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Statistical Physics on the Space (x, v) for Dissipative Systems and Study of an Ensemble of Harmonic Oscillators in a Weak Linear Dissipative Medium

G. V. López,[1,3] P. López,[1] and X. E. López[2]

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We use the phase space position-velocity (x, v) to deal with the statistical properties of velocity dependent dynamical systems, like dissipative ones. Within this approach, we study the statistical properties of an ensemble of harmonic oscillators in a linear weak dissipative media. Using the Debye model of a crystal, we calculate at first order in the dissipative parameter the entropy, free energy, internal energy, equation of state and specific heat using the classical and quantum approaches. For the classical approach we found that the entropy, the equation of state, and the free energy depend on the dissipative parameter, but the internal energy and specific heat do not depend of it. For the quantum case, we found that all the thermodynamical quantities depend on this parameter.

KEY WORDS: space (x, v); dissipation; harmonic oscillators.

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1. INTRODUCTION

Our foundation of classical and quantum statistical mechanics (Kubo, 1999) is based on the Hamiltonian formalism (Goldstein, 1950) of conservative systems. These systems are particular cases of much more general ones called autonomous systems which are those where the total force acting on the particle does not depend explicitly on time, otherwise they are called non-autonomous. For conservative systems, the Hamiltonian is a constant of motion of the system, and, in principle, one can calculate all the thermodynamic characteristics of an ensemble of

[1] Departamento de Física, Universidad de Guadalajara, Apartado Postal 4-137, 44410 Guadalajara, Jalisco, México.
[2] Facultad de Ciencias, Universidad Nacional Autónoma de México, Apartado Postal 70-348, Coyoacán 04511, México D.F.
[3] To whom correspondence should be addressed at Departamento de Física, Universidad de Guadalajara, Apartado Postal 4-137, 44410 Guadalajara, Jalisco, México; e-mail: gulopez@udgserv.cencar.udg.mx

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N particles governed by this Hamiltonian, through the acknowledge of its associated partition function. For dynamical systems which depend explicitly on the velocity, for example dissipative systems. There are mainly two approaches to study these systems. The first one uses the kinetic equation (Vlasov or Boltzmann equations) to find the density distribution and, then, to calculate the desired statistical property. The other one tries to find an effective or phenomenological Hamiltonian and, then, to estimate the desired thermodynamic quantities from the stationary statistical mechanics (statistical ensemble) (López *et al.*, 1997). This last approach is possible since for autonomous systems sometimes is possible to find time-independent constant of motion, Lagrangian, and Hamiltonian. However, it is known that the Lagrangian and Hamiltonian formulation have some problems. First, the Lagrangian (therefore the Hamiltonian) may not exist for some dynamical systems (Douglas, 1941). Second, There could be two completely different Hamiltonians which describe the same classical mechanical system, but completely different quantum and statistical systems (López, 2005). Third, time-explicitly dependent systems have an ambiguous Lagrangian and Hamiltonian formulation (López and Hernández, 1989). Fourth, Ambiguity Lagrangian and Hamiltonian formulation happens even for the harmonic oscillator (López, 1998, 2002) (where a problem of consistency of units arises). Finally, there are autonomous systems where one can not have explicitly the Hamiltonian of the system because the inverse relation $v = v(x, p)$ can not be given from the original definition of $p = p(x, v)$ (López *et al.*, 2004). This last problem happens particularly on dissipative systems and is the main reason one would like to have an alternative approach in mechanics (López *et al.*, 1997), statistical and quantum mechanics to deal with them.

In this paper, we take the original ideas of Maxwell in statistical mechanics and Heisenberg in quantum mechanics to study these areas from the point of view of coordinates and velocities rather than coordinates and generalized linear momentum. We apply this approach to the ensemble of linear oscillators within a linear dissipative media, and we will do this from the phenomenological point of view and at first order in the dissipation parameter in the constant of motion.

2. DYNAMICAL EQUATION IN THE SPACE (x, v)

In this section, we restrict ourselves to one-dimensional single particle motion to show the main ideas. The approach will be extended immediately to N independent particles moving in a three-dimensional space. The equations of motion of a particle moving under a time-independent force can be written as the following autonomous dynamical system

$$\dot{x} = v, \tag{1a}$$

and

$$\dot{v} = \frac{f(x, v)}{m}, \tag{1b}$$

where m is the mass of the particle, x and v represent its position and velocity, and $f(x, v)$ is the total force acting on the particle. A constant of motion of this system is a function $K(x, v)$ such that $dK/dt = 0$, that is, it satisfies the following equation

$$v\frac{\partial K}{\partial x} + \frac{f(x, v)}{m}\frac{\partial K}{\partial v} = 0.$$

Given this constant of motion, the Lagrangian of the system is given by Kobussen (1979), (Leuber, 1981)

$$L = v\int \frac{K(x, v)}{v^2}dv + A(x)v,$$

where $A(x)$ is an arbitrary function, and the term $A(x)v$ represents the gauge of the Lagrangian. Thus, the generalized linear momentum is given by

$$p = \frac{\partial L}{\partial v}, \tag{4}$$

and it is here where our analysis starts. Suppose now that it is not possible to get $v = v(x, p)$ from (4). Then, the Hamiltonian of the system, $H = vp - L(x, v)$, can not be given explicitly, and it will be given in implicit form through the constant of motion. Therefore, this constant of motion (with units of energy) can help us to avoid this an other problems already mentioned in the introduction.

Consider N particles moving in the three-dimensional space and under a time-independent force acting on them (autonomous system). The motion of these particles is restricted on the hypersurface of the space $\Re^{6N}$ defined by the time-independent constant of motion $K(\mathbf{x}, \mathbf{v})$, where $\mathbf{x}, \mathbf{v} \in \Re^{3N}$. Thus, for a canonical ensemble of N-particles , the classical partition function would be given by

$$Z = \frac{m^{3N}}{h^{3N}\eta}\int e^{-\beta K(\mathbf{x},\mathbf{v})}d\mathbf{x}d\mathbf{v}, \tag{5}$$

where m is the mass of the particles, h is the Plank's constant, $\eta = 1$ for distinguishable particles and $\eta = N!$ for non distinguishable particles, $\beta = 1/kT$ with k being the Boltzmann's constant and T the temperature of the system, and $d\mathbf{x}d\mathbf{v}$ is the measure in the space $\Re^{6N}$,

$$d\mathbf{x}d\mathbf{v} = \prod_{j=1}^{3N} dx_j dv_j. \tag{6}$$

For a quantum canonical ensemble of N particles in a batch temperature T, the quantum partition function would be

$$Z = \sum_i \omega_i e^{-\beta E_i}, \tag{6}$$

where ω_i represents the degeneration of the eigenvalue E_i, where this eigenvalues comes from the solution of the equation

$$\widehat{K}(\widehat{\mathbf{x}}, \widehat{\mathbf{v}})\psi_i = E_i \psi_i. \tag{8a}$$

$\widehat{K}$, $\widehat{\mathbf{x}}$ and $\widehat{\mathbf{v}}$ are the Hermitian operator associated to the constant of motion $K(\mathbf{x}, \mathbf{v})$, the position $\mathbf{x}$, and the velocity $\mathbf{v}$. $\psi_i(\mathbf{x})$ is the eigenfunction which is related with the wave function $\Psi(\mathbf{x}, t)$ of the Schrödinger equation,

$$i\hbar \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} = \widehat{K}(\widehat{\mathbf{x}}, \widehat{\mathbf{v}})\Psi_i(\mathbf{x}, t), \tag{8b}$$

as

$$\Psi(\mathbf{x}, t) = \sum_i C_i e^{-iE_i t/\hbar} \psi_i(\mathbf{x}), \tag{8c}$$

where $|C_i|^2$ represents the probability that the system be on the state ψ_i. The position and velocity operators are defined and related by the following expressions

$$\widehat{x_j} = x_j, \quad \widehat{v_j} = -\frac{i\hbar}{m}\frac{\partial}{\partial x_j}, \quad [x_l, \widehat{v_j}] = \frac{i\hbar}{m}\delta_{lj}, \quad [x_i, x_j] = [v_i, v_j] = 0. \tag{8d}$$

In this way, with Eq. (5) and Eq. (7) it is possible, in principle, to study the thermodynamic characteristics of an ensemble of N particles of any autonomous system through the classical or quantum canonical partition functions. Of course, this approach is reduced to that one of the Hamiltonian formalism whenever this one exists explicitly (López *et al.*, 1997). Note that the same approach can be made for any other type of ensemble.

3. CONSTANT OF MOTION

In López (1996), a constant of motion $K_\alpha(x, v)$ was given for the dynamical system

$$\dot{x} = v \tag{9a}$$

and

$$\dot{v} = -\omega^2 x - \frac{\alpha}{m} v, \tag{9b}$$

where ω is the free natural frequency of oscillations, m is the mass of the particle, and α is the coefficient of the dissipative force which arises phenomenologically as an average effect of the interaction with the particles of the medium. The constant of motion of this system is given by

$$K_\alpha(x, v) = \frac{m}{2}(v^2 + 2\omega_\alpha x v + \omega^2 x^2) e^{-2\omega_\alpha G(v/x, \omega, \omega_\alpha)}, \tag{10a}$$

where ω_α and the function G are defined as

$$\omega_\alpha = \frac{\alpha}{2m}, \tag{10b}$$

and

$$G(\xi, \omega, \omega_\alpha) = \begin{cases} \frac{1}{2\sqrt{\omega_\alpha^2 - \omega^2}} \ln\left[\frac{\omega_\alpha + \xi - \sqrt{\omega_\alpha^2 - \omega^2}}{\omega_\alpha^2 + \xi + \sqrt{\omega_\alpha^2 - \omega^2}}\right] & \text{if } \omega^2 < \omega_\alpha^2 \\ \frac{1}{\omega_\alpha + \xi} & \text{if } \omega^2 = \omega_\alpha^2 \\ \frac{1}{\sqrt{\omega^2 - \omega_\alpha^2}} \arctan\left(\frac{\omega_\alpha + \xi}{\sqrt{\omega^2 - \omega_\alpha^2}}\right) & \text{if } \omega^2 > \omega_\alpha^2 \end{cases} \tag{10c}$$

This constant of motion has the following limit

$$\lim_{\alpha to 0} K_\alpha(x, v) = K_0(x, v) = \frac{1}{2} m v^2 + \frac{1}{2} m \omega^2 x^2. \tag{11}$$

For very weak dissipation ($\omega_\alpha \ll \omega$) and at first order in ω_α, the constant of motion can be written as

$$K(x, v) = K_0(x, v) + \frac{\omega_\alpha}{\omega}\left[m\omega x v - 2K_0(x, v) \arctan\left(\frac{v}{\omega x}\right)\right]. \tag{12}$$

In principle, one can get the Lagrangian of the system through the expression (3), and from this Lagrangian one could get the generalized linear momentum of the system $p = p(x, v)$. However, it is not possible to know $v = v(x, p)$, even for the very weak dissipation case. Thus, the Hamiltonian is given implicitly through the above constant of motion.

The quantization of (12) was carried out in López and López (2006), where the modification of the eigenvalues of the harmonic oscillator ($E_n^{(0)} = \hbar\omega(n + 1/2)$) were given at first order in perturbation theory as

$$E_n(\omega) = \hbar\omega\left(n + \frac{1}{2}\right)\left(1 - \frac{\pi\omega_\alpha}{\omega}\right) - \frac{\hbar\omega_\alpha^2}{\omega}\left[\left(\frac{2}{3}n + \frac{1}{4}\right)\right.$$

$$\left. - \sum_{l=0}^{\infty}\sum_{s=0}^{2l+1}\binom{-1/2}{l}^2\binom{2l+1}{s}^2 \frac{(2n - 2l - s)^2}{(2l+1)^2(2l+1+s)}\right], \tag{13}$$

where the correction has been made up to second order in ω_α.

4. CLASSICAL APPROACH

Consider an ensemble of N particles moving independently which their equation of motion is given by the following dynamical system

$$\frac{d}{dt}\begin{pmatrix} x_j \\ v_j \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega_j^2 & \frac{-\alpha}{m} \end{pmatrix}\begin{pmatrix} x_j \\ v_j, \end{pmatrix}, \quad j = 1, \ldots, 3N \tag{14}$$

where ω_j is the natural free frequency of oscillations. The dissipative coefficient is the same of all oscillators since they are inside the same medium. One can think, for example, in a crystal which is inside a bosonic or fermionic medium where the wave length of the particles of this medium is less than the separation of the crystal components (Jones and March, 1985). The average interaction of the crystal components with the particles of the medium may be modeled by Eq. (14). In Astrophysics, one could think about the core of a neutron star as a superconducting lattice of protons inside a dissipative medium generated by the huge amount of neutrinos (antineutrinos) appearing from the weak decay of neutrons and protons. Since the density in the core of these stars is very big (10^{15} gr/cm^3) (Fang and Ruffini, 1983; Özel, 2006) the interaction with neutrinos (antineutrinos) is not so neglectful. Thus, maybe the local motion of an ensemble of nucleons in the core could be model by Eq. (14).

Let us see first the implications of using classical canonical partition function to study the thermodynamical characteristics of the system. To do this, let us make the following change of variable

$$x_j = \sqrt{\frac{2J_j}{m\omega_j}}\cos\phi_j, \qquad \text{and} \qquad vi = \sqrt{\frac{2\omega_j J_j}{m}}\sin(\phi_j), \tag{15}$$

where the variables ϕ_j and J_j have the following variation $\phi_j \in [0, 2\pi]$ and $J_j \in [0, \infty)$. Then, from (12), the jth-constant of motion and measure are given with this coordinates as

$$K_j = \omega_j J_j - \omega_\alpha J_j(\sin 2\phi_j - 2\phi_j), \tag{15a}$$

and

$$dx_j dv_j = \frac{1}{m} dJ_j d\phi_j. \tag{15b}$$

In this way, the partition function (5) is written as ($\eta = 1$ since the particles in the crystal are distinguishable)

$$Z = \frac{m^{3N}}{h^{3N}}\prod_{j=1}^{3N}\int e^{-\beta K_j(x_j,v_j)}dx_j dv_j = \prod_{j=1}^{3N}\frac{1}{h}\int e^{-\beta J_j[\omega_j-\omega_\alpha(\sin 2\phi_j-2\phi_j)]}dJ_j d\phi_j \tag{16}$$

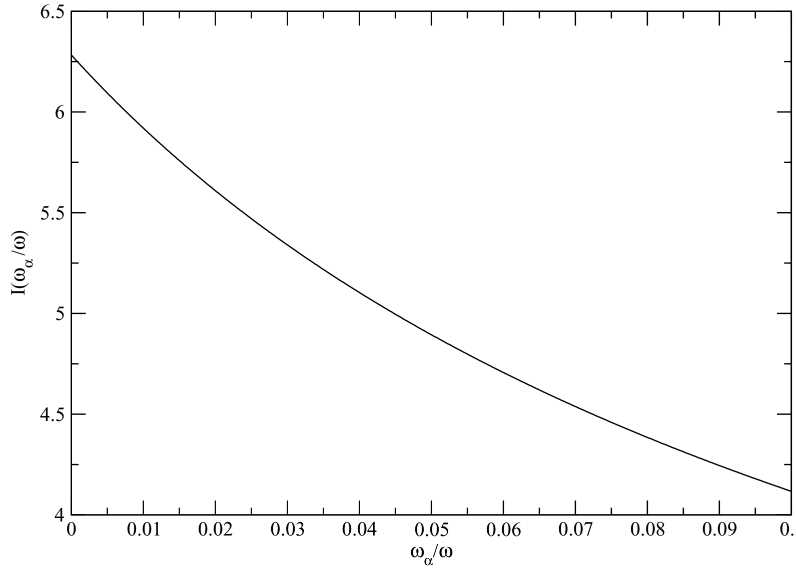

Fig. 1. Function $I\,(\alpha/\omega)$.

which can be integrated, bringing about the following result

$$Z = \prod_{j=1}^{3N} \frac{I(\omega_\alpha/\omega_j)}{\beta h \omega_j}, \tag{17a}$$

where the function $I(\xi)$ has been defined as

$$I(\xi) = \int_0^{2\pi} \frac{d\phi}{1 - \xi(\sin 2\phi - 2\phi)}. \tag{17b}$$

Figure 1 shows the behavior of this function as a function of ω_α/ω. Note that $I(0) = 2\pi$, and that ω_α/ω must be less than the unit, according to our approximations of expression (5). From (17a), one gets

$$\ln Z = -3N \ln h + \sum_{j=1}^{3N} \ln\left(\frac{I(\omega_\alpha/\omega_j)}{\beta\omega_j}\right). \tag{18}$$

Since N is big and there are $3N$ normal modes of oscillations in the crystal, one can assume continuity in the frequency spectrum and write (18) as

$$\ln Z = U_0 + \int_0^{\infty} \ln\left(\frac{I(\omega_\alpha/\omega)}{\beta\omega}\right) g(\omega)\, d\omega, \tag{19a}$$

where U_0 has been defined as $U_0 = -3N \ln h$, and $g(\omega)$ is the density spectral which must satisfied the condition

$$\int_0^\infty g(\omega)\, d\omega = 3N. \tag{19b}$$

Using the Debye's model of solids (Wannier, 1966; Mc Quarrie, 1976; Huang, 1987; Pathrio, 1996; Toda *et al.*, 1998; Schwabl, 2002), the spectral density is given by

$$g(\omega) = \begin{cases} \dfrac{9N\omega^2}{\omega_D^3} & \text{if } 0 \le \omega \le \omega_D \\ 0 & \text{if } \omega > \omega_D \end{cases}, \tag{20a}$$

where ω_D is the Debye's frequency of the solid which is defined by the cutoff frequency such that

$$\int_0^{\omega_D} g(\omega)\, d\omega = 3N. \tag{20b}$$

and it is given by

$$\omega_D = \left(\frac{3N}{4\pi V}\right)^{1/3} v_c. \tag{20c}$$

The variable V represents the volume of the solid, and v_c is the average velocity of the elastic waves in the solid which is given in terms of the longitudinal (v_l) and transversal (v_t) waves as

$$\frac{3}{v_c} = \frac{2}{v_t^3} + \frac{1}{v_l^3}. \tag{20d}$$

Substituting (20a) in (19a), it follows that

$$\ln Z = U_0 + \frac{9N}{\omega_D^3} \int_0^{\omega_D} \omega^2 \ln\left(\frac{I(\omega_\alpha/\omega)}{\beta\omega}\right) d\omega. \tag{21}$$

In this way, one can calculate the thermodynamic characteristics of the system. The internal energy of the system, its entropy, its specific heat, its equation of state, and its free energy are given by

$$U = -\frac{\partial \ln Z}{\partial \beta} = 3NkT, \tag{22a}$$

$$S = k\left[U_0 + \frac{9N}{\omega_D^3} \int_0^{\omega_D} \omega^2 \ln\left(\frac{I(\omega_\alpha/\omega)}{\beta\omega}\right) d\omega + 3N\right], \tag{22b}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = 3Nk, \tag{22c}$$

$$p = \frac{3NkT}{V} \ln\left(\frac{I(\omega_\alpha/\omega_D)}{\beta\omega_D}\right) - \frac{9N}{V\omega_D^3}\int_0^{\omega_D} \omega^2 \ln\left(\frac{I(\omega_\alpha/\omega)}{\beta\omega}\right) d\omega, \quad (22d)$$

and

$$F = -kT\left[U_0 + \frac{9N}{\omega_D^3}\int_0^{\omega_D} \omega^2 \ln\left(\frac{I(\omega_\alpha/\omega)}{\beta\omega}\right) d\omega\right]. \quad (22e)$$

As one can see, the internal energy and the specific heat of the ensemble of oscillators do not depend on the dissipative media, at first order in the dissipation parameter. We must remain here that the whole system is made up of the crystal and the medium. So, in the above quantities one needs to add the contribution coming purely from the medium. On the other hand, we have used the classical canonical statistical partition function and the Debye's model for our study of the thermodynamic quantities of the system. However, this is somewhat a little bite incorrect since Debye's model works fine to relative low temperatures, and classical canonical partition function is expected to work fine to relatively high temperatures. Thus, let us make everything consistent by using quantum canonical partition function.

5. QUANTUM APPROACH

In this case, using (7), (20a), the condition (20b), and the same hypothesis of continuity in the frequencies, one has the following expression

$$\begin{aligned}\ln Z &= \ln \prod_{j=1}^{3N}\left(\sum_n e^{-\beta E_n(\omega_j)}\right)\\ &= \sum_{j=1}^{3N} \ln\left(\sum_n e^{-\beta E_n(\omega_j)}\right) \approx \int_0^\infty \ln\left(\sum_n e^{-\beta E_n(\omega)}\right) g(\omega)\, d\omega\\ &= \frac{9N}{\omega_D^3}\int_0^\infty \omega^2 \ln\left(\sum_n e^{-\beta E_n(\omega)}\right) d\omega, \end{aligned} \quad (23)$$

Now, using (13) at first order in the dissipation parameter, one has

$$\sum_n e^{-\beta E_n(\omega)} = \frac{\lambda_\alpha e^{-\beta\hbar\omega/2}}{1 - \lambda_\alpha^2 e^{-\beta\hbar\omega}}, \quad (24a)$$

where λ_α has been defined as

$$\lambda_\alpha = e^{\beta\pi\hbar\omega_\alpha/2}. \quad (24b)$$

Thus, Eq. (23) is written in the following way

$$\ln Z = \frac{9N}{\omega_D^3} \int_0^{\omega_D} \omega^2 \ln \left(\frac{\lambda_\alpha e^{-\beta\hbar\omega/2}}{1 - \lambda_\alpha^2 e^{-\beta\hbar\omega}} \right) d\omega. \tag{25}$$

Therefore, the internal energy, the entropy, the specific heat, the equation of state and the free energy of the system are given by

$$U = \frac{9N}{2\omega_D^3} \int_0^{\omega_D} \omega^2 (\hbar\,\omega - \hbar\,\omega_\alpha \pi) \coth \left(\frac{\beta\,\hbar\,\omega}{2} - \frac{\beta\,\hbar\,\omega_\alpha \pi}{2} \right) d\omega\,, \tag{26}$$

$$S = \frac{9Nk}{\omega_D^3} \int_0^{\infty} \omega^2 \left[\ln \left(\frac{\lambda_\alpha e^{-\beta\,\hbar\,\omega/2}}{1 - \lambda_\alpha^2 e^{-\beta\,\hbar\,\omega}} \right) + \frac{\beta}{2} (\hbar\,\omega\, - \hbar\,\omega_\alpha \pi) \coth \left(\frac{\beta\hbar\omega}{2} - \frac{\beta\,\hbar\,\omega_\alpha \pi}{2} \right) \right] d\omega, \tag{27}$$

$$C_V = \frac{9N}{4kT^2 \omega_D^3} \int_0^{\omega_D^2} \frac{\omega^2 (\hbar\,\omega - \hbar\,\omega_\alpha \pi)\, d\omega}{\sinh^2 \left(\frac{\beta\,\hbar\,\omega}{2} - \frac{\beta\,\hbar\,\omega_\alpha \pi}{2} \right)}. \tag{28}$$

$$p = \frac{3NkT}{V} \ln \left(\frac{\lambda_\alpha e^{-\beta\,\hbar\,\omega_D/2}}{1 - \lambda_\alpha^2 e^{-\beta\,\hbar\,\omega_D}} \right) - \frac{9NkT}{V\omega_D^3} \int_0^{\infty} \omega^2 \ln \left(\frac{\lambda_\alpha e^{-\beta\,\hbar\,\omega/2}}{1 - \lambda_\alpha^2 e^{-\beta\hbar\omega}} \right) d\omega, \tag{29}$$

and

$$F = -\frac{9NkT}{\omega_D^3} \int_0^{\infty} \omega^2 \ln \left(\frac{\lambda_\alpha e^{-\beta\,\hbar\,\omega/2}}{1 - \lambda_\alpha^2 e^{-\beta\,\hbar\,\omega}} \right) d\omega. \tag{30}$$

Figure 2 shows the variation of C_V/Nk as a function of the temperature for several values the dissipative parameter ω_α. The effect at first order of the dissipation is to increases the specific heat a low temperatures.

6. CONCLUSIONS

We have used the phase space $(\mathbf{x}, \mathbf{v})$ to study the statistical properties of an ensemble of harmonic oscillators within a dissipative medium, where its effect on the oscillators is to create a linear velocity depending force. We have made the study at first order in the dissipation parameter for classical partition function and quantum partition function, taking the Debye's model of solids as an example for possible applications. The classical canonical partition function lead us to have an internal energy and specific heat which are independent on the dissipation. However, quantum canonical partition function brings about dependence on the dissipation for all thermodynamical variables of the system. It is our feeling that

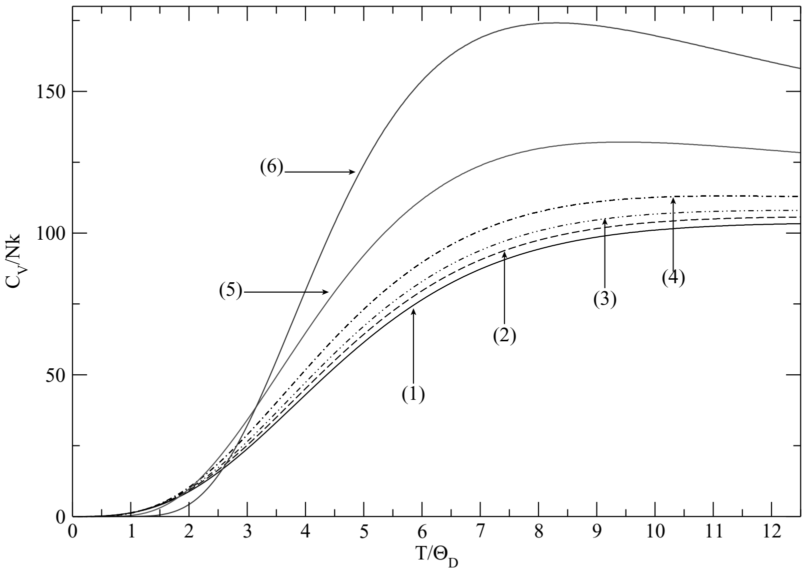

Fig. 2. Specific heat with $\theta_D = \hbar\omega_D/k = 150\ K$ (corresponding to Sodium). (1): $150\omega_\alpha\pi/\omega_D = 0.0$, (2): $150\omega_\alpha\pi/\omega_D = 0.5$, (3): $150\omega_\alpha\pi/\omega_D = 1.0$, (4): $150\omega_\alpha\pi/\omega_D = 2.0$, (5): $150\omega_\alpha\pi/\omega_D = 5.0$, (6): $150\omega_\alpha\pi/\omega_D = 10.0$.

the use of the space (**x**, **v**) for statistical physics studies has less restrictions that the space (**x**, **p**).

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