Nosé equation for a one-dimensional oscillator: Resonance zones and the transition to large-scale irregular dynamics

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Recently, attempts have been made to alter the equation of motion of a multiparticle system so that the temperature rather than the energy is constant. Nosé introduced a modified multiparticle equation of motion involving an auxiliary equation with a free parameter Q. We consider the Nosé-Hoover equation for a one-dimensional oscillator as the equation of motion for a coupled oscillator system with two degrees of freedom. For different values of Q, we consider the dynamics in the four-dimensional phase space by examining two-dimensional surfaces of section. We show that the overlapping of resonance zones causes a transition to large-scale irregular dynamics for a limited range of Q.

Many studies have considered the classical mechanics of a multiparticle system. The multiparticle equation of motion is deterministic and reversible and the energy is constant. Many experiments are performed at constant temperature rather than constant energy, and various attempts[1-5] have been made to modify the multiparticle equation of motion so that the temperature is constant. However, the resulting equations had been restricted to systems with a large number of particles[3] or had been either nondeterministic[4] or nonreversible[5] until Nosé[1,2] introduced a modification involving an auxiliary equation with a free parameter Q. The Nosé equation is both deterministic and reversible and, not surprisingly, has received a considerable amount of attention.[6] Most studies, including those of Nosé, have considered systems with a large number of particles and it has been established that for an N-particle system the Nosé equation with a wide range of Q thermostats the system in the large-N limit.

In this Brief Report we consider the Nosé-Hoover equation for a one-dimensional oscillator as the equation of motion for a coupled oscillator system with two degrees of freedom. This system was previously considered by Hoover[7] and by Posch, Hoover, and Vesely[8] who established a clear connection between the ability of the Nosé-Hoover equation to thermostat the oscillator and the extent to which the dynamics is irregular. The purpose of this Brief Report is to examine the mechanism of the transition to large-scale irregular dynamics and to gain thereby a qualitative understanding of the optimum range of Q.

The Nosé Hamiltonian is[1,2,7]

$$H_N=p_q^2/2ms^2+p_s^2/2Q+V(q)+kT\ln(s)\ . \tag{1}$$

For convenience, we choose m and kT to be 1.0. In (1) q is the oscillator variable and s is an auxiliary variable while p_q and p_s are their conjugate momenta, respectively. $V(q)$ is the oscillator potential which in previous studies[7,8] was chosen to be harmonic. We are interested in modeling a diatomic for which, in general, the potential is anharmonic and we therefore choose

$$V(q)=q^2/2+Aq^3/3+0.01q^4/4\ . \tag{2}$$

Below we present results for $A=0.05$ (weak nonlinearity) and $A=0.20$ (stronger nonlinearity). It will be seen that the overall mechanism of the transition to large-scale irregular dynamics is the same although there are quantitative differences. We note that the amount of nonlinearity displayed by a diatomic typically depends on its excitation energy relative to its dissociation energy. As a rough guide, for H_2, weak and stronger nonlinearity here correspond to approximately 100 and 1000 K, respectively. The kinetic energy of the oscillator is $E_k=p_q^2/2$ and the energy of the oscillator is $E_{\rm osc}=E_k+V(q)$. The initial values of q and p_q must be specified while the initial values of s and p_s are chosen to be 1.0 and 0.0, respectively. In (2) the q^4 term ensures that the oscillator equation of motion is bound for all initial conditions.

The Nosé-Hoover equation of motion (obtained by scaling and redefining variables[7]) is

$$\begin{aligned}\dot q&=p_q\ ,\\ \dot s&=p_s\ ,\\ \dot p_q&=F(q)-p_sp_q\ ,\\ \dot p_s&=(p_q^2-1.0)/Q\ ,\end{aligned} \tag{3}$$

where $F(q)=-dV(q)/dq$. In (3) the q and s degrees of freedom are coupled via the $-p_sp_q$ term; when p_q^2 is greater than 1.0, p_s is increasing and, on average, p_q is decreasing. It is clear that decreasing Q both increases the coupling to the oscillator equation and increases the frequency of the auxiliary equation.

For the Nosé-Hoover equation of a one-dimensional oscillator, the trajectories traverse a four-dimensional phase space. We construct two-dimensional q-p_q surfaces of section by plotting points (q,p_q) when p_s passes through zero. The q-p_q surface of section is symmetric with respect to reflection in the q axis but not the p_q axis,

because of the anharmonic term in the potential. If there is a second constant of the motion, the points (q,p_q) lie on closed curves and the dynamics is regular. Many studies[9,10] have been made of coupled oscillator systems with two degrees of freedom in which the dynamics is primarily regular for small coupling but primarily irregular for large coupling. It was established by Posch, Hoover, and Vesely[8] that there is a clear connection between the ability of the Nosé-Hoover equation to thermostat the oscillator and the extent to which the dynamics is irregular. Over a number of years, Chirikov[11] has developed a theory of the transition to irregular dynamics based on the overlap of resonance zones and Walker and Ford[12] have demonstrated the relevance of this theory for coupled oscillator systems with two degrees of freedom. Large-scale irregular dynamics is generally associated with the overlap of low-order resonance zones.

We first consider results for $A=0.05$ (weak nonlinearity). Figure 1(a) shows q-p_q surfaces of section for $Q=10.0$ for initial conditions (1.0,0.0), (1.5,0.0), (2.0,0.0). As indicated previously, these are the initial values of q and p_q, respectively, and the initial values of s and p_s are chosen to be 1.0 and 0.0, respectively. It may be seen that there are closed curves showing that the dynamics is primarily regular. Each trajectory switches between an $E_{\rm osc}>1.0$ curve and an $E_{\rm osc}<1.0$ curve and the closed curves for initial condition (1.5,0.0) are strongly perturbed by a resonance zone in the region $E_{\rm osc}=1.0$. This 2-1 resonance zone, which consists of four islands (two for which $|p_q|$ is greater than 1.0 and two for which $|p_q|$ is less than 1.0), occurs when the frequency of the auxiliary equation is twice that of the oscillator equation. A 2-1 resonance zone must exist for any form of the auxiliary equation of motion and we therefore call it the primary resonance zone. Figure 1(b) shows q-p_q surfaces of section for $Q=1.0$ for initial conditions (2.0,0.0), (0.0,2.0), and (0.0,1.0). It may be seen that, as in Fig. 1(a), there are closed curves showing that the dynamics is primarily regular. It may also be seen that the primary resonance zone is now larger.

Even for $Q=10.0$ and 1.0, there are large regions of irregular dynamics at large (and small) values of $E_{\rm osc}$. However, there is no large-scale irregular dynamics in the sense that there are tori around $E_{\rm osc}=1.0$ that separate these regions. For an irregular trajectory the kinetic energy peaks at $E_k=0.0$ but the E_k distribution is not well approximated by $2.0\exp(-2.0E_k)$. To gain a qualitative understanding of the transition to large-scale irregular dynamics we now examine the location (to the nearest 0.05) of the primary resonance zone and several secondary resonance zones as defined by the position of the $(c,0.0)$ elliptic point which is one of the centers. These correspond to the re-entrant periodic trajectories of Posch, Hoover, and Vesely[8] who gave the p_q axis intercept. We have altered their prescription because the resonance overlap occurs along the q axis on the q-p_q surfaces of section. Also, the secondary 2-2 resonance zone (see below) corresponds to an $n=1$ reentrant periodic trajectory that has no p_q axis intercept.

Over the range of Q from 1.0 to 0.3, the primary resonance zone remains in the area $E_{\rm osc}=1.0$, and c is close

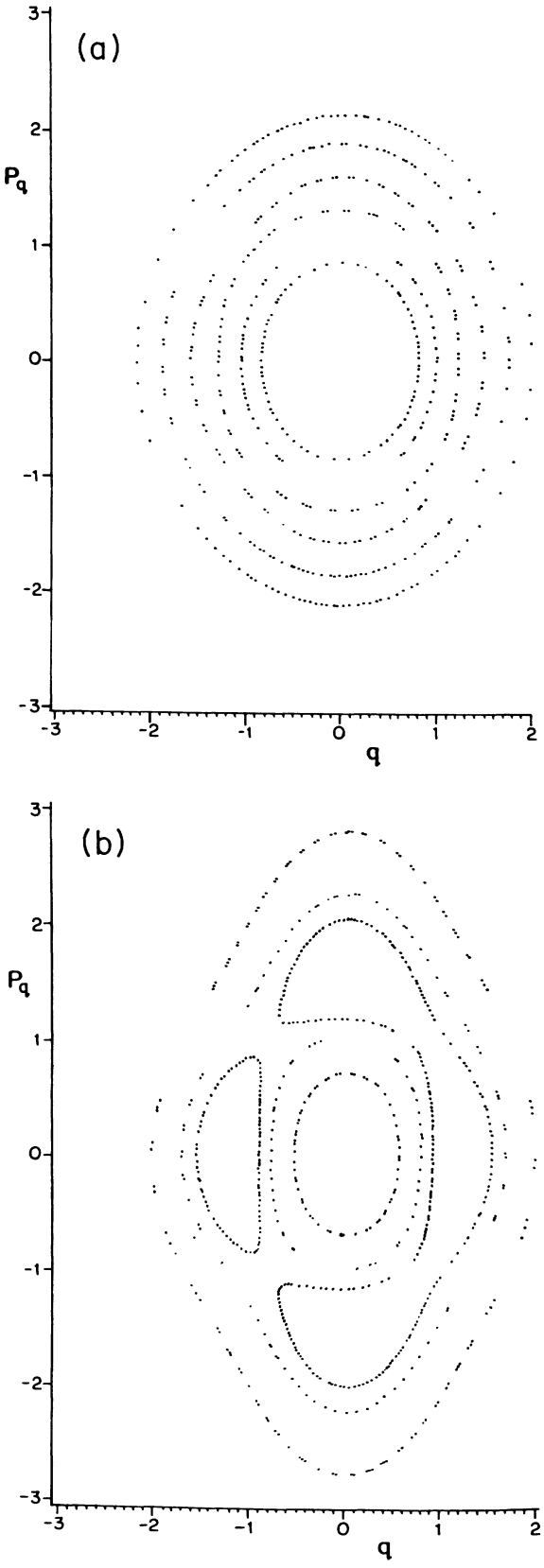

FIG. 1. q-p_q surfaces of section [for potential (2) with $A=0.05$] for (a) $Q=10.0$ and (b) $Q=1.0$ for initial conditions (1.0,0.0), (1.5,0.0), (2.0,0.0) and (2.0,0.0), (0.0,2.0), (0.0,1.0), respectively.

to 1.25. However, a secondary 2-2 resonance zone arises in the area $E_{osc} > 1.0$ and its location varies greatly; for $Q=0.9$ and 0.8, $c=2.60$ and 2.40, respectively. In Figs. 2(a) and 2(b) we show q-p_q surfaces of section for $Q=0.7$ and $Q=0.6$, respectively, for initial conditions (2.0,0.0), (0.0,2.0), and (0.0,1.0). The primary and secondary 2-2 resonance zones are clearly visible and it may be seen that for the primary resonance, c remains close to 1.25 while for the secondary 2-2 resonance, $c=2.20$ and 1.85, respectively. The secondary 2-2 resonance zone begins to overlap with the primary resonance zone for Q between 0.7 and 0.6. It may be seen from Fig. 2(b) that for $Q=0.6$ the tori around $E_{osc}=1.0$ have been destroyed and there is a small region of large-scale irregular dynamics.

In fact, for $Q=0.5$, the secondary 2-2 resonance zone has passed into the area $E_{osc}=1.0$ and there is no large-scale irregular dynamics, but a secondary 4-2 resonance zone arises in the region $E_{osc} > 1.0$ and its location also varies greatly; for $Q=0.6$, 0.5, 0.4, and 0.3, $c=2.65$, 2.45, 2.25, and 2.00, respectively. The secondary 4-2 resonance zone begins to overlap with the primary resonance zone for Q between 0.4 and 0.3 For $Q=0.3$ the tori around $E_{osc}=1.0$ have again been destroyed and there is an extensive region of large-scale irregular dynamics.

We now consider results for $Q=0.20$ (stronger nonlinearity). For $Q=10.0$ and $Q=1.0$, the situation is similar to that described above for weak nonlinearity. Again, over the range of Q from 1.0 to 0.3, the primary resonance zone remains in the area $E_{osc}=1.0$. However, the primary resonance zone is somewhat larger and c is close to 1.35. Consequently, the secondary 2-2 resonance zone begins to overlap with the primary resonance zone for Q between 0.8 and 0.7. For $Q=0.6$, 0.5, 0.4, and 0.3, there are extensive regions of large-scale irregular dynamics (although the secondary 4-2 resonance zone may still be identified). Therefore, not surprisingly, for stronger nonlinearity the transition to large-scale irregular dynamics takes place for a larger value of Q, and the dynamics is more irregular for smaller values of Q.

Thus the transition to large-scale irregular dynamics may be qualitatively understood as being due to the sequential overlap of successively higher-order secondary resonance zones with the primary resonance zone in the area $E_{osc}=1.0$ as Q is decreased. Maximum irregular dynamics occurs for a limited range of Q (larger for stronger nonlinearity) when several secondary low-order resonance zones effectively overlap with the primary resonance zone. Thus for Q between 0.1 and 0.05 the dynamics is primarily irregular. Then, for an irregular trajectory, the kinetic energy peaks at $E_k=0.0$ and the E_k distribution is well approximated by $2.0\exp(-2.0E_k)$.

As Q is further decreased the frequency of the auxiliary equation increases until the dynamics is eventually dominated by high order resonance zones. In this case there is no longer effective overlap of low-order resonance zones and the dynamics is primarily regular (albeit very complicated). Then, for an irregular trajectory, the kinetic energy typically peaks at $E_k > 0.0$ although the average E_k is very close to 0.5.

In this Brief Report we considered the Nosé-Hoover equation for a one-dimensional oscillator. For different

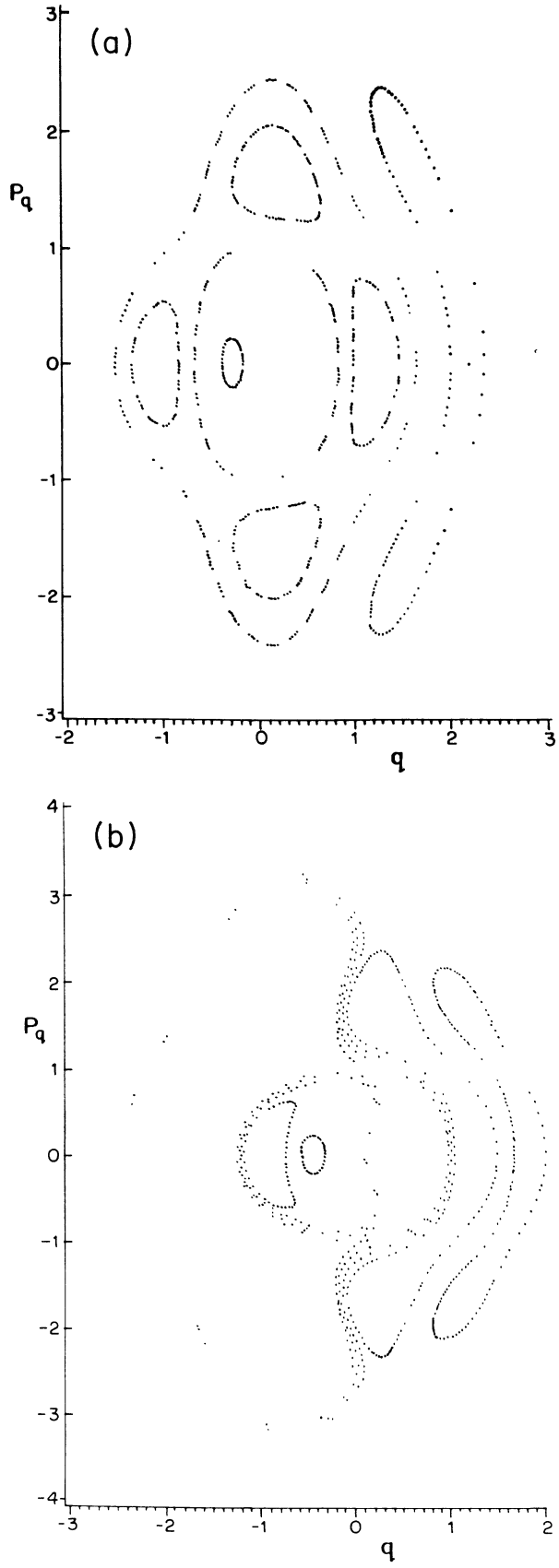

FIG. 2. q-p_q surfaces of section [for potential (2) with $A=0.05$] for (a) $Q=0.7$ and (b) $Q=0.6$ for initial conditions (2.0,0.0), (0.0,2.0), (0.0,1.0).

values of Q we considered the dynamics in the four-dimensional phase space by examining two-dimensional surfaces of section. For large (and small) values of Q there are isolated resonance zones and the dynamics is primarily regular. However, we have shown that for a limited range of Q there is effective overlap of low-order resonance zones and the dynamics is primarily irregular. Note that by causing the dynamics to be primarily irregular, the Nosé-Hoover equation creates the circumstances that are required for it to work. We believe that these results are also relevant for a multidimensional oscillator. If the Nosé-Hoover equation thermostats such systems for a much broader range of Q it is either because the multidimensional oscillator dynamics is primarily irregular or because it is sufficiently complicated that it is effectively irregular. That is, recurrence times are longer than typical limiting times (such as the collision time).

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