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→∞, 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 ε=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→∞. 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

\[ H = \left( \frac{p_1^2 + p_2^2}{2} \right) + \frac{q_1^4}{2} + \frac{q_2^4}{2} + \frac{\alpha}{2} q_1^2 q_2^2, \] (1)

where \( q \)'s and \( p \)'s are generalized coordinates and momenta, respectively, and \( \alpha \) 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 \( \alpha > 6 \). 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 \( \Gamma \) is the phase-space volume bounded by the constant energy (E) surface. Thus,