

Exact Gibbs statistical mechanics of a system of quadratic Liénard type oscillators^{a)}

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Hamiltonian dynamics and exact Gibbs statistical mechanics of a system of quadratic Liénard type oscillators have been investigated. The work has shown that the canonical ensemble for the harmonic oscillator is a particular case of the Gibbs ensemble theory developed in this paper.

Keywords: Hamilton equations, phase plane analysis, quadratic Liénard equation, harmonic oscillator, Gibbs ensemble theory.

I. INTRODUCTION

A number of problems in statistical mechanics are solved on the basis of particules without interactions. This is for example the case of the theory of ideal gas in order to simplify the complexity of mathematical analysis. However the obtained results are in practice not satisfactory so that statistical mechanics where particule interactions are taken into consideration is required¹. The Gibbs statistical mechanics satisfied to this requirement. In other words, the Gibbs statistical mechanics introduces the ensemble theory that is microcanonical, canonical and grand canonical ensembles in which interactions between particules may be taken into account. So the canonical ensemble for harmonic oscillator has been developed to study the statistical thermodynamics of a variety of physical systems^{1,2}. But it is well known that the linear harmonic oscillator could not represent with efficiency the vibration of particules of real material systems which exhibit several nonlinearity properties like geometric, material and damped nonlinearities². On the other hand, it is well known that the canonical ensemble theory for classical harmonic oscillators predicted for example, a temperature-independent specific heat at constant volume in opposition with observations. The experiments have shown that such a constant value is only adequate for large temperatures. This has been known as the law of Dulong and Petit, that is to say, this statistical mechanical model fails at intermediate temperatures. There appears then reasonable to be interested to investigate the Gibbs statistical mechanics for classical nonlinear oscillator. Therefore to overcome the preceding difficulties, the Gibbs statistical mechanics of thermodynamical materials has been developed in the framework of dynamical systems where quadratic dissipation was taken

into account². However there are few literatures on such a theory taking into consideration quadratic dissipation. Moreover this theory is particularly developed by means of approximation, due to the fact that the Hamiltonian functions are of complicated expressions. As exact analytical theories are of high importance for the modern engineering calculations, there appears more again logic to propose exact analytical studies of canonical ensemble for classical systems of quadratic Liénard type. A physically interesting case of quadratic Liénard type oscillator is that exhibiting exact trigonometric periodic solutions. Such a class of quadratic Liénard type oscillators has been recently highlighted by Akande and co-workers³. Let us consider in this way the oscillator defined by

$$\ddot{x} - ax\dot{x}^2 + bx \exp(ax^2) = 0 \quad (1)$$

which belongs to the above mentioned class of quadratic Liénard type differential equations³. As $a \rightarrow 0$, (1) reduces to the well known linear harmonic oscillator equation for $b = \omega_0^2$, where ω_0 is the angular frequency. The problem to be investigated now is to show that the canonical ensemble for (1) provides the law of Dulong and Petit for $a \rightarrow 0$ in particular, and in general includes the canonical ensemble for harmonic oscillator as special case. So the question to be addressed becomes: Can we generalize the canonical ensemble theory for harmonic oscillator so that the law of Dulong and Petit may be recovered for $a \rightarrow 0$? The present work predicts such a generalization, which is of high interest for theoretical and practical perspectives, since the law of Dulong and Petit is recovered as a limiting case and the formula to compute the specific heat at constant volume for intermediate temperatures is provided. In other words the possibility for controlling the temperature-dependent specific heat is analytically formulated so that the developed theory may be used for experimental data fitting procedures. To demonstrate the preceding hypothesis, the Hamiltonian dynamics⁴ of (1) is briefly recalled (section 2), which gives the ability to compute the canonical ensemble partition function (section 3). In this regard the specific heat at constant volume and other thermodynamical functions are deduced (section 4), the preceding results are discussed (section 5) and a conclusion of the work is finally addressed.

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II. HAMILTONIAN DYNAMICS

The Hamiltonian dynamics of (1) has been studied in⁴. This section is devoted to briefly review some main results and to represent the dynamics of the system in the phase plane.

A. Hamiltonian function

The equation (1) is of position-dependent mass so that the mass distribution function may be written as⁴

$$m(x) = m_0 \exp(-ax^2) \quad (2)$$

and the potential energy takes the form

$$V(x) = \frac{b}{2} m_0 x^2 \quad (3)$$

In this way the Hamiltonian for (1) becomes

$$H(x, p) = \frac{p^2}{2m_0} \exp(ax^2) + \frac{1}{2} b m_0 x^2 \quad (4)$$

which allows then the formulation of Hamiltonian equations.

B. Canonical equations

The Hamilton equations called also canonical equations are defined as

$$\dot{x} = \frac{\partial H}{\partial p} \quad (5)$$

$$\dot{p} = -\frac{\partial H}{\partial x} \quad (6)$$

that is to say

$$\dot{x} = \frac{p}{m_0} \exp(-ax^2) \quad (7)$$

$$\dot{p} = b m_0 x + \frac{ax}{m_0} p^2 \exp(ax^2) \quad (8)$$

which express the equations of the dynamical system (1) in the (x, p) phase plane when the initial conditions are specified.

C. Position variation of mass and phase trajectories

This section shows graphically the variation of mass distribution as a function of position (Figure 1) and simulated phase diagrams (Figure 2) from (5), and (6). The Figure 1 is obtained for $m_0 = 1$ and several $a = 1, 2, 3$. Phase diagrams in Figure 2 are plotted for $m_0 = 1$, and several values of the Hamiltonian $H = 2, 4, 8$. As illustrated by Figure 2 the phase curves are closed orbits showing the periodic behavior of the system (1) which is said to be conservative, so that the statistical mechanics for classical Hamiltonian systems may be applied.

III. CANONICAL ENSEMBLE

The objective of this section is to use the canonical ensemble theory to calculate the thermodynamical functions for classical nonlinear oscillator (1).

A. Canonical partition function

Let us consider classical system of N decoupled quadratic Liénard type oscillators defined by (1), in contact with a reservoir at temperature T . In this perspective the canonical partition function of the system of N independent quadratic Liénard oscillators is given by

$$Z(T, N) = Z_1^N(T) \quad (9)$$

where $Z_1(T)$ designates the partition function of a single quadratic Liénard type oscillator that is^{1,2}

$$Z_1(T) = \frac{1}{h} \int \int dpdq \exp(-\beta H) \quad (10)$$

where

$$H(q, p) = \frac{p^2}{2m_0} \exp(aq^2) + \frac{b}{2} m_0 q^2$$

according to (4), $\beta = \frac{1}{kT}$, k is the Boltzmann constant and h is the Planck constant. In this regard the canonical partition function $Z(T, N)$ becomes⁵.

$$Z(T, N) = \left[\frac{2\pi\sqrt{m_0}}{h\sqrt{\beta(a + \beta m_0 b)}} \right]^{3N} \quad (11)$$

Knowing the canonical partition function expression, one may immediately determine the main other thermodynamical functions expressions.

B. Other thermodynamical functions

1. Heat capacity

The heat capacity also called specific heat at constant volume C_v is of high importance since it may be experimentally evaluated to immediately assess the internal energy and entropy. Analytically this may be calculated using the formula²

$$C_v(T) = \frac{\partial}{\partial T} (kT^2 \frac{\partial \log Z}{\partial T})$$

which may read using (11)

$$C_v(T) = \frac{3Nk}{2} \left[1 + \frac{m_0^2 b^2}{(m_0 b + akT)^2} \right] \quad (12)$$

from which the internal energy and entropy may be analytically expressed.

2. Internal energy, entropy and free energy

From (12) the internal energy may be written as

$$E(T) = \frac{3N}{2} \left[kT + \frac{m_0 b k T}{m_0 b + a k T} \right] \quad (13)$$

and the entropy takes the form

$$S(T) = 3Nk \left[\ln Z + \frac{a + 2m_0 b \beta}{2(a + m_0 b \beta)} \right] \quad (14)$$

and finally the Helmholtz free energy may read

$$F = -3NkT \ln \left[\frac{2\pi}{h \sqrt{\beta(a + \beta m_0 b)}} \right] \quad (15)$$

So with that, the analytical predictions of the proposed theory may be discussed regarding, the well known canonical ensemble for harmonic oscillator.

IV. DISCUSSION

In many cases the Gibbs canonical ensemble for harmonic oscillator is used to describe the statistical property of thermodynamical systems¹. In such a situation, the specific heat at constant volume is $C_v = 3Nk$, known as the law of Dulong and Petit. This relationship is temperature-independent heat capacity so that it fails at intermediate temperature. In this regard it was appropriate to develop a more satisfactory theory. The present work has proposed a new law which is temperature-dependent specific heat at constant volume on the basis of Gibbs canonical ensemble for classical quadratic Liénard type nonlinear oscillator exhibiting harmonic periodic behavior. So the theoretically predicted heat capacity is given by (12). The fundamental question was to know for $a \rightarrow 0$, if the law of Dulong and Petit is recovered. One may see that the substitution of $a = 0$ into (12) yields, immediately the law of Dulong and Petit, as expected, since $a \rightarrow 0$, corresponds to the case of harmonic oscillator equation regarding the quadratic Liénard type equation (1). For $b = 0$, the interaction potential is null, the Hamiltonian H becomes $H = \frac{p^2}{2m_0} \exp(ax^2)$, and the heat capacity (12) reduces to $C_v = \frac{3}{2}Nk$, which is, as expected, the heat capacity of the ideal gases for the

translation¹. This result is also obtained for $T \rightarrow \infty$. As $T \rightarrow 0$, the heat capacity (12) may be, by expanding the second term in (12) in Taylor series, approximated at first order by $C_v = 3Nk \left[1 - \frac{akT}{m_0 b} \right]$. However, as well mentioned in the literature¹ the classical heat capacity fails at low temperatures so that quantum approach is required. That being so the conclusion of the work may be addressed.

V. CONCLUSION

The Gibbs canonical ensemble for harmonic oscillator is in many cases used to describe the statistical property of thermodynamical systems. However, this model suffers from a number of shortcomings such as a constant heat capacity. To remedy, the Gibbs ensemble theory for quadratic Liénard type nonlinear oscillator is proposed. The fundamental question was to know what happens to this theory when some parameters take their critical value. In this perspective it is observed that the canonical ensemble for harmonic oscillator is nothing but a particular case of the theory developed in this paper. So it is established that the law of Dulong and Petit may be recovered from the temperature-dependent heat capacity expression developed in the current theory as the nonlinearity parameter tends to its critical value. There appears the specific heat of ideal gases may be also recovered as the interaction potential becomes zero, so that the theory formulated in this research contribution may have many practical implications.

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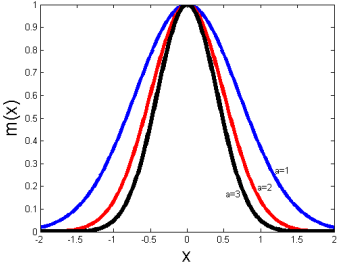


FIG. 1. Curve of position-dependent mass $m(x)$ for $m_0 = 1$ and $a = 1, 2, 3$

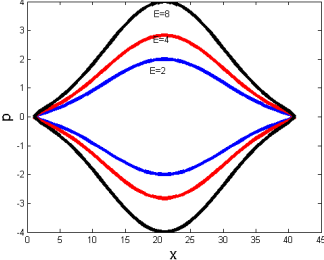


FIG. 2. Phase plane trajectories (x, p) of Hamiltonian H