

Finite Horizon Model Reduction and the Appearance of Dissipation in Hamiltonian Systems

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Abstract

An apparent paradox in classical statistical physics is the mechanism by which conservative, time-reversible microscopic dynamics, can give rise to seemingly dissipative behavior. In this paper we use system theoretic tools to show that dissipation can arise as an artifact of incomplete observations over a finite horizon. In addition, this approach allows us to obtain finite-time, low order, approximations of systems with moderate size, and to establish how the approach to the thermodynamic limit depends on the different physical parameters.

1 Introduction and Motivation

Loschmidt's classic paradox [5] arises in the context of Statistical Mechanics and can be stated as follows: how can the dynamics of an ensemble of particles governed by time-reversible, conservative laws give rise to seemingly dissipative, irreversible macroscopic behavior? The essential challenge is to reconcile the emergence of an accurate, phenomenological dissipative description from the underlying conservative microscopic dynamics. A standard illustration of this phenomenon in either classical or quantum mechanics is the model of an oscillator coupled to a thermal bath shown schematically in Figure 1, (see for example [3, 9]). This is the model system used by Caldeira and Leggett to study the dephasing effects of thermal coupling in quantum mechanics [1].

In this model, a harmonic oscillator is linearly coupled to a thermal bath—itself modelled as a large collection of harmonic modes with a distribution of frequencies, leading to the Hamiltonian:

$$H = \frac{p^2}{2m} + \frac{m\Omega^2 q^2}{2} - u(t)q + \sum_{i=1}^N \left[\frac{p_i^2}{2m_i} + \frac{m_i}{2} (\omega_i q_i - g_i q)^2 \right] \quad (1)$$

The generality of (1) resides in the freedom to

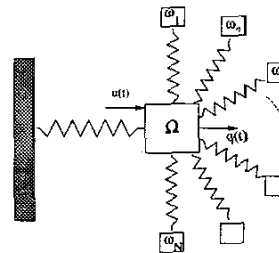


Figure 1: Model of a harmonic oscillator in a thermal bath.

choose the bath frequencies ω_i and the coupling strengths g_i . Letting $m_i = 1$ without loss of generality, one can consider for instance an Ohmic bath with frequencies evenly spaced in the interval $(0, \omega_c]$ and constant couplings $g_i^2 = 4m\gamma\omega_c/\pi N$. In this case, standard results [3, 9] indicate that the observed oscillator will behave like a damped oscillator with frequency Ω and damping rate 2γ in the limit $N, \omega_c \rightarrow \infty$. However, we emphasize that most approximation techniques used in the Physics literature to resolve Loschmidt's paradox are *ad hoc*, with no approximation error bounds, and often requiring formal limits with some infinite scaling. They also lack an algorithmic content and thus provide just a qualitative description of the appearance of dissipation from microscopic Hamiltonian dynamics.

In contrast, our approach is based on control-theoretical tools. By considering the input-output system associated with (1), our problem can then be viewed as that of obtaining low-order approximations, over a finite time horizon, of a high-dimensional LTI operator. Indeed, as suggested by the impulse response (dashed line in Figure 3), the observed dynamics of the system at *early times* may be very close to that of a damped oscillator even for

a moderate number of bath modes.

Note, however, that the operator all its poles on the $j\omega$ -axis, and thus standard infinite horizon model reduction techniques cannot be directly applied. To circumvent this difficulty, we use recent results [8] that allow model reduction over finite horizons of not necessarily stable LTI systems by recasting the problem into a Hankel norm model reduction form. We illustrate the potential of this approach through the analysis of different frequency distributions for the bath oscillators, and of situations far from the thermodynamic limit.

2 Finite Horizon Model Reduction of Unstable Systems

In this section we recall, for ease of reference, some recent results showing that finite horizon model reduction of unstable systems can be accomplished through a modified version of Glover's well-known balanced truncation algorithm.

2.1 Notation and Preliminaries

\mathcal{L}_∞ denotes the Lebesgue space of complex valued matrix functions essentially bounded on the $j\omega$ axis, equipped with the norm $\|G(s)\|_\infty \doteq \text{ess sup}_\omega \bar{\sigma}(G(j\omega))$, where $\bar{\sigma}$ is the largest singular value. \mathcal{H}_∞ denotes the subspace of functions in \mathcal{L}_∞ with a bounded analytic continuation in $\mathcal{R}(s) \geq 0$. $\mathcal{L}_2[0, T]$ denotes the space of vector valued real functions essentially bounded in the interval $[0, T]$, equipped with the norm $\|f\|_{\mathcal{L}_2[0, T]}^2 \doteq \int_0^T f'(t)f(t)dt$. Let \mathcal{L} represent the space of LTI, causal, bounded operators in $\mathcal{L}_2[0, T]$. The induced norm of an operator $M \in \mathcal{L}$ is given by

$$\|M\|_{\mathcal{L}_2[0, T], \text{ind}} \doteq \sup_{\|u\|_{\mathcal{L}_2[0, T]} \neq 0} \frac{\|Mu\|_{\mathcal{L}_2[0, T]}}{\|u\|_{\mathcal{L}_2[0, T]}}$$

A standard result states that the $\mathcal{L}_2[0, \infty)$ -induced norm of a LTI *stable* operator G coincides with the peak value of its frequency response: $\|G\|_{\mathcal{L}_2[0, \infty), \text{ind}} = \|G\|_\infty$.

Let $G: \mathcal{L}_2[0, \infty) \rightarrow \mathcal{L}_2[0, \infty)$ be a stable, finite dimensional operator with McMillan degree n . Its associated Hankel operator [7] $\Gamma_G: \mathcal{L}_2(-\infty, 0] \rightarrow \mathcal{L}_2[0, \infty)$ can be thought off as mapping past inputs in $(-\infty, 0]$ to the corresponding output in $[0, \infty)$. Let $\Gamma_G^*: \mathcal{L}_2[0, \infty) \rightarrow \mathcal{L}_2(-\infty, 0]$ denote the adjoint operator of Γ_G .

The Hankel singular values σ_i^H of G , defined as

the square roots of the eigenvalues of the operator $\Gamma_G^* \Gamma_G$, coincide with the eigenvalues of the product of the controllability and observability Gramians of G (see for instance [7], Chapter 6). Moreover, a rank r approximation G_r to G can be obtained by considering a balanced realization of $G(s)$, and discarding the states associated with the smallest $n - r$ Hankel singular values $\sigma_i^H, i = r + 1, \dots, n$. The corresponding approximation error is then bounded [4] by $\|G - G_r\|_\infty \leq 2 \sum_{i=r+1}^n \sigma_i^H$.

2.2 Model Reduction of Non-Hurwitz Systems

The following theorem is key to the developments in the paper. It relates the $\mathcal{L}_2[0, T]$ -induced norm of a finite dimensional LTI operator G to the $\mathcal{L}_2[0, \infty)$ -induced norm (and thus to the \mathcal{H}_∞ norm) of G_a , a shifted version of G .

Theorem 1 Consider a strictly proper, finite dimensional, LTI, (not necessarily stable system) G with state space realization $G = \left(\begin{array}{c|c} A & B \\ \hline C & \end{array} \right)$. If there exists a $a > 0$ such that $G_a \doteq \left(\begin{array}{c|c} A - aI & B \\ \hline C & \end{array} \right)$ is stable, with $\|G_a\|_\infty < \gamma$, then the following bound holds:

$$\|G\|_{\mathcal{L}_2[0, T], \text{ind}} < \gamma e^{aT}. \quad (2)$$

Proof: See [8].

Straightforward application of this result leads to the following algorithm for finite horizon model reduction of non-Hurwitz systems:

Algorithm 1

0.- Take as inputs a state space realization $G(s) = C(sI - A)^{-1}B + D$, and a number $a \in \mathcal{R}^+$ such that $G(s + a) \in \mathcal{H}_\infty$.

1.- Find a stable reduced order approximation $G_{r,a} \doteq \left(\begin{array}{c|c} A_r & B_r \\ \hline C_r & D_r \end{array} \right)$ to the shifted system $G_a \doteq \left(\begin{array}{c|c} A - aI & B \\ \hline C & D \end{array} \right)$. If, for instance, we use balanced truncations [4], the approximation error is bounded by

$$\|G_a - G_{r,a}\|_\infty \leq 2 \sum_{i=r+1}^n \sigma_{a,i}^H, \quad (3)$$

where $\sigma_{a,i}^H$ denotes the Hankel singular values of G_a (ordered in decreasing order).

2.- Use the system $G_r \doteq \left(\begin{array}{c|c} A_r + aI & B_r \\ \hline C_r & D_r \end{array} \right)$ as an approximation to G in the interval $[0, T]$. From Theorem 1 it follows that

$$\|G - G_r\|_{\mathcal{L}_2[0, T], \text{ind}} \leq 2e^{aT} \sum_{i=r+1}^n \sigma_{a,i}^H. \quad (4)$$

Remark 1 From equation (4) it follows that the proposed algorithm gives error bounds comparable to those of the stable LTI case when $a \sim 1/T$.

3 Finite Horizon Approximations and the Appearance of Dissipation

One of our main conclusions is that, from a systems theoretic viewpoint, the origin of dissipation is not particularly paradoxical: it arises as a parsimonious description of incomplete observations of the dynamics over a finite horizon. The mathematical basis underlying this general statement is the empirical observation that large Hamiltonian systems often result in a state space model with strongly observable and strongly controllable subspaces that are nearly orthogonal. Thus, in a systematic search for simple descriptions of these systems, dissipative dynamics will usually arise, unless conservation of energy is artificially enforced. Indeed, conservative descriptions will typically be of higher order.

In this section we use the canonical coupled-oscillator heat bath model as a prototype to illustrate our ideas. Viewed as an input-output system, the Hamiltonian (1) leads to the following LTI state-space realization:

$$\begin{aligned} \dot{q} &= p/m \\ \dot{p} &= -m\Omega^2 q + u(t) + \sum_{i=1}^N g_i (\omega_i q_i - g_i q) \\ \dot{q}_i &= p_i \\ \dot{p}_i &= -\omega_i^2 q_i + g_i \omega_i q \\ y &= p \end{aligned} \quad (5)$$

As seen in Fig. 1, the variables q and p describe, respectively, the position and momentum of a harmonic oscillator of frequency Ω subject to an external driving force $u(t)$, and linearly coupled to a thermal bath modelled by oscillators with position and momenta q_i and p_i . This system is sufficiently general in that a model of this form can be obtained from any linear bath by finding a canonical transformation that diagonalizes the bath Hamiltonian. The standard assumptions in the Physics literature, commonly referred to as an Ohmic bath, are:

$$g_i^2/m = 4\omega_c \gamma / \pi N, \quad \omega_i = i \omega_c / N \quad (6)$$

i.e. constant couplings and frequencies evenly distributed up to a cut-off $\omega_c \rightarrow \infty$.

3.1 The Classical Physics Viewpoint: Dissipation and the Thermodynamic Limit

Some insight may be obtained by means of a formal solution to system (5) that leads to an integro-differential equation for the dynamics of the observed oscillator [9]. It is cumbersome but straightforward to show that

$$\begin{aligned} \dot{p} &= -m\Omega^2 q + u(t) + F(t) \\ &\quad - \int_0^t \kappa(t-t') p(t') dt' \\ \kappa(t) &= \sum_{i=1}^N (g_i^2/m) \cos(\omega_i t) \\ F(t) &= \sum_i \left[g_i \omega_i \left(q_i(0) - \frac{g_i}{\omega_i} q(0) \right) \cos \omega_i t \right. \\ &\quad \left. + g_i p(0) \sin \omega_i t \right], \end{aligned} \quad (7)$$

where the first term corresponds to the harmonic oscillation; the second to the external drive; and the third to a quasi-random forcing that results from the initial positions and momenta of the bath modes.

The properties of the fourth and last term depend on the integration kernel $\kappa(t)$. Under the Ohmic assumptions (6), and in the limit where the gap between the frequencies $\Delta\omega = \omega_c/N \rightarrow 0$, one gets $\kappa(t) \rightarrow 4\gamma\delta(t)$, where $\delta(t)$ is the Dirac delta (generalized) function. Now Eq. (7) formally leads to the simple expression:

$$\dot{p} = -m\Omega^2 q + u(t) + F(t) - 2\gamma p. \quad (8)$$

Although we will not address this question in detail, it is not hard to show that if the initial positions and momenta of the bath oscillators are thermally distributed at some temperature τ then the sharply peaked behavior of the integration kernel in Eq. (7) also guarantees that

$$\langle F(t) \rangle = 0, \quad \langle F(t)F(t') \rangle = 4mk_B\tau\gamma\delta(t-t'),$$

where k_B is Boltzmann's constant. Hence, from an input-output standpoint, F may be taken to be white noise, and the observed dynamics of the (infinite-dimensional) oscillator system is described by the Langevin equation of a damped harmonic oscillator forced by Brownian motion. This intimate connection between the magnitude of the fluctuations in the system and its rate of return to equilibrium is termed the *fluctuation-dissipation theorem* [6].

We emphasize that this formal procedure sheds little light for systems with a finite number of oscillators, or with a non-zero gap between bath frequencies. Note also that the resulting equation does not conserve energy: if $u = 0$, energy leaves the system

oscillator for the bath and never returns. Clearly, for any finite system all of the bath oscillators will eventually rephase to their original positions and momenta, and the original energy will return to the system oscillator (see Fig. 3). Thus, for a finite number of oscillators, the Langevin equation can only be at best an approximation valid for a finite time.

3.2 The Systems Theoretical Viewpoint: Dissipation as a model reduction problem

In order to move beyond this framework, we proceed along a different path: we obtain reduced approximations valid only over a finite horizon for a finite number of oscillators, and compare those with the limiting model of a damped oscillator. Specifically, we exploit Algorithm 1 to approximate the input/output behavior of our system by: (i) shifting the corresponding transfer function by some $a > 0$, $G(s) \rightarrow G(s+a) \doteq G_a(s)$; (ii) model-reducing the shifted G_a using balanced truncations; and (iii) shifting back the resulting reduced model G_{red} . The error in this procedure is bounded by (3) and (4).

We have analyzed the finite Ohmic system (5), (6) with N modes. The expectation is that, as N and ω_c increase and for a given horizon T , the system will approximate, in the $\mathcal{L}_2[0, T]$ norm sense, a damped oscillator with frequency Ω and damping rate 2γ . This should be evidenced by a Hankel operator with only two large singular values, with the sum of the rest, and the bound (4), tending to zero.

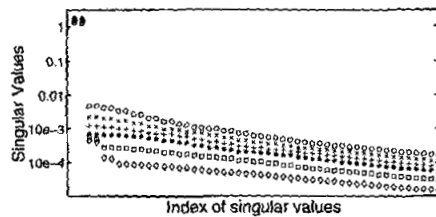


Figure 2: Singular values of the Hankel operator for the shifted oscillator system with $N = 100, 150, 200, 250, 350, 500$ (circles, crosses, plus, stars, squares and diamonds, respectively). The other parameters are $\Omega = 1$, $\gamma = 0.1$, $a \propto N^{-1/3}$ and $\omega_c \propto N^{1/3}$.

Figure 2 shows the Hankel singular values of the shifted system G_a for several values of N . As expected, the system has only two significant Hankel singular values with the remaining ones typically orders of magnitude smaller and tailing off rapidly. Surprisingly, this is so even for moderate numbers of oscillators, far from the $N \rightarrow \infty$ limiting behavior commonly invoked in the Physics literature. In

essence, this is an algorithmic derivation of the fact that, in a rigorous sense, the best model of the dynamics over a finite horizon is a damped oscillator.

This is corroborated in Fig. 3, which compares the impulse responses of the full system (5) and its second order approximation. Indeed, the reduced model for these parameters has the state-space realization:

$$G_{red} = \left(\begin{array}{cc|c} -0.30 & -1.02 & 1.01 \\ 1.02 & 0.10 & -0.05 \\ \hline 1.01 & 0.05 & \end{array} \right),$$

and even for this relatively small number of oscillators ($N = 100$) the error over a time horizon T is bounded by $\|G_{CO} - G_{red}\|_{\mathcal{L}_2[0, T]}$, and $\leq 0.12e^{0.1T}$.

Our numerics show small approximation errors if $a \approx 1/T$. This is intuitive: if the horizon T is to lead to significant simplification of the dynamics, the weighting e^{-aT} should ensure that times $t > T$ do not contribute significantly to the norm. Note also that dissipative models appear when the horizon T is smaller than the characteristic recurrence time of the system (e.g., $t \leq 10$ in Fig. 3).

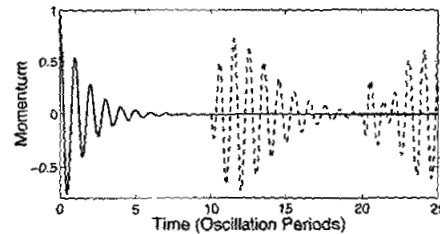


Figure 3: Impulse response of the coupled oscillator system (5),(6) with $\Omega = 1$, $\gamma = 0.1$, $N = 100$, $\omega_c = 10$. The dashed line is the output of the full system, while the solid line corresponds to the second order approximation with $a = 0.1$ ($T = 10$).

We also investigated the approximation error of the second order reduced models as N, ω_c and T are varied. The physical intuition is that it should be possible to consider arbitrarily long horizons by increasing N and ω_c . Indeed, this is shown numerically in Figure 4 where we plot the bounds on the approximation error as $N, T, \omega_c \rightarrow \infty$ such that $(\omega_c/Na) \rightarrow 0$ and $(a\omega_c/\Omega^2)$ is held constant.

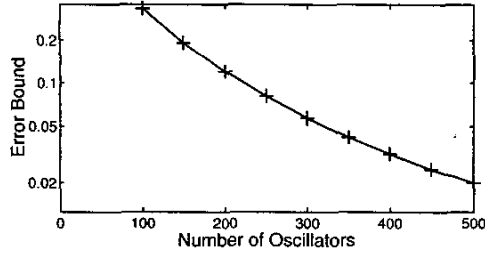


Figure 4: Upper bound on the approximation error as a function of the number of oscillators.

3.3 The Approach to the Limiting Behavior: Analytical Results

Figure 4 gives numerical evidence that the error in replacing the full Ohmic system by a second order Langevin equation may be made arbitrarily small. As long as some scaling ratios hold, this algorithmic result remains robust to changes in the parameters of the system: the damping γ , the cut-off frequency ω_c , the number of bath modes N , the horizon T , and the shifting factor a . In fact, our approach offers the possibility of unravelling the dependence of the approximation error on those parameters *analytically*.

To see this, consider the transfer function from momentum driving to momentum output (the position output case is identical) for the model (5),(6):

$$G_{CO}(s) = \frac{s}{s^2 + \Omega^2 + 2\gamma s \left[\frac{2}{\pi} \frac{\omega_c}{N} \sum_i \frac{s}{s^2 + (i\omega_c/N)^2} \right]}.$$

We must now show that some sequence of oscillator models approaches a damped oscillator in the appropriate limits $\omega_c \rightarrow \infty$, $N \rightarrow \infty$, $a \rightarrow 0$. Thus, $G_{CO}(s)$ should approach the transfer function

$$G_{red}(s) = \frac{s}{s^2 + \Omega^2 + 2\gamma s}$$

in the precise sense of a vanishing approximation error bound over a finite time horizon.

In order to use the bound (4), we should establish that the \mathcal{H}_∞ bound on the relative error vanishes: $\|(G_{CO,a} - G_{red,a})/G_{CO,a}\|_\infty \rightarrow 0$. After algebraic manipulations this is equivalent to:

$$\left\| \frac{G_{CO}(\omega_c \mathcal{S}) - G_{red}(\omega_c \mathcal{S})}{G_{CO}(\omega_c \mathcal{S})} \right\|_\infty = 2\gamma \left\| G_{red}(\omega_c \mathcal{S}) \left(1 - \frac{2}{\pi} \sum_{i=1}^N \frac{N\mathcal{S}}{(N\mathcal{S})^2 + i^2} \right) \right\|_\infty \rightarrow 0,$$

where $\mathcal{S} = (a + j\omega)/\omega_c$. Note that this leads naturally to a *weighted* model reduction problem, where the weight comes into play because of our interest in approximating the “closed-loop” behavior

resulting from the interaction of the oscillator and the bath. On the other hand, the classical Physics approach is akin to “open-loop” model reduction, where the term $\left[\frac{2}{\pi} \frac{\omega_c}{N} \sum_i \frac{s}{s^2 + (i\omega_c/N)^2} \right]$ is approximated by 1, or equivalently $\sum_i \cos \omega_i t \approx \delta(t)$. Note that this is a sufficient (but conservative) condition for $\|G_{CO} - G_{red}\|_{\mathcal{L}_2[0,T]}$, $\text{ind} \approx 0$.

Using some properties of the digamma function ψ and its asymptotic expansion, we get

$$\begin{aligned} \frac{2}{\pi} \sum_{i=1}^N \frac{N\mathcal{S}}{(N\mathcal{S})^2 + i^2} &= \coth(\pi N\mathcal{S}) - (\pi N\mathcal{S})^{-1} \\ &\quad + \frac{j}{\pi} [\psi(1 + N + jN\mathcal{S}) - \psi(1 + N - jN\mathcal{S})] \\ &= \coth(\pi N\mathcal{S}) - \frac{(\pi N\mathcal{S})^{-1}}{1 + \mathcal{S}^2} + \frac{j}{\pi} \ln \frac{1 + j\mathcal{S}}{1 - j\mathcal{S}} + \mathcal{O}\left(\frac{Na}{\omega_c}\right)^{-2} \end{aligned}$$

where the last term is bounded by a finite multiple of $(Na/\omega_c)^{-2}$. The logarithmic term can be shown to have a norm of $\mathcal{O}(\omega_c^{-1} \ln(\omega_c/a))$ and it is also easy to show that

$$\begin{aligned} \|1 - \coth(\pi N\mathcal{S})\|_\infty &\leq \frac{2 \exp(-2\pi Na/\omega_c)}{1 - \exp(-2\pi Na/\omega_c)} \\ &< \pi^{-1} (Na/\omega_c)^{-1} \\ \left\| \frac{1}{\pi N\mathcal{S}} \frac{1}{1 + \mathcal{S}^2} \right\|_\infty &< \pi^{-1} (Na/\omega_c)^{-1}. \end{aligned}$$

Hence, the dominant term in the approximation error is the ratio (ω_c/Na) and if this approaches zero then so does the $\mathcal{L}_2[0,T]$ -induced norm of the error resulting from using the damped oscillator approximation. (This has an intuitive meaning: the frequency spacing should be larger than the peak width ($a \simeq 1/T$) introduced by the finite horizon.) With these scalings the reduced model is shown to converge to the damped oscillator.

3.4 Applicability of the Algorithm

Finally we highlight the methodological advantages of algorithmic approximation methods for large, possibly Hamiltonian systems. Note that our technique needs no modification to be applied to non-Ohmic, non-Markovian baths, or to models which are not of the simple form of equation (1). In those cases, the description in terms of the memory kernel $\kappa(t)$ will generally be non trivial even in the limit of large number of bath modes. The model reduction procedure will typically accommodate this through a larger number of state variables for comparable performance. For the Markovian (Ohmic) system, the number of state variables was no greater than the number of variables describing the system of interest; in general, the approximate models will appropriately retain some chosen degrees of freedom of the environment.

While it is beyond the scope of this article to consider a broad range of models, we illustrate these

points with a simple example of a non-Ohmic bath where the results may again be compared to those obtainable by existing techniques. Consider the system (1) with

$$\begin{aligned} g_i^2/m &= 4\omega_c\gamma f(\omega_i)/\pi N f(\Omega) \\ \omega_i &= i\omega_c/N \\ f(\omega) &= \frac{\gamma_b(\omega^2 + \omega_b^2 + \gamma_b^2)}{(\omega^2 - \omega_b^2 + \gamma_b^2)^2 + 4\gamma_b^2\omega_b^2}. \end{aligned} \quad (9)$$

The frequency dependence is a function of two new parameters ω_b and γ_b , whose meaning becomes clear when carrying out the formal limiting procedure to approximate the memory function $\kappa(t) \rightarrow 2\gamma e^{-\gamma_b t} \cos(\omega_b t)/f(\Omega)$.

In the limit, it is clear that this new bath behaves as if it were an oscillator with frequency ω_b which decays at rate γ_b as it is in turn coupled to an Ohmic bath. This suggests that an accurate model should require four state variables rather than just two, with the extra variables referring to the effective bath oscillator. Indeed, our model reduction algorithm finds four significant singular values with the rest being much smaller. Figure (5) shows the time dynamics of the full non-Ohmic model and of a four-dimensional reduced model valid for early times. Note how the energy is radiated from the system oscillator and back again, all inside the envelope of an overall decay into the environment. In fact, it is to capture this non-Markovicity that the extra reduced system degrees of freedom are needed.

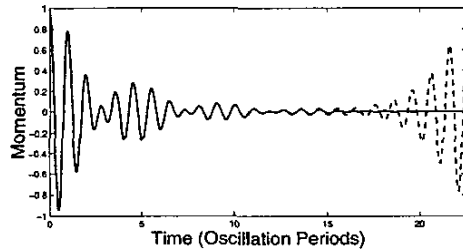


Figure 5: Same as Fig. 3 for the non-ohmic oscillator system (5), (9) with $\Omega = 1, \gamma = 0.1, N = 250, \omega_c = 12, \omega_b = 1, \gamma_b = 0.09, a = 0.05$.

4 Conclusions

In this paper we have shown how system-theoretic approximation methods can be systematically applied to obtain low order approximations, valid over finite intervals, to the collective behavior of the interconnection of a large number of simpler subsystems. These tools were illustrated in the context of

Loschmidt's paradox: the seemingly dissipative behavior of a collection of non-dissipative oscillators. From a model approximation perspective, the origin of this dissipation is no particular mystery: it arises as a parsimonious description of incomplete observations of the dynamics over a finite horizon. Remarkably, the algorithmic results presented in this paper are robust to changes in the parameters of the system (5) (such as $\Gamma, \omega_c N$), the horizon T and the shifting factor a , as long as some general scaling ratios hold. Indeed, a key feature of our approach is that it offers the possibility of unravelling the dependence of the approximation error on all of those parameters.

In addition, our approach provides algorithmic tools for a more meaningful reinterpretation of experimental data in terms of data-driven, parsimonious reduced models (as opposed to the current fitting of data in terms of generalized Markov models).

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