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Statistical mechanics of quartic oscillators

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We study statistical mechanics of quartic oscillator with two degrees of freedom, which is known to be chaotic almost everywhere except in a few regions of the parameter range. We obtain exact expressions for temperature, entropy, and distribution functions. Temperature is also obtained numerically by time averaging the kinetic energy and using equipartition theorem and agrees with our expressions when the system is almost chaotic. We further generalize our model to quartic oscillators with N degrees of freedom, and exact expressions for thermodynamic quantities are obtained. As $N\rightarrow\infty$, standard statistical mechanics results are recovered. We also discuss pressure, density, and equation of state of this system. [S1063-651X(97)09803-6]

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I. INTRODUCTION

Statistical mechanics (SM) [1] is normally used to study a system with a large number of particles (degrees of freedom) in thermal equilibrium. In recent years, however, many Hamiltonian systems (e.g., the Henon-Heiles oscillator) with a few ($N=2,3$) degrees of freedom have been found that are almost chaotic [2] in nature. Further, it has been shown that, just as for systems with many degrees of freedom, one can define ''macroscopic'' variables such as temperature, entropy, and distribution function, for these chaotic systems with $N=2,3$. The ''macroscopic'' (thermodynamics or SM) quantities characterize the ''macroscopic'' state of the $N=2,3$ chaotic systems. It is therefore natural to expect that in these cases the macroscopic quantities may enable one (as in thermodynamics and SM of large systems) to learn about many aspects of the system without explicitly carrying out detailed calculations involving the orbits of the particles.

A large number of studies in the thermodynamics of the Henon-Heiles (HH) oscillator have been carried out but they have some limitations. First, the HH oscillator is almost chaotic only for energy $\varepsilon=1/6$ and second, due to resonance coupling between the two oscillators the role of chaotic behavior in the determination of thermodynamics of such a system is not clear. In view of this, we consider a quartic oscillator (QO) model, which does not have the difficulties associated with the HH oscillator mentioned above. Another major advantage of the quartic oscillator is that we are able to derive analytic expressions for temperature, entropy, and distribution function for the system.

For the $N=2$ quartic oscillator we also estimate numerically the time average of kinetic energies of each degree of freedom. We find thermalization of energy and estimate the temperature from equipartition theorem, which matches the temperature obtained analytically. In this model, the temperature has a very simple linear variation with the total energy. The equipartition of energy takes place because of the nonlinear interaction so that system as whole is almost chaotic. Further, we are able to generalize the model from two-degrees of freedom to N degrees of freedom and again analytically derive thermodynamic quantities and distribution functions. From the expressions we can explicitly see that the definition of entropy used for a finite N system and that used in SM matches for $N\rightarrow\infty$. Similarly, the particle momentum distribution goes from a flat distribution to a Gaussian as N goes from 2 to ∞. We also derive the equation of state for a chaotic quartic oscillator with $N=2$.

In Sec. II we describe the quartic oscillator with $N=2$ and evaluate it's thermodynamic functions. A discussion of the quartic oscillator with N degrees of freedom follows in Sec. III. The distribution functions and the equation of state are derived in Sec. IV. Summary and conclusions are given in Sec. V.

II. $N=2$ QUARTIC OSCILLATOR

The Hamiltonian of this model is

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

where q's and p's are generalized coordinates and momenta, respectively, and α is a parameter. Some of the classical and quantum mechanical properties were studied in [3–5]. Here we investigate the statistical mechanics and thermodynamics of this system when it is almost chaotic. It was shown by Berdichevsky and Alberti [2] that one can apply SM to a chaotic system, even though it has a few degrees of freedom, with a slight modification of the definition of entropy and distribution function from that of usual SM. More precisely, they studied the SM of the HH oscillator. Here we study the quartic oscillator model because it does not have problems of resonance coupling between oscillators and is almost chaotic for a wide range of energy and parameter value α $(\alpha>6)$. It is fully integrable for $\alpha=0,2$.

Following Berdichevsky and Alberti [2] for a system with a few degrees of freedom entropy is defined as $S(E)=\ln\Gamma(E)$, where Γ is the phase-space volume bounded by the constant energy (E) surface. Thus,

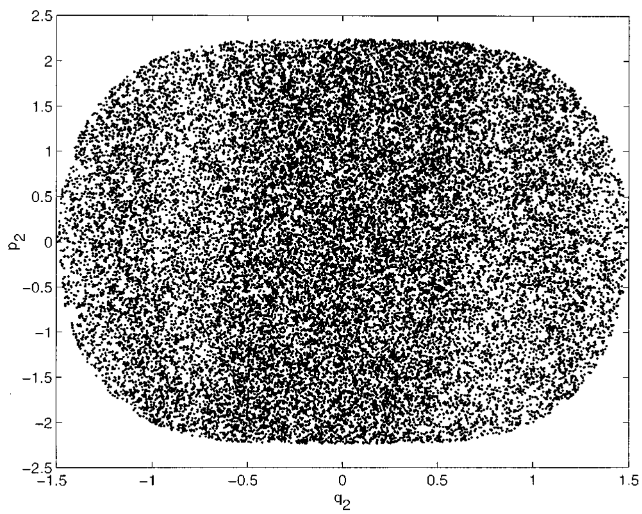

FIG. 1. Poincaré section (q_2,p_2) of 2 QO for $E=2.5$ and $\alpha=500$, where q_2 and p_2 are coordinate and momentum of particle 2, respectively.

$$\Gamma(E)=\int_{H\leq E} dp_1 dp_2 dq_1 dq_2, \tag{2}$$

and on integration over momenta, we get

$$\Gamma(E)=\int dq_1 dq_2 (E-U), \tag{3}$$

which on integration by parts gives

$$\Gamma(E)=2\pi\int_0^E A(e)de. \tag{4}$$

Here $A(e)$ is the area in the (q_1,q_2) plane, bounded by the curves $U(q_1,q_2)=e$, i.e.,

$$A(e)=\int_{U\leq e} dq_1 dq_2, \tag{5}$$

which on integration over one of the variable gives

$$A(e)=4\int_0^{(2e)^{1/4}} dx\left(-\frac{\alpha x^2}{2}+\frac{1}{2}\sqrt{(\alpha^2-4)x^4+8e}\right)^{1/2}, \tag{6}$$

in our QO model. As an example, we take $E=2.5$, and $\alpha=500$. For this set of parameter values the $N=2$ quartic oscillator is almost chaotic, as can be seen from Fig. 1. From the expression for entropy we can obtain the temperature $T_B^{-1}=\partial S/\partial E$ and by explicit integration we can very easily get $T_B=\frac{2}{3}E$. With the usual definition of entropy in SM, $S=\ln(\partial\Gamma/\partial E)$ we would have got a temperature, say, $T_s=2E$. Our numerical result for temperature, which is obtained by taking time average of momentum square of particles 1 and 2, is shown in Fig. 2. We can see that asymptotically the values approach each other and equal to $T_B=2E/3$.

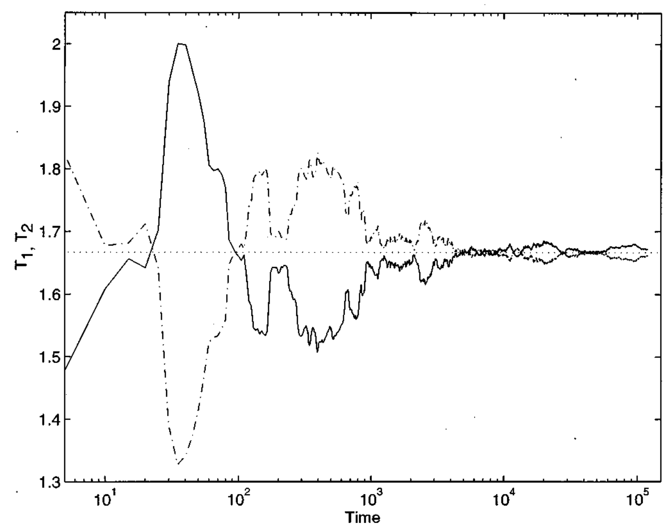

FIG. 2. Time averaged momentum square of particle 1 (solid curve), particle 2, (dash-dotted curve), and T_B (dotted curve) plots for $N=2$ quartic oscillators (2 QO) for $E=2.5$ and $\alpha=500$.

III. *N* DEGREES OF FREEDOM QUARTIC OSCILLATOR

Consider N coupled quartic oscillators. The Hamiltonian is

$$H=\frac{1}{2}\sum_{i=1}^{N} p_i^2+\frac{1}{2}\sum_{i,j=1}^{N}\alpha_{ij}q_i^2q_j^2\equiv\frac{1}{2}p^2+U, \tag{7}$$

where α_{ij} are parameters. This system reduces to our earlier $N=2$ quartic oscillator for $\alpha_{11}=\alpha_{22}=1$ and $\alpha_{12}=\alpha_{21}=\alpha/2$. In Eq. (7) U is the potential energy. We follow Khinchin's [1] procedure to evaluate the thermodynamic quantities, assuming that parameters are such that the system is almost chaotic. The phase space volume $\Gamma(E)$ is

$$\Gamma(E)=\int_{H\leq E} dp_1\cdots dp_N dq_1\cdots dq_N=C_1E^{3N/4}, \tag{8}$$

where C_1 is a constant. Equation (8) follows from a simple scaling argument by noting that q_i has dimensions $E^{1/4}$ and p_i has dimension $E^{1/2}$. The structure function $\Omega(E)$ is given by

$$\Omega(E)\equiv\frac{\partial\Gamma}{\partial E}=C_1\frac{3N}{4}E^{(3N/4-1)}, \tag{9}$$

and the generating function

$$\Phi(\alpha)=\int_0^\infty dx e^{-\alpha x}\Omega(x)=C_2\alpha^{-3N/4}, \tag{10}$$

so that

$$\ln\Phi(\alpha)=\ln C_2-\frac{3N}{4}\ln\alpha, \tag{11}$$

where C_2 is a constant. Temperature, which is defined by the relation

$$\left.\frac{\partial \ln \Phi(\alpha)}{\partial \alpha}\right|_{\alpha=1/T}=-E, \tag{12}$$

immediately gives

$$T=\frac{4}{3N}E. \tag{13}$$

For the $N=2$ QO the above relation gives $T=2E/3$, which we obtained earlier using Berdichevsky's definition of entropy. The entropy is given by

$$S=\frac{E}{T}+\ln\Phi(T)+\text{const}=\frac{3N}{4}\ln E+\text{const}=\ln\Gamma(E)+\text{const}, \tag{14}$$

which is different from the usual SM defintion of entropy, viz.,

$$S_s=\ln\frac{\partial\Gamma}{\partial E}=(3N/4-1)\ln E+\text{const}. \tag{15}$$

Note that for large N, $S_s \rightarrow S$.

We emphasize that for the above results to be true the parameters α_{ij} should be such that system is almost chaotic. In this case, an equipartition of energy between the N degrees of freedom takes place and one has

$$\left\langle p_1\frac{\partial H}{\partial p_1}\right\rangle=\left\langle p_2\frac{\partial H}{\partial p_2}\right\rangle=\cdots=\left(\frac{\partial \ln\Gamma}{\partial E}\right)^{-1}. \tag{16}$$

We then obtain

$$\left(\frac{\partial \ln\Gamma}{\partial E}\right)^{-1}=\left(\frac{3N}{4E}\right)^{-1}=T, \tag{17}$$

which we find in our numerical results for $N=2$. Since we have self interaction as well as mutual interactions between the coupled oscillators, equipartition of energy takes place not only between kinetic energies but also with interaction energy. In other words, one also has

$$\left\langle q_1\frac{\partial H}{\partial q_1}\right\rangle=\left\langle q_2\frac{\partial H}{\partial q_2}\right\rangle=\cdots=\left(\frac{\partial \ln\Gamma}{\partial E}\right)^{-1}=T. \tag{18}$$

We also notice in the $(N=2)$ numerical results that the average value of twice the time averaged kinetic energy of the two oscillators is equal to T, even though for each oscillator it is not. This is because of virial theorem, which states that

$$\sum_{i=1}^{N}\left\langle p_i\frac{\partial H}{\partial p_i}\right\rangle=4\sum_{i=1}^{N}\left\langle q_i\frac{\partial U}{\partial q_i}\right\rangle=4\langle U\rangle, \tag{19}$$

and hence the total energy

$$E=\frac{1}{2}\sum_{i=1}^{N}\left\langle p_i\frac{\partial H}{\partial p_i}\right\rangle=\frac{1}{4}\sum_{i=1}^{N}\left\langle p_i\frac{\partial H}{\partial p_i}\right\rangle, \tag{20}$$

or

$$\frac{1}{N}\sum_{i=1}^{N}\left\langle p_i\frac{\partial H}{\partial p_i}\right\rangle=\frac{4}{3N}E=T. \tag{21}$$

Therefore, even though full thermalization has not taken place still the average temperature is always related to the total energy whose value is T. This is true even for that value of α_{ij} for which system is integrable and has nothing to do with chaotic trajectories. So the proper test of thermalization is equipartition theorem, which states that time averaged kinetic energy of each oscillator should approach the same value, which is equal to T, given by Eq. (13).

IV. PROBABILITY DENSITY FUNCTIONS

Following either Khinchin or Berdichevsky, the probability density function of the ith particle is

$$f_1(q_i,p_i,E)=\frac{\Omega^i(E-e_i)}{\Omega(E)}, \tag{22}$$

where $\Omega(E)$ is the structure function of full system and $\Omega^i(E-e_i)$ is that of system excluding ith particle. For $N=2$ QO, the probability density functions (PDF) of one of the oscillators is obtained as an elliptic function. That is,

$$\Gamma_1(q_1,p_1,E)=\int dp_2\,dq_2 = 2\int_0^{q_{max}} dq_2\sqrt{2E-p_1^2-q_1^4-q_2^4-\alpha q_1^2q_2^2}, \tag{23}$$

where

$$q_{max}\equiv\left[-\frac{\alpha}{2}q_1^2+\frac{1}{2}\sqrt{(\alpha^2-4)q_1^4+4(2E-p_1^2)}\right]^{1/2}, \tag{24}$$

the maximum allowed value of q_2. Once we know the expressions for Γ_1 and Γ [Eqs. (23) and (8), respectively) using Eq. (22) for f we get, after some algebra,

$$f_1(q_1,p_1,E)=A\frac{K(z)}{[(\alpha^2-4)q_1^4+4\,(2E-p_1^2)]^{1/4}}, \tag{25}$$

where

$$A^{-1}=2\,\pi E^{1/2}\int_0^1 dy\sqrt{-\alpha y^2+\sqrt{(\alpha^2-4)y^4+4}}, \tag{26}$$

$$z=\sqrt{\frac{1}{2}-\frac{\alpha q_1^2/2}{\sqrt{(\alpha^2-4)q_1^4+4\,(2E-p_1^2)}}}, \tag{27}$$

and $K(z)$ is an elliptic function of second kind.

For the N degrees quartic oscillator system the calculation involves complicated angular integration to get one degree of freedom PDF. However, we can evaluate one degree of freedom momentum distribution by integrating out the position of one particle PDF. That is,

$$f(p)=\int f_1(p,q,E)\,dq, \tag{28}$$

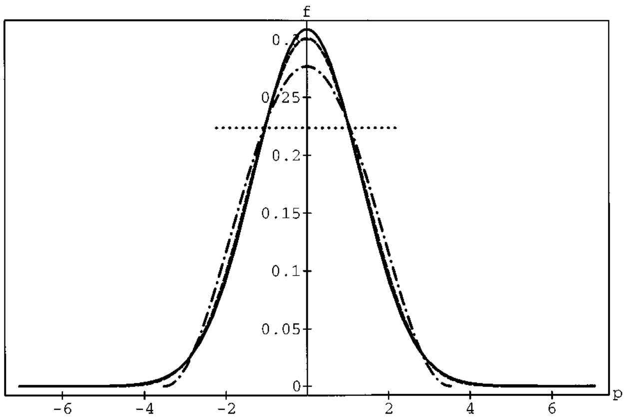

FIG. 3. One particle momentum distribution $[f \equiv f(p)]$ of N degrees quartic oscillator for $N=2$ (dotted curve), $N=5$ (dash-dotted curve), $N=20$ (dashed curve), and Gaussian $N=\infty$ (solid curve).

which after some algebra gives

$$f(p)=\frac{\left[1-\frac{p^2/(2T)}{3N/4}\right]^{(3N-6)/4}}{\sqrt{\frac{3NT}{2}}B\left(\frac{3N-2}{4},\frac{1}{2}\right)}, \tag{29}$$

where $B(x,y)$ is the beta function. Here we made use of Eq. (13) to relate energy and temperature. The plot of $f(p)$ is given in Fig. 3 for $E=2.5$ and for $N=2$, 5, 20, and a Gaussian ($N=\infty$). We can see that as N increases the distribution changes from a flat distribution to a Gaussian. This can also be seen from Eq. (29). As $N \rightarrow \infty$,

$$f(p)\rightarrow \frac{1}{\sqrt{2\pi T}}e^{-p^2/(2T)}, \tag{30}$$

the Maxwellian distribution.

Next let us derive other thermodynamics quantities such as pressure, density, and equation of state (EOS). For the N QO system pressure is given by [1]

$$P=\sum_{i=1}^{N}\frac{1}{\Omega(E)}\int dp_i p_i^2 \Omega^{(i)}(E-e_i), \tag{31}$$

where Ω^i is the structure function of the system except the ith particle and e_i is the energy of the ith particle. On explicitly summing and evaluating the above integral we get

$$P(q)=\theta_0 2^{N/2}\frac{1}{\Omega(E)}\int dq_1 \ldots dq_N(E-U)^{N/2}, \tag{32}$$

where θ_0 is a constant and P is a function of one coordinate q. Defining

$$f(E,q)=\int dq_2 \ldots dq_N(E-U)^{N/2}, \tag{33}$$

the pressure is given by

$$P(q)=\theta_0 2^{N/2}\frac{1}{\Omega(E)}f(E,q). \tag{34}$$

On integrating the one particle probability density function [Eq. (22)] over momentum we get

$$\overline{n(q)}=\theta_0 2^{N/2}\frac{1}{N\Omega(E)}\frac{\partial}{\partial E}f(E,q). \tag{35}$$

From Eqs. (34) and (35) we eliminate $\Omega(E)$ to get EOS,

$$P(q)=\frac{1}{\frac{\partial}{\partial E}\ln f}n(q)\equiv T_{eff}(q)n(q), \tag{36}$$

where $n(q)\equiv N\overline{n}$ is the density and $T_{eff}\equiv(\partial \ln f/\partial E)^{-1}$ is a position-dependent effective thermodynamic temperature. Note that P, n, and T_{eff} all depend on position in the case of a finite N system. For our special case of $\alpha_{ii}=1$ and $\alpha_{ij}=\alpha_{ji}=\alpha/2$,

$$f(E,q)=\int d^{N-1}\theta\int_0^{q_0'}dq'^{N-2} \times\left[E-\frac{1}{2}q^4-\frac{\alpha}{2}q^2q'^2-q'^4 f_\theta(\theta)\right]^{N/2}, \tag{37}$$

where q' and θ are the radial and angular coordinates in $(N-1)$ dimensional space. $f_\theta(\theta)$ is a function of angles. It may be also written as

$$f(E,q)=E^{(3N-1)/4}f_1(\overline{q}), \tag{38}$$

where f_1 is the above integral after factoring out E's and $\overline{q}\equiv q/E^{1/4}$. Therefore,

$$T_{eff}^{-1}=\frac{3N-1}{4}\frac{1}{E}-\frac{\overline{q}}{4E}\frac{1}{f_1}\frac{\partial f_1}{\partial \overline{q}}. \tag{39}$$

From the above equations, in the region where $q \ll E^{1/4}$,

$$T_{eff}\approx\frac{4E}{3N-1}=\frac{3N}{3N-1}T, \tag{40}$$

and for $N\rightarrow\infty$ (again, the second term in $\partial \ln f/\partial E$ is negligible) $T_{eff}\rightarrow T$. Hence thermodynamic temperature of a finite N system goes to that of SM for $N\rightarrow\infty$. In Fig. 4, we have plotted EOS for an $N=2$ QO system for $E=2.5$ and $\alpha=500$. T_{eff}, the slope of the curve at large n (small q) is ≈ 1.7 close to $2E/3$ and asymptotically ($q\rightarrow 0$) it approaches 2 [see Eq. (40)].

V. SUMMARY AND CONCLUSIONS

We have studied some aspects of statistical mechanics and thermodynamics of quartic oscillators. Exact expressions for temperature, entropy, and one particle momentum distribution for N-degrees quartic oscillators are obtained analytically. These results approach standard statistical mechanics results as $N\rightarrow\infty$. The one particle probability function for $N=2$ case is obtained analytically and is an elliptic function of second kind. We have verified numerically that when the

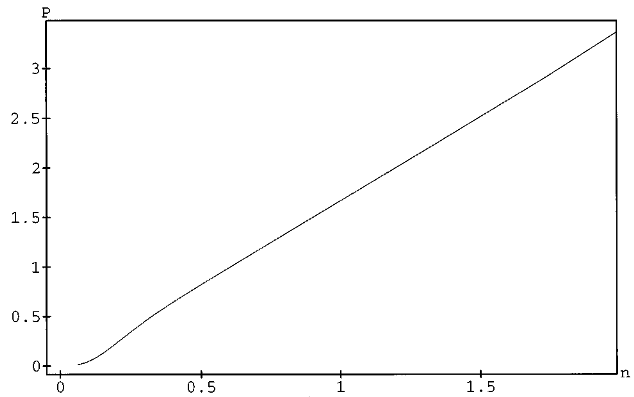

FIG. 4. Equation of state (P vs n) for the 2 QO system.

system is almost chaotic, equipartition of energy takes place. The time average and the phase average gives the same result for the parameters for which the system is almost chaotic. Pressure, density, and EOS of our system are also studied. For parameters for which the system is integrable, for example $N=2$, $\alpha_{11}=\alpha_{22}=1$, and $\alpha_{12}=\alpha_{21}=0$ or 2, equipartition of energy does not take place and each oscillator reaches average kinetic energy separately, determined by their initial separate energies. Each oscillator exchanges energy with its potential and comes to some kind of equipartition of energy and twice the average kinetic energy is again given by Eq. (13) for $N=1$. It can also be seen that the mean value of the average temperature of oscillators matches very closely with $4E/3N$ both for chaotic as well as integrable case. This result has nothing to do with chaos and follows from virial theorem.

In conclusion, the quartic oscillator is a useful model with chaotic or ergodic properties for a wide range of parameters. There is no resonance effect, which one has in the case of the HH model. Statistical mechanics of this model is studied analytically. Various other thermodynamic quantities, transport coefficients, etc. of a chaotic system may be studied by using this model, and some work along this line is under progress.

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