PRAMANA — journal of physics

Vol. 72, No. 2
February 2009
pp. 315–323

Formulation of statistical mechanics for chaotic systems

VISHNU M BANNUR[1,*] and RAMESH BABU THAYYULLATHIL[2]
[1]Department of Physics, University of Calicut, Kozhikode 673 635, India
[2]Department of Physics, Cochin University of Science and Technology, Kochi 682 022, India
*Corresponding author. E-mail: vmbannur@yahoo.co.in

MS received 14 July 2008; revised 21 August 2008; accepted 26 August 2008

Abstract. We formulate the statistical mechanics of chaotic system with few degrees of freedom and investigated the quartic oscillator system using microcanonical and canonical ensembles. Results of statistical mechanics are numerically verified by considering the dynamical evolution of quartic oscillator system with two degrees of freedom.

Keywords. Statistical mechanics; chaotic system; quartic oscillators.

PACS Nos 05.45.-a; 05.20.Gg; 05.70.-a

1. Introduction

The study of statistical mechanics and thermodynamics of chaotic systems with few degrees of freedom is very important in understanding its various formal aspects from a dynamical point of view [1] and for the study of chaotic system using the well-developed concepts of statistical mechanics [2,3]. Since the trajectory of a chaotic system is almost ergodic in phase-space, it can be approximately described by the principles of statistical mechanics. The chaotic systems like quartic oscillator (QO), Henon–Heiles oscillator (HHO) etc., with two degrees of freedom exhibit chaos depending on the value of parameters of the system. Hence it is possible to study the thermodynamics of the system from the dynamical point of view. Issues related to the definition of various thermodynamical quantities such as entropy, temperature etc., are discussed in the literature [2–4]. There are also other highly debated issues like, the study of Fourier heat law, thermalization of oscillator chain etc. [5–12] using chaotic systems. We know that in a thermodynamical system, as the number of microsystems $N \to \infty$ the system is driven to ergodicity and the statistical property comes from the implicit assumption of collisions. On the contrary, in a chaotic system, N is finite and the nonlinear interactions present in the Hamiltonian drive the system to an almost ergodic region, provided the system is in a chaotic region. There may be few non-chaotic islands depending on the values of the parameters, where the system may not show any ergodicity and the statistical properties and thermodynamics of the system may not have much meaning in that region.

An initial study of statistical mechanics of chaotic system was carried out by Berdichevsky and Alberti [2] using Henon–Heiles oscillator and later it was extended to quartic oscillator [3] also. Various issues like concepts of temperature, entropy and distribution function and equipartition of energy were studied in detail and also verified numerically using the formulation of microcanonical ensemble.

Here, we again strengthen the idea of statistical mechanics of chaotic systems using Kinchin's formulation based on microcanonical ensemble [13]. Further, we extend the study to canonical ensemble of such a system and as an example, we consider QO and obtain various thermodynamic quantities and the results are verified numerically.

2. Henon–Heiles oscillator and quartic oscillator

First we briefly discuss QO and HHO models, studied extensively in the context of chaos and statistical mechanics of chaos [2,3]. Both are Hamiltonian systems with two degrees of freedom and the Hamiltonians are given by

$$H = \frac{(p_1^2 + p_2^2)}{2} + \frac{(1-\alpha)}{12}(q_1^4 + q_2^4) + \frac{1}{2}q_1^2 q_2^2, \tag{1}$$

and

$$H = \frac{(p_1^2 + p_2^2)}{2} + \frac{q_1^2}{2} + \frac{q_2^2}{2} + q_1^2 q_2 - \frac{1}{3}q_2^3, \tag{2}$$

for QO and HHO respectively. Here q's and p's are generalized coordinates and momenta respectively and α is a parameter. QO is chaotic except for the values of $\alpha = -\infty$, -2 and 0, and is highly chaotic for α close to 1 as shown in refs [14–16]. HHO is chaotic for energy $E = 1/6$ and develops non-chaotic islands as the energy is decreased. In order to study the statistical mechanics using microcanonical ensemble first we need to evaluate the bounded phase-space volume for a given energy E and it is given by

$$\Sigma(E) = \int_{H \le E} \mathrm{d}p_1\, \mathrm{d}p_2\, \mathrm{d}q_1\, \mathrm{d}q_2 = CE^{3/2}, \tag{3}$$

for QO with $\alpha \neq 1$ and for HHO

$$\Sigma(E) = \pi E^2 \left(1 + \frac{E}{2} + \frac{35}{32}E^2 + \cdots\right), \tag{4}$$

as discussed in detail in ref. [3]. Note that for $\alpha = 1$ the phase-space volume of QO is infinite and hence undefined. In our numerical work we chose $\alpha = 0.99$. In ref. [3] we also discussed the generalized QO with N degrees of freedom for the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2}\sum_{i,j=1}^{N} \alpha_{ij}\, q_i^2 q_j^2, \tag{5}$$

where α_{ij} are parameters. This system reduces to our earlier $N = 2$ quartic oscillator if $\alpha_{11} = \alpha_{22} = (1-\alpha)/6$ and $\alpha_{12} = \alpha_{21} = 1/2$. Phase-space volume for this system is given by

$$\Sigma(E) = \int_{H\leq E} \mathrm{d}p_1 ... \mathrm{d}p_N\, \mathrm{d}q_1 ... \mathrm{d}q_N = C_1 E^{3N/4}, \tag{6}$$

where C_1 is a constant.

3. Microcanonical ensemble

In the microcanonical ensemble, one consider a system with constant energy and in our case we consider a Hamiltonian system like HHO or QO with constant energy. Depending on the value of the parameters, the system may exhibit chaos and their phase-space trajectory is almost ergodic in the whole or some region of the phase-space. In those chaotic regions we may have averages of any observable O given as

$$\langle O\rangle_{\mathrm{t}} = \langle O\rangle_{\mathrm{ph}} = \langle O\rangle_{\mathrm{en}}, \tag{7}$$

which follows from ergodic theorem. Here $\langle O\rangle_{\mathrm{t}}$, $\langle O\rangle_{\mathrm{ph}}$ and $\langle O\rangle_{\mathrm{en}}$ refers to time, phase-space and ensemble averages respectively. For example, the average of momentum square of ith degrees of freedom $\langle p_i^2\rangle$ approaches the same value on both time average and phase-space average, as verified in ref. [3]. The phase-space average is defined as

$$\langle O\rangle_{\mathrm{ph}} \;\equiv\; \frac{1}{\Gamma}\int_{E\leq H\leq E+\Delta} \mathrm{d}\Sigma\, O, \tag{8}$$

where Σ, Γ and $\Omega \equiv (\partial\Sigma/\partial E)$ are the number of microstates in phase-space hypersphere, hypershell and on the hypersphere surface respectively. Using the above definition of average we now have the equipartition theorem,

$$\langle p_1^2\rangle = \langle p_2^2\rangle = \cdots = \left[\frac{\partial \ln\Sigma}{\partial E}\right]^{-1} \equiv T_B. \tag{9}$$

Here T_B may be identified as a temperature by considering a thought experiment of equilibration of two systems in thermal contact. Suppose we have two systems 1 and 2 and they are brought into thermal contact. After equilibration, the average momentum square of ith particle in system 1 is,

$$\langle p_i^2\rangle_{(1)} = \left[\frac{\partial \ln\Sigma_1}{\partial E_1}\right]^{-1} = T_{B1}\ ,$$

by equipartition theorem (EPT) on system 1. It may be also evaluated by considering the combined system $(1+2)$ as

$$\langle p_i^2\rangle_{(1+2)} = \left[\frac{\partial \ln \Sigma}{\partial E}\right]^{-1} = T_B,$$

by EPT on system (1+2) together. Similarly, for the other system

$$\langle p_j^2\rangle_{(2)} = \left[\frac{\partial \ln \Sigma_2}{\partial E_2}\right]^{-1} = T_{B2},$$

by EPT on system 2 which is also equal to

$$\langle p_j^2\rangle_{(1+2)} = \left[\frac{\partial \ln \Sigma}{\partial E}\right]^{-1} = T_B,$$

by EPT on system (1+2) together. Therefore, once the system is equilibrated $T_{B1} = T_{B2}$ and hence we may call

$$T_B = (\partial \ln \Sigma/\partial E)^{-1} \tag{10}$$

as the temperature of the system. Note that it is different from normal definition of temperature,

$$T_S = \left[\frac{\partial \ln(\partial\Sigma/\partial E)}{\partial E}\right]^{-1} = \langle \Phi\rangle^{-1},$$

where $\Phi = \nabla\cdot(\nabla H/|\nabla H|^2)$, which was found recently [4] and reformulated and verified using quartic oscillators as well as Henon–Heiles oscillators in ref. [3]. In the limit $N\to\infty$ both are the same.

Let us now discuss the entropy of our system which is an extensive variable. Following Khinchin [13] for a system with energy E, which consists of two subsystems 1 and 2 we have,

$$\Omega(E) = \sum_{E_1} \Omega_1(E_1)\Omega_2(E-E_1),$$

which can be written as

$$\Omega(E) = \int_0^\infty \mathrm{d}E_1 \Omega_1(E_1)\Omega_2(E-E_1). \tag{11}$$

Since the relation given in eq. (11) is a convolution integral, it is convenient to work with Laplace transform of various $\Omega(E)$. Defining $\phi(\alpha) = \int_0^\infty \mathrm{d}E\mathrm{e}^{-\alpha E}\Omega(E)$ we write $\phi(\alpha) = \phi_1(\alpha)\phi_2(\alpha)$ where ϕ_1 and ϕ_2 are Laplace transforms of Ω_1 and Ω_2 respectively. Again, following Khinchin, we choose $\alpha=\theta$ as the simple root of the equation

$$-\left.\frac{\mathrm{d}\ln\phi(\alpha)}{\mathrm{d}\alpha}\right|_{\alpha=\theta} = E. \tag{12}$$

In simple systems like N-quartic oscillators [3] where $\Sigma(E) = CE^{3N/4}$ or ideal gas [17] with

$$\Sigma(E) = \left(\frac{V}{h^3}\right)^N \frac{(2\pi m)^{3N/2}}{(3N/2)!} E^{3N/2},$$

etc., this θ is related to T_B via EPT. To see this connection consider systems with $\Sigma(E) = CE^l$ and the corresponding $\Omega(E) = ClE^{l-1}$. Then EPT gives us

$$T_B^{-1} = \frac{\partial \ln \Sigma}{\partial E} = \frac{\Omega}{\Sigma} = \frac{l}{E}. \tag{13}$$

Since

$$\phi(\alpha) = \int_0^\infty \mathrm{d}E\, \mathrm{e}^{-\alpha E} ClE^{l-1} = \frac{Cl!}{\alpha^l} \tag{14}$$

and using eq. (14) in eq. (12) gives us the relation

$$\theta = \frac{l}{E}. \tag{15}$$

Comparing eqs (13) and (15) we get the important relation $\theta = T_B^{-1}$. Now the extensive property reads as

$$\phi(\alpha) = \phi_1(\alpha)\phi_2(\alpha) \to \phi(T_B) = \phi_1(T_B)\phi_2(T_B).$$

In this formalism [13] the entropy is defined as

$$S = E\,\theta + \ln \phi(\theta) \to \frac{E}{T_B} + \ln \phi(T_B), \tag{16}$$

and it becomes

$$S = \frac{E_1 + E_2}{T_B} + \ln(\phi_1(T_B)\phi_2(T_B)) = S_1 + S_2, \tag{17}$$

where S_1 and S_2 are entropies of the subsystems. Hence the extensive property of the entropy defined by eq. (16) is very well-established. For our examples,

$$\Sigma = CE^l \to \ln \Sigma = \ln C + l \ln E$$

and this gives us

$$S = \ln \Sigma + \ln l! - (l \ln l - l) + \text{constant}.$$

Finally, it leads to

$$\frac{\partial S}{\partial E} = \frac{\partial \ln \Sigma}{\partial E} = T_B^{-1},$$

which is the well-known thermodynamic relation.

4. Canonical ensemble formulation of quartic oscillators

In the classical theory we have the canonical partition function

$$Q = \int \mathrm{d}p_1\, \mathrm{d}p_2\, \mathrm{d}q_1\, \mathrm{d}q_2\; \mathrm{e}^{-\beta[\frac{p_1^2+p_2^2}{2}+\frac{1}{2}((1-\alpha)/6\;(q_1^4+q_2^4)+q_1^2\,q_2^2)]}, \tag{18}$$

which reduces to

$$Q = (2\,\pi\,T)^{3/2}\; 2\,\sqrt{\frac{1-\alpha}{2(4-\alpha)}}\; K\left(\sqrt{\frac{2+\alpha}{4-\alpha}}\right), \tag{19}$$

where T is the temperature and $\beta = 1/T$ and $K(z)$ is the complete elliptical integral of the first kind. From the partition function Q one can obtain the density of states which may be useful for the study of transition from chaos to integrability of a system [18].

For a more general quartic oscillator with N degrees of freedom we have

$$Q_N = \int d^N p d^N q \mathrm{e}^{-\beta H},$$

where

$$H = \sum_i \frac{p_i^2}{2} + \sum_{i,j} \frac{\alpha_{ij}}{2} q_i^2\, q_j^2,$$

which on simplification reduces to

$$Q_N = T^{3N/4} C_N, \tag{20}$$

where C_N is independent of T. Following the standard procedure, various thermodynamic quantities may be derived from the Helmholtz free energy,

$$A = -T \ln Q_N = -\frac{3N}{4}\, T\; \ln T - T\; \ln C_N. \tag{21}$$

The entropy S and the average energy U are

$$S = \frac{3N}{4}\, \ln T + \frac{3N}{4} + \ln C_N$$

and

$$U = \frac{3}{4} N T.$$

Further, the specific heat C_V and square of the energy fluctuation ΔE^2 are obtained as

$$C_V = \frac{3}{4} N, \quad \frac{\Delta E^2}{U^2} = \frac{1}{3N/4}.$$

It is interesting to note that the energy–temperature relation here is the same as that of the microcanonical ensemble formulation, i.e. $T_B^{-1} = (3N/4)/E$, provided we take the temperature T to be the same as T_B. Also note that the temperature $T_S \equiv \langle \Phi \rangle^{-1}$ defined in ref. [4] is obtained from the definition

$$\langle \Phi \rangle = \frac{1}{Q_N} \int d^N p d^N q \mathrm{e}^{-\beta H} \nabla \cdot \frac{\nabla H}{|\nabla H|^2},$$

and after some algebra it gives us

$$\langle \Phi \rangle = \beta = \frac{1}{T},$$

which is also the same as T. This means that T_B and T_S are the same and equal to T, since T is the temperature of the reservoir with the number of degrees of freedom $N \to \infty$ and at this limit $T_B = T_S$. Thus, for the dynamical evaluation of temperature in canonical ensemble formulation T_B may be more preferable, contrary to the observation in ref. [4], since the expression for Φ is more complicated than p_i^2 for very large N.

5. Numerical results

Numerical results for microcanonical ensemble of QO were reported earlier [3] where we have showed that the temperatures, which are obtained by time averaging, agrees with that of the phase-space averaging whenever the system and the initial points are chosen to be in the chaotic region. Here, in the case of canonical ensemble also, the time averages almost agree with that of the phase-space averages for the chaotic QO system. To establish this we have performed a dynamical calculation of various quantities like temperatures (T_B and T_S), average energy (U) and specific heat (C_V). In doing this we couple one of the degrees of freedom q_1 of our QO to a thermal bath. And the thermal bath is modelled by Nose–Hoover thermostats given by

$$\dot{\eta} = \frac{\dot{q}_1^2}{T} - 1, \tag{22}$$

where T is the temperature. The final equations of motion which follows from the Hamiltonian in eq. (1) are

$$\ddot{q}_1 = -\frac{(1-\alpha)}{3} q_1^3 - q_1 q_2^2 - \eta \dot{q}_1 \tag{23}$$

and

$$\ddot{q}_2 = -\frac{(1-\alpha)}{3} q_2^3 - q_2 q_1^2. \tag{24}$$

And we need the solutions to eqs (22)–(24). To check for the accuracy of the numerical method we may use the following constant of motion of the above set of equations:

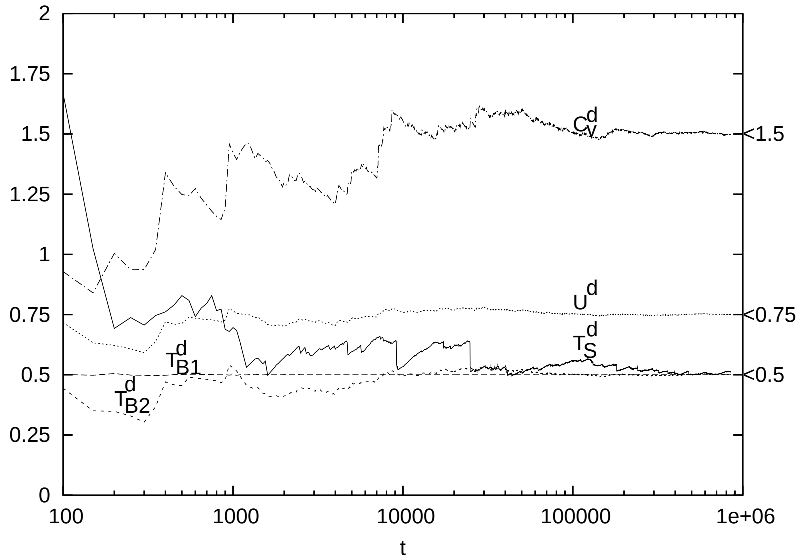

Figure 1. Plots of T_B^d of q_1 (T_{B1}^d) and q_2 (T_{B2}^d) degrees of freedom, T_S^d, U^d and C_V^d of chaotic QO system as a function of time.

$$E \equiv \frac{(p_1^2+p_2^2)}{2} + \frac{(1-\alpha)}{12}(q_1^4+q_2^4) + \frac{1}{2}q_1^2q_2^2 + T\,\frac{\eta^2}{2} + T\int_0^t \mathrm{d}\tau\eta(\tau). \quad (25)$$

Results are plotted in figure 1 for the thermostat temperature $T = 0.5$. Here T_B^d, T_S^d, U^d and C_V^d are obtained by time averaging of dynamical quantities. These are plotted as a function of time in figure 1 and asymptotically they all approach the values obtained from the phase-space averages, i.e., from eq. (21) for $N = 2$, which are given by $T_B = 0.5$, $T_S = 0.5$, $U = 0.75$ and $C_V = 1.5$. The QO system is chosen to be highly chaotic with α close to 1. For reasons of numerical stability we took $\alpha = 0.99$. As can be seen from the plot, T_{B1}^d immediately approaches 0.5, the temperature of the thermostats, since it is in direct contact with the reservoir. But the other dynamical quantities T_{B2}^d, T_S^d, U^d and C_V^d slowly approach the values 0.5, 0.5, 0.75 and 1.5 respectively in accordance with the ergodic theorem.

6. Conclusions

The formulation of statistical mechanics of chaotic systems based on Khinchin's formalism [13] of statistical mechanics for a finite N system is presented. We investigated both microcanonical and canonical ensemble systems of quartic oscillators. The microcanonical ensemble of chaotic systems were studied and numerically verified earlier by Berdichevsky and Alberti [2], and also by one of us [3]. Here we strengthened the earlier observations and extended the study to canonical ensemble and numerical verification is done using a chaotic QO system. Various quantities like temperatures, energy and specific heat are numerically evaluated by time averaging and they are almost in agreement with our formalism.

References

[1] M Bianucci, R Manella, B J West and P Grigolini, *Phys. Rev.* **E51**, 3002 (1995)
[2] V L Berdichevsky and M V Alberti, Phys. Rev. **A44**, 858 (1991)
[3] V M Bannur, P K Kaw and J C Parikh, *Phys. Rev.* **E55**, 2525 (1997)
V M Bannur, *Phys. Rev.* **E58**, 407 (1998)
[4] H H Rugh, *Phys. Rev. Lett.* **78**, 772 (1997)
[5] B Hu, L Yang and Y Zhang, *Phys. Rev. Lett.* **97**, 124302 (2006)
[6] L Yang, P Grassberger and B Hu, *Phys. Rev.* **E74**, 062101 (2006)
[7] G R Lee-Dadswell, B G Nickel and C G Gray, *Phys. Rev.* **E72**, 031202 (2005)
[8] S Corezzi, M Bianucci and P Grigolini, *Phys. Rev.* **E52**, 6881 (1995)
[9] G Casati, J Ford, F Vivaldi and W M Visscher, *Phys. Rev. Lett.* **52**, 1861 (1984)
[10] S Lepri, R Livi and A Politi, *Phys. Rev. Lett.* **78**, 1896 (1997)
[11] B Müller and T Trayanov, *Phys. Rev. Lett.* **68**, 3387 (1992)
C Gong, *Phys. Lett.* **B298**, 257 (1993)
T S Biro, C Gong, B Müller and T Trayanov, *Int. J. Mod. Phys.* **C5**, 113 (1994)
[12] V M Bannur, *Phys. Rev.* **C72**, 024904 (2005)
[13] A I Khinchin, *Mathematical foundations of statistical mechanics* (Dover Pub., 1949)
[14] M Lakshmanan and R Sahadevan, *Phys. Rep.* **224**, 1 (1993)
[15] M P Joy and M Sabir, *Pramana – J. Phys.* **40**, 17 (1993)
[16] M S Santhanam and J N Bandyopadhay, *Phys. Rev. Lett.* **95**, 114101 (2005)
[17] R K Pathria, *Statistical mechanics* (Butterworth-Heinemann, Oxford, 1997)
[18] H Aiba and T Suzuki, *Phys. Rev.* **E72**, 066214 (2005)