1}\mathbf{F}_{li}(\mathbf{x}_i - \mathbf{x}_l)$, describing the redial interaction of the ith-particle with all the others (nonseparable case)

$$K(\mathbf{x},\mathbf{v}) = \sum_{i=1}^{n}\frac{1}{2}mv_i^2 + \sum_{i,l}^{N}V_{il}(\mathbf{x}_i - \mathbf{x}_l), \quad V_{il}(\mathbf{x}_i - \mathbf{x}_l) = -\int \mathbf{F}_{il}\cdot \mathrm{d}\mathbf{x}_i \tag{31}$$

Let us recall that for the relativistic (special) cases [31], the modified Newton's equation of motion is carried out by to incert the relativistic gama factor, $\gamma^{-1} = \sqrt{1-\beta^2}$, with $\beta = \mathbf{v}/c$ in the usual (nonrelativistic) momentum of the body, $m\mathbf{v}$.

$$\frac{\mathrm{d}(\gamma m\mathbf{v})}{\mathrm{d}t} = \mathbf{F}. \tag{32}$$

So, let us see some cases.

(b1) $\gamma_i \gg 1$ and $\mathbf{F}_i = \mathbf{0}$, corresponding to free relativistic noninteracting particles (relativistic ideal gas) ,

$$K(\mathbf{x},\mathbf{v}) = \sum_{i=1}^{N}(\gamma_i - 1)mc^2, \ \gamma_i = \left(1 - v_i^2/c^2\right)^{-1/2} \tag{33}$$

(b2) $\gamma \gg 1$ and $\mathbf{F}_i = \mathbf{F}_i(\mathbf{x}_i)$, corresponding to relativistic particles under the same conservative force,

$$K(\mathbf{x},\mathbf{v}) = \sum_{i=1}^{N}\left\{(\gamma_i - 1)mc^2 + V(\mathbf{x}_i)\right\}, \ V(\mathbf{x}_i) = -\int \mathbf{F}_i(\mathbf{x}_i)\cdot \mathrm{d}\mathbf{x}_i. \tag{34}$$

(b3) $\gamma_i \gg 1$, $F_{ij} = -\alpha v_{ij}, j = 1,2,3; i = 1,\cdots,N_1$, $\mathbf{F}_l = \mathbf{0}, l = 1,\cdots,N_2$, corresponding to N_1 relativistic particles of mass m moving in a linear dissipative medium formed by N_2 noninteracting relativistic particles of mass $\tilde{m}$,

$$K(\mathbf{x},\mathbf{v}) = \sum_{j=1}^{3}\sum_{i=1}^{N_1}\left\{(\gamma_{ij} - 1)mc^2 + 2\alpha c^2 x_{ij}\right\} + \sum_{l=1}^{N_2}(\gamma_l - 1)\tilde{m}c^2, \tag{35}$$

where $\gamma_{ij} = \left(1 - v_{ij}^2/c^2\right)^{-1/2}$ and $\gamma_l = \left(1 - v_l^2/c^2\right)^{-1/2}$. In the next section, one selects one of the most drastic situation where there is a big difference by making classical statistic mechanics in the configuration space and the impossibility of doing this with the Hamiltonian formulation.

4. Harmonic Oscillator with Linear Dissipation

This problem associated with (a4) is of particular interest since it shows that there are cases where the application of Mechanics Statistical in the phase space $(\mathbf{x},\mathbf{p})$

may have no meaning at all, meanwhile, the application of Mechanical Statistical in the configuration space $(\mathbf{x},\mathbf{v})$ has full meaning. Let us recall that on the phase space $(\mathbf{x},\mathbf{p})$ for a 1-D conservative potential and linear dissipation, it is usual to define $L(x,v,t)=\left(mv^2/2-V(x)\right)\mathrm{e}^{\alpha t}$ as the Lagrangian for this type of system since the application of Euler-Lagrange equation to this Lagrangian bring about the equation $\mathrm{d}(mv)/\mathrm{d}t=-\mathrm{d}V/\mathrm{d}x-\alpha mv$, which represents the evolution equation of a linear dissipation problem with known potential energy. The Hamiltonian associated with this system depends explicitly on time and is given by $H(x,p,t)=p^2\mathrm{e}^{-\alpha t}/2m+V(x)\mathrm{e}^{\alpha t}$, and this means that the system of many particles described by this type of interaction can not be in thermodynamical equilibrium, and the application of the usual canonical ensemble with the partition function $Z=\left(1/N!h^N\right)\int \mathrm{e}^{-\beta H}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{p}$ has not meaning for any potential $V(x)$, in particular for the harmonic oscillator potential $V(x)=kx^2/2$. Of course, the main problem with this approach is explicitly proposing time depending quantities on an autonomous system. However, as we saw in the last section, example (4), the harmonic oscillator with linear dissipation is an autonomous system that has a constant of motion (27) which is time independent. Therefore, the Mechanics Statistical on the configuration space $(\mathbf{x},\mathbf{v})$ has full sense, and one can talk about equilibrium thermodynamic and thermodynamic states. For practical proposes, one will use the constant of motion at first order of approximation on the dissi-pation parameter α (29). According to this expression and (23), and the factorization of the coordinates of each particle, it follows that $Z=Z_{N_1}Z_{N_2}$, where Z_{N_i} are defined by (14) according to the constant of motion.

$$Z_i=\left(\frac{m}{2\pi\hbar}\right)\prod_{j=1}^{3}\int_{\Re\times L_{ij}}\mathrm{e}^{-\beta K_i(x_{ij},v_{ij})}\mathrm{d}x_{ij}\mathrm{d}v_{ij}=\left(\frac{m}{2\pi\hbar}\right)\left(\frac{2\pi}{b}\right)^{3/2}f_i(\alpha), \tag{36}$$

where $x_{ij},v_{ij}\in\Re$, and one has made the definitions

$$f_i(\alpha)=\prod_{j=1}^{3}\int_{\sqrt{\alpha/m\omega_i^2}v_{ij}}^{L_{ij}+\sqrt{\alpha/m\omega_i^2}v_{ij}}\mathrm{e}^{-a\xi^2/2}\mathrm{d}\xi, \tag{37}$$

$$a=\sqrt{\frac{m\beta}{2}}\ \text{ and }\ b=\sqrt{\frac{m\beta}{2}\left(1-\frac{\alpha}{2m}\right)}. \tag{38}$$

r The canonical partition function in the configuration space is then given by $\mathcal{Z}=\mathcal{Z}_{N_1}\cdot\mathcal{Z}_{N_2}$ where

$$Z_{N_1}=\frac{1}{N_1!}\left(\frac{m}{2\pi\hbar}\right)_1^N\left(\frac{2\pi}{b}\right)^{3N_1/2}f_i^{N_1}(\alpha), \tag{39}$$

the function $f_i(\alpha)$ contains the information of the system's volume. The partition function Z_{N_2} corresponds to a set of N_2 noninteracting particles in a volume $V=L_{i1}L_{i2}L_{i3}$ for any ith-particle, that is

$$Z_{N_2}=\frac{1}{N_2!}\left(\frac{\tilde m}{2\pi\hbar}\right)^{N_2}V^{N_2}\left(\frac{2\pi}{\sqrt{\tilde m\beta/2}}\right)^{3N_2/2} \tag{40}$$

Given this partition function $Z=Z_{N_1}Z_{N_2}$, the thermodynamic characteristics (15), (16), (17), and (18) can be calculated.

5. Formulation: (*x*, *p*) vs (*x*, *v*)

In addition to the above clear advantage to use the formulation $(\mathbf{x},\mathbf{v})$ to determine the thermodynamics characteristics in equilibrium of the system, it will show in this section that the formulation $(\mathbf{x},\mathbf{p})$ can bring about even different results for systems where forces depend explicitly on the velocity of the particles. Consider a system of N_1 particles of mass m moving in a dissipative medium of N_2 particles where the dynamical system is modeled by the equations

$$\dot{x}_i = v_i,\ \dot{v}_i = -\frac{\alpha}{m} v_i^2 \ \text{ for } i = 1,\cdots,3N_1 \ (v_i > 0), \tag{41}$$

where α is the parameter of dissipation, and

$$\dot{x}_j = v_j,\ \dot{v}_i = 0 \ \text{ for } j = 1,\cdots,3N_2. \tag{42}$$

Ignoring the contribution of the N_2 particles to the thermodynamics characteristics of the system, one has from [32], one has the constant of motion, Lagrangian, generalized linear momentum, and Hamiltonian as

$$K_i = \frac{1}{2} m v_i^2 \mathrm{e}^{+2\alpha x_i/m}, \tag{43}$$

$$L_i = \frac{1}{2} m v_i^2 \mathrm{e}^{+2\alpha x_i/m}, \tag{44}$$

$$p_i = m v_i \mathrm{e}^{+2\alpha x_i/m} \ \text{ and } \ p_i > 0, \tag{45}$$

and

$$H_i = \frac{p_i^2}{2m} \mathrm{e}^{-2\alpha x_i/m}, \tag{46}$$

where the constant of motion was chosen such that $\lim_{\alpha\to 0} K_i = (1/2) m v_i^2$, and the Lagrangian was obtained from the KLL's formula $L = v_i \int K(x_i, s_i)\, ds_i / s_i^2$ [29]. The partition functions in the formulation $(\mathbf{x},\mathbf{p})$ and $(\mathbf{x},\mathbf{v})$ are

$$Z_H = \frac{1}{N_1!(2\pi\hbar)^{N_1}} \prod_{i=1}^{3N_1} \int \mathrm{e}^{-\beta\left(p_i^2/2m\right)\mathrm{e}^{-2\alpha x_i/m}} \mathrm{d}x_i \mathrm{d}p_i \tag{47}$$

making the integration over the linear momentum components it follows that

$$Z_H = \frac{1}{N_1!(2\pi\hbar)^{N_1}} \frac{1}{2^{3N_1}} \left(\frac{2m\pi}{\beta}\right)^{3N_1} \prod_{i=1}^{3N_1} \int \mathrm{e}^{\alpha x_i/m} \mathrm{d}x_i \tag{48}$$

On the other hand, for the configuration formulation one has

$$Z_K = \frac{1}{N_1!} \left(\frac{m}{2\pi\hbar}\right)^{N_1} \prod_{i=1}^{3N_1} \int \mathrm{e}^{-\beta\left(m v_i^2/2\right)\mathrm{e}^{+2\alpha x_i/m}} \mathrm{d}x_i \mathrm{d}p_i \tag{49}$$

making the integration over the linear momentum components it follows that

$$Z_K = \frac{1}{N_1!(2\pi\hbar)^{N_1}} \frac{1}{2^{3N_1}} \left(\frac{2\pi}{m\beta}\right)^{3N_1} \prod_{i=1}^{3N_1} \int \mathrm{e}^{-\alpha x_i/m} \mathrm{d}x_i \tag{50}$$

Spatial integration in (48) and (50) is done to certain volume *V*, and as one can see they bring about different results. Thus, for explicitly velocity depending autonomous system one can expect that statistical mechanics formulation on the spaces $(\mathbf{x},\mathbf{v})$ and $(\mathbf{x},\mathbf{p})$ give different results, representing an experimental case to see which formulation is the correct for these type of autonomous systems.

Now, one will extend the above ideas to Quantum Statistical Mechanics.

6. Quantum Statistical Mechanics

Despite the enormous success of the Quantum Mechanics in the phase space $(\mathbf{x},\mathbf{p})$, described mainly by the Schrödinger's equation

$$i\hbar\frac{\partial\Psi}{\partial t}=\hat{H}(\mathbf{x},\hat{\mathbf{p}},t)\Psi, \tag{51}$$

where $\Psi=\Psi(\mathbf{x},t)$ is the so called wave function, $\hat{H}=\hat{H}(\mathbf{x},\hat{\mathbf{p}},t)$ is the linear operator (Hermitian or no-Hermitian) associated to the classical Hamiltonian function $H=H(\mathbf{x},\mathbf{p},t)$ (as mentioned before), one knows that the Lagrangian-Hamiltonian formulation of Classical Mechanics is not free of ambiguities, which are then transmitted to Quantum and Statistical Mechanics.

For this reason, on the reference [34], a formulation of the Schrödinger's equation in the configuration space $(\mathbf{x},\mathbf{v})$ was given, where instead of using the classical Hamiltonian $H=H(\mathbf{x},\mathbf{p},t)$ function, it is used a classical function $K=K(\mathbf{x},\mathbf{v},t)$ to define a linear operator and the Schrödinger equation. This is done by assigning to the velocity, the linear operator

$$\hat{\mathbf{v}}=-i\frac{\hbar}{m}\nabla,\ \text{such that}\ [x_l,\hat{v}_k]=i\frac{\hbar}{m}\delta_{lk}I, \tag{52}$$

where "I" is the identity operator. The Schrödinger's equation is now written as

$$i\hbar\frac{\partial\Psi}{\partial t}=\hat{K}(\mathbf{x},\hat{\mathbf{v}},t)\Psi, \tag{53}$$

where $\hat{K}$ is the linear operator associated to the function $K=K(\mathbf{x},\mathbf{v},t)$, and determines the quantum integrable system. For autonomous systems, the classical function K can be a constant of motion of the system (like the functions shown before), depending only on the variables $\mathbf{x}$ and $\mathbf{v}$, $K=K(\mathbf{x},\mathbf{v})$. Therefore, the associated linear operator will not depend explicitly on time, $\hat{K}(\mathbf{x},\hat{\mathbf{v}})$ and the equation (53) is of variable separable in space-time through the proposition $\Psi(\mathbf{x},t)=\Phi(\mathbf{x})\mathrm{e}^{-iEt/\hbar}$, bringing about the eigenvalue equation

$$\hat{K}(\mathbf{x},\hat{\mathbf{v}})\Phi=E\Phi. \tag{54}$$

Solving this equation, one gets the set of values $\{E_n,\Phi_{nl}\}_{l=1,\cdots,g_n}$ (assuming discrete spectrum), where E_n represents the nth-eigenvalue and the set $\{\Phi_{nl}\}_{l=1,\cdots,g_n}$ represents the eigenfunctions associated to the same eigenvalue E_n, g_n represents its degeneration. As it is well known, the solution of (53) would be given by

$$\Psi(\mathbf{x},t)=\sum_{n,l}C_{nl}\mathrm{e}^{-iE_nt/\hbar}\Phi_{nl}(\mathbf{x}). \tag{55}$$

In this way, one could define the Quantum Canonical Partition Function (QCPF) by

$$Z = \sum_n g_n e^{-\beta E_n}, \tag{56}$$

and the probability to find the system in the state with energy E_n would be given by

$$P_n = \frac{g_n e^{-\beta E_n}}{Z}. \tag{57}$$

7. Quantum Harmonic Oscillator with Linear Dissipation

One wants to focus on this particular case, as it was done in the classical case, since it shows dramatically the big difference between Quantum Statistical Mechanics in the phase spaces $(\mathbf{x},\mathbf{p})$ and $(\mathbf{x},\mathbf{v})$. As with the example done in Classical Statistical Mechanics, one will restrict oneself to the weak dissipation case described by the approximated constant of motion (29) in 1-D, with $N_2 = 0$ and the expression is at first order in the dissipative parameter α

$$K(x,v) = \frac{1}{2}mv^2 + \frac{1}{2}m\omega^2 x^2 + \frac{\alpha}{2}xv. \tag{58}$$

The Hermitian linear operator associated to this function is

$$\hat{K}(x,\hat{v}) = \frac{1}{2}m\hat{v}^2 + \frac{1}{2}m\omega^2 x^2 + \frac{\alpha}{2}(x\hat{v} + \hat{v}x). \tag{59}$$

This operator can be written in terms of the non-Hermitian operators (as one knows from usual Hamiltonian Quantum Mechanics)

$$a = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega x + im\hat{v}) \quad \text{and} \quad a^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega x + im\hat{v}) \tag{60}$$

where the inverse relations are given by

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a) \quad \text{and} \quad \hat{v} = i\sqrt{\frac{\omega\hbar}{2m}}(a^\dagger - a), \tag{61}$$

as

$$\hat{K} = \hbar\omega(a^\dagger a + 1/2) + i\frac{\alpha\hbar}{2m}(a^{\dagger 2} - a^2), \tag{62}$$

Since one is dealing with weak dissipation, let us note that (62) can be written as

$$\hat{K} = \hat{K}_0 + \alpha W, \tag{63}$$

with $\hat{K}_0 = \hbar\omega(a^\dagger a + 1/2)$ and $W = i(\hbar/2m)(a^{\dagger 2} - a^2)$, which can be considered as a perturbation to the system. The operators $a^\dagger$ and a satisfy the following relations

$$[a, a^\dagger] = I,\ a^\dagger a|n\rangle = n|n\rangle,\ a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \text{ and } a|n\rangle = \sqrt{n-1}|n-1\rangle, \tag{64}$$

where $\{|n\rangle\}_{n\in Z^+}$ represents the set of abstract eigenvector of the eigenvalue equation $\hat{K}_0|n\rangle = E_n^0|n\rangle$, with $\{E_n^0 = \hbar\omega(n+1/2)\}_{n\in \mathcal{Z}^+}$ being the set of eigenvalues without perturbation (there is not degeneration on the system, that is, $g_n = 1$ for any n). The function $\langle x|n\rangle$ associated to the vector state $|n\rangle$ is

(normalized harmonic oscillator)

$$\langle \xi | n \rangle = \Phi_n(\xi) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}\xi^2} H_n(\xi), \tag{65}$$

where $H_n(z)$ are the Hermit polynomials. Using perturbation theory, the eigenvalues E_n and eigenvectors $|\tilde{n}\rangle$ of the equation

$$\hat{K} |\tilde{n}\rangle = E_n |\tilde{n}\rangle \tag{66}$$

can be calculated [XX], and one is concerned mainly with the eigenvalues which at second order of approximation can be given by

$$E_n = E_n^0 + \alpha \langle n | W | n \rangle + \alpha^2 \sum_{n' \neq n} \frac{|\langle n | W | n' \rangle|^2}{E_{n'}^0 - E_n^0}. \tag{67}$$

From (64) , it follows that

$$\langle n | a^{\dagger 2} - a^2 | n' \rangle = \sqrt{(n'+1)(n'+2)}\, \delta_{n,n'+2} - \sqrt{n'(n'-1)}\, \delta_{n,n'-2}, \tag{68}$$

and

$$E_{n'}^0 - E_n^0 = \hbar\omega(n' - n). \tag{69}$$

Therefore, there is no contribution at first order, and the eigenvalues at second order in perturbation theory are

$$E_n = \hbar\omega(n+1/2) - \frac{\alpha^2 \hbar}{8m^2\omega} \left\{ \sqrt{n(n-1)} + \sqrt{(n+1)(n+2)} \right\}. \tag{70}$$

In this way, the canonical quantum partition function is (using the fact of weak dissipation)

$$\begin{aligned} Z &= \sum_n e^{-\beta E_n} = \sum_n e^{-\beta\hbar\omega(n+1/2) + (\beta\alpha^2\hbar/8m^2\omega)\left\{\sqrt{n(n+1)} + \sqrt{(n+1)(n+2)}\right\}} \\ &\approx \sum_n e^{-\beta\hbar\omega(n+1/2)} \left\{ 1 + \frac{\beta\alpha^2\hbar}{8m^2\omega} \left(\sqrt{n(n+1)} + \sqrt{(n+1)(n+2)} \right) \right\} \\ &\approx \sum_n e^{-\beta\hbar\omega(n+1/2)} + \frac{\beta\alpha^2\hbar}{8m^2\omega} \sum_n e^{-\beta\hbar\omega(n+1/2)} \left(\sqrt{n(n+1)} + \sqrt{(n+1)(n+2)} \right) \end{aligned}$$

Thus, the partition function can be given as

$$Z = e^{-\beta\hbar\omega/2} \sum_n e^{-\beta\hbar\omega n} + \frac{\beta\alpha^2\hbar}{8m^2\omega} e^{-\beta\hbar\omega/2} \sum_n e^{-\beta\hbar\omega n} \left(\sqrt{n(n+1)} + \sqrt{(n+1)(n+2)} \right). \tag{71}$$

As we know [19], the first term brings about the partition function associated with Planck's formula,

$$Z_p = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}, \tag{72}$$

and the second term is the dissipation contribution, which results in a second order in the dissipation parameter.

8. Results and Comments

It has been shown that Statistical Mechanics can be done in the configuration space $(\mathbf{x},\mathbf{v})$, where instead of having a Hamiltonian, $H(\mathbf{x},\mathbf{p})$ to describe the dynamics of the particles, one can have a constant of motion, $K(\mathbf{x},\mathbf{v})$, associated to the autonomous system. Both formulation are totally equivalent for conservative systems, but dealing with autonomous non conservative dynamical system (dissipation), both formulation could give drastic different results. One has used the set of harmonic oscillators with linear dissipation to see that there can be a great difference in Statistical Mechanics in these spaces. Since the Hamiltonian associated with this system depends explicitly on time, it is impossible to determine the system's thermodynamic characteristics in equilibrium, either from the classical or quantum point of view. However, in the configuration space one is dealing with an autonomous system, and one can find a constant of motion $K(\mathbf{x},\mathbf{v})$ which allows us to make Statistical Mechanics in equilibrium, either from the classical or the quantum point of view.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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Appendix

$$
\begin{aligned}
Z_i &= \left(\frac{m}{2\pi\hbar}\right)\prod_{j=1}^{3}\int_{\Re\times L_{ij}} \mathrm{e}^{-\beta K_i\left(x_{ij},v_{ij}\right)}\mathrm{d}x_{ij}\mathrm{d}v_{ij}, \quad x_{ij}, v_{ij} \in \Re \\
&= \left(\frac{m}{2\pi\hbar}\right)\prod_{j=1}^{3}\int_{\Re\times L_{ij}} \mathrm{e}^{-\beta\left(mv_{ij}^2/2+m\omega_i x_{ij}^2/2+\alpha x_{ij}v_{ij}\right)}\mathrm{d}x_{ij}\mathrm{d}v_{ij} \\
&= \left(\frac{m}{2\pi\hbar}\right)\prod_{j=1}^{3}\int_{\Re} \mathrm{e}^{-m\beta(1-\alpha/2m)v_{ij}^2/2}\mathrm{d}v_{ij}\int_{\sqrt{\alpha/m\omega_i^2}v_{ij}}^{L_{ij}+\sqrt{\alpha/m\omega_i^2}v_{ij}} \mathrm{e}^{-a\xi^2/2}\mathrm{d}\xi, \quad a=\sqrt{\frac{m\beta}{2}} \qquad \text{(A1)} \\
&= \left(\frac{m}{2\pi\hbar}\right)\prod_{j=1}^{3}\sqrt{\frac{2\pi}{b}}\int_{\sqrt{\alpha/m\omega_i^2}v_{ij}}^{L_{ij}+\sqrt{\alpha/m\omega_i^2}v_{ij}} \mathrm{e}^{-a\xi^2/2}\mathrm{d}\xi, \quad b=\sqrt{\frac{m\beta}{2}\left(1-\frac{\alpha}{2m}\right)}. \\
&= \left(\frac{m}{2\pi\hbar}\right)\left(\frac{2\pi}{b}\right)^{3/2} f_i(\alpha), \quad \text{with } f_i(\alpha)=\prod_{j=1}^{3}\int_{\sqrt{\alpha/m\omega_i^2}v_{ij}}^{L_{ij}+\sqrt{\alpha/m\omega_i^2}v_{ij}} \mathrm{e}^{-a\xi^2/2}\mathrm{d}\xi.
\end{aligned}
$$