Dissipation dynamics with two distinct chaotic baths

Diptanil Roy\textsuperscript{1} and A.V. Anil Kumar\textsuperscript{1}

\textsuperscript{1}School of Physical Sciences, National Institute of Science Education and Research, HBNI, Jatni - 752050, India

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I. INTRODUCTION

The dissipation of energy occurs in diverse systems and it is one of the most fundamental processes in dissipative dynamical systems. In the Langevin description of Brownian motion, the damping force together with the randomly fluctuating force are used to model dissipation\textsuperscript{1, 2}. These forces relate the effect of the collisions of the system with the particles in the thermal bath and are related by the dissipation-fluctuation theorem\textsuperscript{2}. The dissipative dynamics of physical systems have been studied extensively\textsuperscript{3–10}. In modelling energy dissipation, these studies used a small system coupled to the environment. The environment can be of two types: one with an infinite collection of modes\textsuperscript{3} and another with a small number of chaotic modes\textsuperscript{1, 4–6, 9, 10}. These investigations have led to several interesting results. For example, Wilkinson\textsuperscript{4} showed that the rate of exchange of energy between the system and the chaotic bath depends on the classical motion of the particles comprising the chaotic bath. The rate of energy exchange increases when the bath shows chaotic motion. Later Marchiori and de Aguiar showed that energy dissipation occurs in the chaotic regime even if the bath is composed of small number of particles\textsuperscript{9}. Xavier \textit{et al.}\textsuperscript{10} also improved upon the model in \textsuperscript{9} and showed that the damping rate can be expressed in terms of the mean Lyapunov exponent of the chaotic bath. Also they have shown that the dissipation is more effective if there is resonance between the system and bath frequencies.

In this paper, we extend this study to the case of a small system coupled to multiple baths. The purpose of this investigation is to study the dissipative dynamics of the system if it is connected to two distinct baths with different chaoticity. We use linear response theory following the approach presented in \textsuperscript{9}. We also carry our numerical simulations and compare the theoretical results with those obtained from simulations.

II. THE MODEL

Our model comprises of a particle, with generalised coordinates \((q, p)\) in a one dimensional harmonic oscillator potential with angular frequency \(\omega_0\). The particle is connected to two baths comprising of \(N\) quartic oscillators each. The two baths are not connected to each other, but are coupled indirectly through the harmonic oscillator. The quartic oscillators are two dimensional and the \(n_{th}\) particle of the \(i_{th}\) bath is characterised by the generalised coordinates \((q_n, y_n, p_n, \dot{y}_n, \dot{q}_n)\). The interaction between the baths and the system is through a coupling term of the form \(H_I\), where \(\lambda_N = \frac{1}{\sqrt{N}}\) is a measure of the effective coupling \[9\]. The Hamiltonian governing the dynamics of the system can be written as

\[ H = H_{HO} + H_{E_1} + H_{E_2} + H_I \]  

\begin{align*}
H_{HO} &= \frac{p^2}{2m} + \frac{m\omega^2_0 q^2}{2} \\
H_{E_i} &= \frac{N}{\lambda N} \left[ \frac{p_x^2{n_i} + p_y^2{n_i}}{2} + \frac{a_1}{4}(x_{n_i}^4 + y_{n_i}^4) + \frac{x_{n_i}^2 y_{n_i}^2}{2} \right] \\
H_I &= \sum_{n=1}^{N} \lambda_N q(x_{n_1} + x_{n_2})
\end{align*}

The total Hamiltonian is conservative, but the system can exchange energy with the baths and hence behave dissipatively. The non-linear dynamics of the baths is determined completely by the parameters \(a_i\), where the systems are integrable for \(a_i = 1.0\), mildly chaotic for \(a_i = 0.1\) and strongly chaotic for \(a_i = 0.01\). We numerically solve the \(8N + 2\) equations of motion arising from the Hamiltonians \(H_{HO}, H_{E_1}, H_{E_2}\) and \(H_I\) respectively and compare our analytical results to them. The chaotic dynamics of the baths acts as a sink of energy for the system. A temperature for the environment can be defined by using the general equipartition theorem, where every quadratic degree of freedom has a contribution of \(k_B T/2\) to the total energy \(E\). It is clear here that the \(T\) represents the equilibrium temperature.
Before we proceed to the results for our model, it is imperative to discuss the behaviour of a particle in harmonic oscillator potential coupled to only one bath. We will compare and contrast our results to those provided in [9] [10]. When $a = 1.0$, the system is in the integrable regime and the environment has very little effect, causing a slight decrease in the oscillator energy. With $a = 0.5$, the energy loss is more and there are slightly pronounced oscillations. The equilibrium energy value for such cases is $0.8E_0$ [9]. For example, for a bath with $N = 100$ QOs [9] [10] and $a = 1$, the energy of the system decreases a bit from $E_S(0)$ and performs tiny oscillations around the decreased value. For $a = 0.1$, the energy decreases further with more prominent oscillations with increasing time. For $a = 0.01$, the situation however is completely different. The energy decay for such a system is exponential and can be fit to $E_S(t) = E_S(0)e^{-\gamma t}$ where $\gamma$ is a function of the bath properties and $\omega_0$.

For small values of $N$, the indirect coupling does not have much effect on the system unless the coupling is strongly chaotic. For example, when the coupling parameter is set in the chaotic regime, we cannot characterise the behaviour by a single realisation for $1 \leq N \leq 6$ because of large fluctuations. For $7 \leq N \leq 20$ however, the onset of dissipation and the transition to an exponential decay are apparent, though the energy fluctuation is still large. With increasing $N$, the system starts to behave differently, allowing dissipation to occur. The effect of different values of the coupling are discussed above.

As is apparent from the numerical results, the value of $E_S(t)$ for large $N$ becomes independent of $N$ over large times. This is possible only when the coupling term $\lambda N$ falls with $N$ as $N \rightarrow \infty$. For one bath, it has been shown in [9] that $\lambda N = \frac{\lambda}{\sqrt{N}}$ using Linear response theory. For large $N$, the system equilibrates with the environment and the equilibrium energy distribution is Boltzmann-like. This allows us to define a temperature; however it is not possible in the regular or mixed regimes.

### III. THEORY

We will try to understand the flow of energy to the two different baths using linear response theory (LRT) [11]. We will follow the formalism developed in [9] to write the final equation of motion for the system. The HO in hamiltonian [1] satisfies the following equation of motion

\[
\dot{q} + \omega_0^2 q = -\frac{\lambda_N}{m} \sum_{n=1}^{N} \{x_n^{(1)}(t) + x_n^{(2)}(t)\} \equiv -\frac{\lambda_N}{m} X(t)
\]

We consider the HO to be perturbed by an external force given by $-\frac{\lambda_N}{m} X(t)$. Under the assumption that the bath coordinates are chaotic, we can replace $X(t)$ with $\langle X(t) \rangle$. LRT has been used to determine $\langle X(t) \rangle$ in terms of the response function. The dynamics of the system is determined by the Liouville equations. The integral form of the Liouville equation is given by

\[
\rho(t) = e^{i(t-t_0)L_0} \rho(t_0) + \int_{t_0}^{t} e^{i(t-s)L_0} L_I(s) \rho(s) ds
\]

where $L_0$ and $L_I$ are the Liouville operators. The Hamiltonian $L_I$ can be estimated using

\[
H = H_E(Q, P) + H_I(Q, P, t)
\]

where $Q$ and $P$ represent the entire set of canonical variables of the environment and $H_I(Q, P, t) = A(Q, P) \chi(t)$ where $A(Q, P)$ is the corresponding displacement ($A = -\frac{\partial}{\partial x} H(q, p; x)$). Under the approximation of a small perturbation, Eq. 3 can be expanded to 1st order in $L_I$ as

\[
\rho(t) = \rho(t_0) + \int_{t_0}^{t} e^{i(t-s)L_0} \{H_I(s), \rho(t_0)\} ds
\]

![FIG. 1: The correlation functions $C_N^{(i)}(t, 0)$ for the two sets of baths for different set of initial parameters. $C_N^{(i)}$ deviates from the delta function approximation in the mixed and integrable regimes.](image-url)
The ensemble average $\langle X(t) \rangle$ can thus be written as

$$\langle X(t) \rangle = \langle X(t) \rangle_0 - \frac{\lambda N}{\lambda N} \int_0^t \phi_{XX}(t-s)q(s) ds$$

where $\langle X(t) \rangle_0$ is equal to 0 due to the parity of $H_E$. Therefore, Eq. 2 reduces to

$$\ddot{q} + \omega_0^2 q \approx \frac{\lambda N}{\lambda N} \int_0^t \left( \phi_{11}(t-s) + \phi_{22}(t-s) \right)q(s) ds$$

(7)

Here $\phi_{XX}(t-s) = \{ \langle X(t), X(s) \rangle \}$ and from [9], it follows that

$$\phi_{XX}(t-s) = N(\phi_{11}(t-s) + \phi_{22}(t-s))$$

(8)

Here, $\phi_{xx}^{(i)}$ is the response function obtained in [12] and is given by

$$\phi_{xx}^{(i)}(t-s) = \frac{5}{4E_QS(0)} \langle x^{(i)}(t)P_x^{(i)}(s) \rangle_0$$

$$+ \frac{t-s}{4E_QS(0)} \langle P_x^{(i)}(t)P_x^{(i)}(s) \rangle_0$$

(9)

or

$$\phi_{xx}^{(i)}(t-s) = \frac{5}{4} \frac{d}{ds} C_N^{(i)}(t,s) + \frac{t-s}{4} \frac{d^2}{dsdt} C_N^{(i)}(t,s)$$

(10)

where $C_N^{(i)}(t,s)$ is the correlation function given by

$$C_N^{(i)}(t,s) = \left( \sum_{n=1}^{N} x_n^{(i)}(t)x_n^{(i)}(s) \right)$$

(11)

Following [9], we make this approximation

$$C_N^{(i)}(t,s) \approx \mu E_n^{(i)} \delta(t-s)$$

(12)

where $A_n^{(i)} = \mu E_n^{(i)} N$ is the maximum amplitude of the correlation function. In the time scale of dissipation, this is a valid approximation when the quartic oscillators are in the chaotic regime. As we transition to the mixed and integrable regimes, the approximation fits poorly, however we will consider the delta function approximation in the mixed regime too for ease of calculations.
From Eq. 7 and Eq. 12 we obtain
\[ \ddot{q} + \omega_0^2 q + \gamma T \dot{q} = 0 \] (13)
where
\[ \gamma_T = \frac{7\lambda^2_N (\mu_1^{(1)} + \mu_1^{(2)}) N}{4m} \] (14)

The \( \gamma_T \) we obtain theoretically compares well with the numerical results (Fig. 2) we obtained.

IV. NUMERICAL SIMULATIONS

We have also simulated the time evolution of our system by solving \( 8N+2 \) equations of motion obtained from the Hamiltonian in Eq. 1 numerically. The second order differential equations were solved using fourth order Runge-Kutta algorithm in a microcanonical ensemble. The time step has been taken to be 0.4 in each case. For all the simulations, the value of \( \lambda \) is taken as 0.01. The mass \( m \) is taken as 1 for all the oscillators and the angular frequency of the harmonic oscillator \( \omega_0 \) is taken to be 0.3. The time is measured in terms of the harmonic oscillator time period \( \tau \approx 20.93 \).

V. RESULTS AND DISCUSSION

The results for our model are obtained both from Linear response theory and numerical simulations. Figure 2 shows the energy of the harmonic oscillator for four different set of initial conditions obtained from both simulations and linear response theory. The parameters for the harmonic oscillators are same for all the four graphs. The theoretical and numerical results are in good agreement with each other. The deviations can be attributed to the \( \delta \)-function approximation for the correlation function used in the liner response theory. In the case of one chaotic bath, this has been improved upon by Xavier et al.\[10\] by incorporating the history and frequency dependence of the system. We intend to incorporate these in our model and the results will be reported elsewhere. Figure 2 confirms that the harmonic oscillator is dissipative and energy flow occurring from the system to the bath. Also we have done simulations in which both the baths are not chaotic. In this case, the harmonic oscillator does not dissipate energy considerably into the baths and the energy dissipation happens only if at least one of the baths is in the chaotic regime.

Next, we have analysed the energy flow from the harmonic oscillator to the chaotic bath. For this, we have calculated the total energy of the system and each bath at regular intervals. This has been shown in Figure 3 and Figure 4. In Figure 3, we have plotted the total energy of the system and the two baths, both of which are in chaotic regime, but with different chaotic parameter and initial energy, versus time. In Figure 3(a) the more chaotic system has less initial energy and less chaotic system has more initial energy. As evident from the figure, more of the dissipated energy from the system goes to the more chaotic system. Figure 2(b) shows an interesting behaviour in the energy flow. In figure 3, the more chaotic system has more energy and less chaotic system has less energy. So naturally one would expect more energy to flow to the bath which has lesser energy (and less chaotic). However, more of the dissipated energy has flown into the more chaotic system even though its energy is higher than the other bath.

Figure 4 shows two graphs which depicts the energy flow into the two different baths, one bath in the chaotic regime and the other in the mixed regime. Here also it is evident that irrespective of the initial energy of the baths, the energy dissipated from the system flows more into the chaotic system. This has been the case with all the simulations, we have done in our model for different parameters. Also, it has been observed that the bath in the mixed regime attained the steady state much faster than the chaotic bath.

This result is rather surprising and nonintuitive. Us-
FIG. 4: The energy flow into two different sets of baths, one in chaotic and one in mixed regime. The central HO has an initial energy of 10.

Using the general equipartition theorem, we can define a temperature for the environment. Therefore, each bath contributes $E^{(i)} = N \frac{kT}{2}$ to the total energy. Therefore, different initial energies for the two baths essentially means coupling the central HO to two baths at two different temperatures, the bath with higher energy being at a higher temperature. In such case, normally one would expect more energy to flow to the bath at lower temperature. This has been the case if the low temperature bath is more chaotic. However, the reverse happens if the low temperature bath is less chaotic.

The seemingly counterintuitive result may be explained in terms of the entropy of the system. The more chaotic system will have more entropy and the energy will flow into the more chaotic bath such that the total entropy of the system will increase. This also causes the more chaotic system to take more time to reach the steady state, which is evident in Figure 4. More analysis are being carried out to quantitatively justify this observed result.

VI. CONCLUSIONS

The dissipative dynamics of a one dimensional harmonic oscillator coupled to two distinct baths has been investigated using linear response theory and numerical simulations. It has been shown that the harmonic oscillator dissipates energy into the baths if the baths are chaotic. The numerical and theoretical results compare well. We have also analysed the dissipative energy flow into the baths from the system. It has been observed that more energy flows into the more chaotic system irrespective of the initial energy of the baths. This rather surprising result may be explained based on the maximization of entropy of the system. One might be able to justify this more precisely by calculating the dynamical entropy of the system for different sets of parameters.

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