Dynamical temperatures of quartic and Henon-Heiles oscillators

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We have numerically verified the recently proposed formulation of dynamical temperature, $T_S^{\rm dy} \equiv$ time average of $\nabla \cdot (\nabla H/|\nabla H|^2)$, by H. H. Rugh [Phys. Rev. Lett. **78**, 772 (1997)], using the quartic and the Henon-Heiles oscillators. We also give a simple, alternative derivation of the dynamical temperature. Our numerical results agree with theory reasonably well. However, contrary to Rugh's claim, we find that it is not computationally efficient compared to the more generally used form of the dynamical temperature, $T_B^{\rm dy} \equiv$ time average of momentum square of each particle, especially for a system with large degrees of freedom (N). For sufficiently large N, both temperatures approach the same value and $T_B^{\rm dy}$ is easier to evaluate.
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Statistical mechanics (SM) is generally used to study the macroscopic properties of a system with many degrees of freedom. A large number of degrees of freedom gives rise to ergodic motion of the system in phase space due to frequent collisions among particles. These collisions are assumed implicitly and are essential for the success of SM [1].

Recently it was found that concepts from SM and thermodynamics may be used to study systems with few degrees of freedom, exhibiting chaotic behavior, like quartic oscillators (QO) and Henon-Heiles oscillators (HHO) [2,3]. Or, conversely, we can gain a physical insight into the dynamical description of SM using such systems [4]. In these systems there are no implicitly assumed collisions and the ergodicity is due to the nonlinearity of the system, which is explicit in the Hamiltonian. The dynamical description of SM and thermodynamics using such models may answer fundamental problems such as the Fourier heat law, thermalization of oscillator chains, etc., from first principles [5–7].

In this paper, we study the temperature of a Hamiltonian dynamical system in the microcanonical ensemble of thermodynamics. In the literature there are two definitions of temperatures derivable from phase space volume, Γ. As discussed by Berdichevsky and Alberti [2] and Bannur *et al.* [3], one definition of temperature is $T_B = (\partial \ln \Gamma/\partial E)^{-1}$, generally used in the study of systems with few degrees of freedom [5–7]. Another definition is $T_S = [\partial \ln(\partial\Gamma/\partial E)/\partial E]^{-1}$, generally used in SM. Both of the above temperatures approach the same value in the limit of large degrees of freedom [2,3]. However, for few degrees of freedom they do differ. For many calculations, in the literature, the more commonly used definition of temperature is the time average of momentum square associated with any one degree of freedom. This is what is called the dynamical temperature $T_B^{\rm dy}$, which is equal to T_B, defined above, by the ergodic theorem [2,1]. For a chaotic system, left for sufficiently long time, $T_B^{\rm dy}$ associated with each degree of freedom approaches T_B. So far, the other definition of temperature, namely, T_S, has not been used in any calculations of dynamical systems with finite degrees of freedom. This is probably because the dynamical temperature ($T_S^{\rm dy}$) corresponding to T_S was not known and also in SM there is no difference between T_B and T_S. Recently Rugh [8] obtained an expression for $T_S^{\rm dy}$ that is equal to the time average of a function, $\Phi(t) \equiv \nabla \cdot (\nabla H/|\nabla H|^2)$, where H is the Hamiltonian, ∇ is the gradient operator in phase space. He verified it using N uncoupled harmonic oscillators (HO). However, this HO system is not chaotic while the theory is for a chaotic system. So it is more appropriate to verify the theory using chaotic systems such as QO or HHO. This is exactly what we present in this paper along with a simple alternative derivation of it, which follows from SM [1]. Earlier, in Ref. [3], we derived analytic expressions for T_B and T_S for N degrees of freedom QO. Here we also derive approximate analytic expressions for T_B and T_S for a HHO system. Note that in Ref. [2], T_B and T_S are integrals that need to be evaluated numerically. Our numerical results show that $T_S^{\rm dy}$ approaches T_S and $T_B^{\rm dy}$ of each particle converges to T_B, when the system is chaotic, for both QO and HHO systems. When the system is nonchaotic, both $T_S^{\rm dy}$ and $T_B^{\rm dy}$ approach constant values, but not equal to T_S and T_B, respectively. In the case of HHO, equipartition of energy still takes place and the corresponding temperature is close to T_B and has an origin different from ergodicity.

We consider QO and HHO as two examples to study the dynamical temperatures of a system with finite N degrees of freedom. We consider here the case of $N=2$ and the Hamiltonians are

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

and

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

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 for $\alpha > 6$. HHO is chaotic for energy $E = 1/6$ and develops nonchaotic islands as energy is decreased. Earlier analysis by Berdichevsky *et al.* shows that

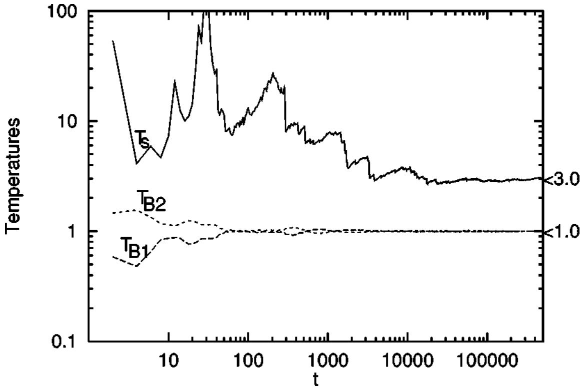

FIG. 1. Dynamical temperatures corresponding to T_{B1}, T_{B2}, and T_S as a function of time t for QO with $E=1.5$ and $\alpha=500$.

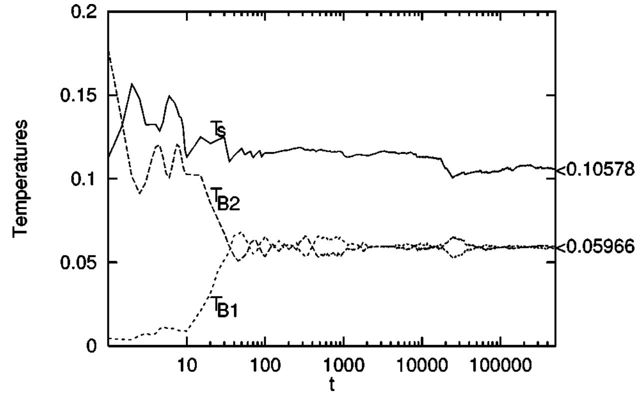

FIG. 2. Dynamical temperatures corresponding to T_{B1}, T_{B2}, and T_S as a function of time t for HHO with $E=1/8$ and initial points on the chaotic region.

even for $E<1/6$, equipartition of energy takes place. When the system is chaotic or ergodic then we have

$$\left\langle p_1 \frac{\partial H}{\partial p_1} \right\rangle = \left\langle p_2 \frac{\partial H}{\partial p_2} \right\rangle = \left\langle q_1 \frac{\partial H}{\partial q_1} \right\rangle = \left\langle q_2 \frac{\partial H}{\partial q_2} \right\rangle = \left(\frac{\partial \ln \Gamma}{\partial E} \right)^{-1} = T_B, \tag{3}$$

where the angular brackets indicate the time average, which is equal to the phase space average. For QO [3], we have

$$\Gamma(E) = \int_{H \leqslant E} dp_1 dp_2 dq_1 dq_2 = C E^{3/2}, \tag{4}$$

and hence $T_B = 2E/3$ and $T_S = 2E$.

For HHO it is not possible to get an exact analytic expression for $\Gamma(E)$, as in the case of QO. However, using the same procedure, one can get a useful expansion for $\Gamma(E)$ in powers of E where E is always $\leqslant 1/6$. That is,

$$\Gamma(E) = \pi E^2 \left(1 + \frac{E}{2} + \frac{35}{32} E^2 + \cdots \right), \tag{5}$$

and hence

$$T_B = \frac{E}{2} \left(1 - \frac{E}{4} - \frac{29}{32} E^2 + \cdots \right) \tag{6}$$

and

$$T_S = E \left(1 - \frac{3}{4} E - \frac{13}{4} E^2 + \cdots \right). \tag{7}$$

The expressions obtained for T_B and T_S above are from SM, phase space average of $X_i\, \partial H(X_i)/\partial X_i$ and $\Phi(t)$, respectively, where X_i is either q_i or p_i. Next let us discuss the corresponding dynamical quantities. $T_B^{\rm dy}$ has a simple form $T_B^{\rm dy} = \langle p_1^2 \rangle = \langle p_2^2 \rangle$, which immediately follows from Eq. (3) and $T_S^{\rm dy} = 1/\langle \Phi(t) \rangle$, where $\Phi(t)$ has very complicated expression. More detailed derivation of $T_S^{\rm dy}$ is given by Rugh [8] and here we give a simple alternative derivation, which follows from SM. Following Khinchin [1], we have

$$\frac{1}{T_S} = \frac{\partial \ln \Omega}{\partial E}, \tag{8}$$

where $\Omega(E) \equiv \int_E (d\Sigma/|\nabla H|) = \partial \Gamma/\partial E$. $\Gamma(E)$ is the phase space volume bounded by energy E. Hence,

$$\frac{1}{T_S} = \frac{1}{\Omega} \frac{\partial}{\partial E} \int_E \frac{d\Sigma}{|\nabla H|} = \frac{1}{\Omega} \frac{\partial}{\partial E} \int_E d\boldsymbol{\Sigma} \cdot \frac{\nabla H}{|\nabla H|^2}, \tag{9}$$

where $d\Sigma$ is the surface element. Note that the surface here is a constant energy surface and hence a unit vector normal to the surface is $\nabla H/|\nabla H|$. Next, using divergence theorem, we get

$$\frac{1}{T_S} = \frac{1}{\Omega} \frac{\partial}{\partial E} \int_{H \leqslant E} d\Gamma \nabla \cdot (\nabla H/|\nabla H|^2) = \frac{1}{\Omega} \int_E d\Omega \Phi = \langle \Phi \rangle. \tag{10}$$

From ergodic theory we know that the phase space average equal to the time average and hence $T_S = T_S^{\rm dy}$ when the system is chaotic.

Numerical results on the evaluation of dynamical temperatures $T_S^{\rm dy}$ and $T_B^{\rm dy}$ for quartic oscillator and Henon-Heiles oscillator systems are presented in Figs. 1–3 with dynamical temperatures along the y axis and time along the x axis in log scale. Note that in Fig. 1, temperature is also plotted in

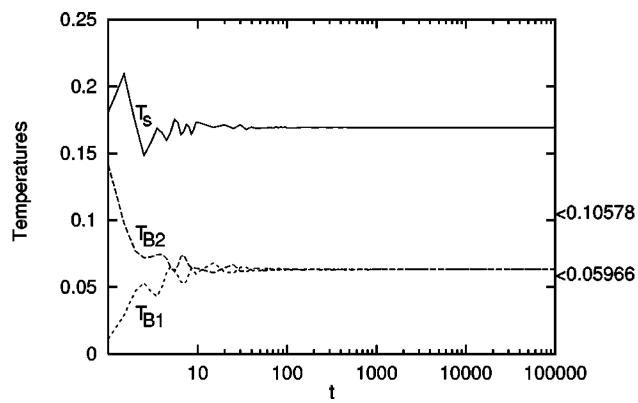

FIG. 3. Dynamical temperatures corresponding to T_{B1}, T_{B2}, and T_S as a function of time t for HHO with $E=1/8$ and initial points on the nonchaotic region.

log scale. These are time averaged quantities and plotted as functions of time. The time average of an observable $O(t)$ is defined as

$$\langle O\rangle(t)=\frac{1}{t}\int_0^t O(\tau)d\tau. \tag{11}$$

The values of T_B and T_S are marked on the y axis at the right.

Figure 1 is for a QO system with parameters $E=1.5$, $\alpha=500.0$, and hence $T_B=1.0$ and $T_S=3.0$ from Eq. (4). As we discussed in Ref. [3], for $\alpha=500$ the system is chaotic and for smaller α phase space contains a lot of nonchaotic islands. We can see that T_S^{dy} approaches T_S and T_B^{dy} of each particle approaches to T_B. Initially, both the temperatures show large fluctuations and then settle around the expected values. T_B^{dy} approaches close to T_B at $t\approx 5000$, which is faster than that of T_S, which is at $t\approx 5\times 10^4$ as we see from the figure. At $t=5\times 10^5$, the percentage difference between T_S and T_S^{dy} is $\approx 1.5\%$ and that of T_{B1} and T_{B2} are both $\approx 0.2\%$. This gives an idea of the convergence of dynamical temperatures to their corresponding SM temperatures. For $\alpha=0$ or 2 the system is integrable and $T_B^{\mathrm{dy}}\neq T_B$ and $T_S^{\mathrm{dy}}\neq T_S$.

For HHO, we have taken $E=1/8$ and hence $T_B\approx 0.059\,66$ and $T_S\approx 0.106\,93$ from Eqs. (6) and (7). The exact values are $T_B=0.059\,657$ and $T_S=0.105\,78$, which are obtained by numerical evaluation of the integral equation, Eqs. (3.5) in Ref. [2]. Results are plotted in Figs. 2 and 3. Figure 2 is for the initial points on the chaotic region and we see the convergence of dynamical temperatures to the corresponding SM temperatures. At $t=5\times 10^5$, the percentage difference between T_S and T_S^{dy} is $\approx 0.01\%$ and that of T_{B1}, T_{B2} is $\approx 2.1\%$ and $\approx 0.3\%$, respectively. Figure 3 is for the initial points on the nonchaotic islands and T_B^{dy} of each particle converges to a value close to T_B but not exactly T_B, whereas T_S^{dy} approaches a value clearly not equal to T_S. Equipartition of energy, $T_{B1}^{\mathrm{dy}}=T_{B2}^{\mathrm{dy}}$, in this case, may be due to the resonance coupling between two oscillators as pointed out by Berdichevsky and Alberti [2]. Note that in all above cases dynamical temperatures oscillate around corresponding SM temperatures with decreasing amplitude with time.

The reason for not considering the case with $E=1/6$ for HHO is that $\Phi(t)$ has a singularity and numerical results are not trustable. For $E<1/6$, $\Phi(t)$ has very sharp peaks, but by taking enough points in the integration one can get results correct to required accuracy. As the system evolves, whenever $|\nabla H|=0$ or minimum, singularity or peaks occur.

In summary, we have studied the dynamical temperatures of QO and HHO and compared with temperatures, derivable from statistical mechanics using the ergodic theorem. The dynamical temperatures obtainable by time averaging momentum squares of the particles was discussed earlier by Berdichevsky and Alberti [2] for HHO and Bannur *et al.* [3] for QO. Here, we have rederived and verified the recently proposed dynamical temperature, T_S^{dy}, by Rugh [8], which corresponds to the usual temperature used in SM, T_S and have compared it with the earlier results on T_B^{dy}. We have also derived approximate analytic expression for T_B and T_S for HHO which reproduce the approximate straight line plot between T_B and E, shown in Fig. 9 of Ref. [2], which was obtained by numerical integration.

In conclusion, we found that T_S^{dy} is a reasonable definition of dynamical temperature, derivable from statistical mechanics based on the ergodic theorem. In both of our models, QO and HHO, which have different properties and symmetries, T_S^{dy} asymptotically approaches T_S, as expected, when the system is almost chaotic, whereas T_B^{dy}, from our study of HHO, asymptotically approaches T_B even for systems that are nonchaotic. Hence, T_B may not be an appropriate temperature. However, for systems with large degrees of freedom one may use T_B^{dy} as a temperature because, for large N, $T_B\approx T_S$ and the expression $\Phi(t)$, for example, QO with N degrees of freedom, is very complicated to handle. In fact, the evaluation of T_S^{dy} is not as efficient as T_B^{dy} for large N. This justifies our usual notion of temperature as T_B^{dy}, which is $\approx T_S^{\mathrm{dy}}$ for a statistical system $(N\rightarrow\infty)$. Our present study also reconfirms our earlier thermodynamic and SM treatment of chaotic systems even with only two degrees of freedom. As a future work, it would be interesting to reanalyze the earlier work on the Fourier heat law, thermalization of oscillator chains, etc., [5–7] using this definition of temperature, T_S^{dy}, where N is finite.

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