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Relaxation in nonlinear systems, nonconvergent infinite continued fractions and sensitive relaxation processes

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Abstract

The Mori–Lee treatment of linear response theory demonstrates that the Laplace transform of any relaxation function of a dynamical variable can be expressed as a continued fraction. For certain simple nonlinear systems, the continued fraction representation of the relaxation functions cannot be evaluated perturbatively. It turns out that many body systems with even a single on-site nonlinearity can dramatically alter the relaxation behavior in such systems. We argue that nonperturbative continued fractions in the Mori–Lee formalism are necessarily associated with systems that exhibit relaxation that is sensitive to the presence of nonlinearities.

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1. Introduction

The Mori–Lee formalism [1,2] for solving the time evolution of some dynamical variable $A(t)$ described as follows via the Liouville equation:

$$\mathrm{d}A(t)/\mathrm{d}t = \mathtt{L}A(t)\,, \tag{1}$$

where the Liouville operator $\mathtt{L} \equiv \sum_{i=1}^{N}(\partial/\partial x_i)(\partial\mathtt{H}/\partial p_i) - (\partial/\partial p_i)(\partial\mathtt{H}/\partial x_i)$, i.e., a Poisson bracket in a classical N particle system and by $\mathtt{L} \equiv (i/\hbar)[\mathtt{H},]$, a commutator bracket for in a quantum system. The Hamiltonian of the system is denoted by $\mathtt{H}$ and $\mathtt{H}$ is assumed

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to be hermitian, i.e., there is no source or sink of energy in our system. The Mori–Lee formalism grew out of the projection operator formalism of Zwanzig [3]. While the formalism provides a prescription for the construction of a complete solution for $A(t)$, a *typical application* concerns constructing the relaxation function associated with some dynamical variable. The Mori–Lee formalism proves that the Laplace transform, $C(z)$, of any normalized relaxation function $C(t) \equiv \langle A(t)A(0)\rangle/\langle A(0)\rangle^2$, where the angular brackets denote canonical ensemble averages, $1 \leqslant C(t) \leqslant -1$, and where as a system approaches equilibrium, $C(t) \to 0$, can be written as a continued fraction (CF) of the form

$$C(z) = 1/(z + \Delta_1/(z + \Delta_2/(z + \Delta_3/(z + \Delta_4/(z + \Delta_5/(z + \ldots)))))) \,. \tag{2}$$

In Eq. (2), the Δ_ν's are constructed out of equilibrium correlation functions of the system according to a prescription to be summarized below. In perfectly nonergodic systems (within the context of the canonical ensemble), $C(z)$ is a finite CF [4]. In systems that exhibit ergodicity or even partial ergodicity in the sense that a part of any external perturbation propagates through the entire system, $C(z)$ is an infinite CF (ICF) [4].

It turns out that in many of the tractable physical systems one can study, Δ_ν's grow in magnitude with increasing ν. If Δ_ν's grow at rate ν^α, where $\alpha \geqslant 2$, then an ICF cannot be replaced by a finite CF or truncated in some manner, no matter how many levels are kept to describe the return to equilibrium of the relaxation function $C(t)$ [5]. In other words, when $\alpha \geqslant 2$, no matter how many levels are retained in $C(z)$, anything short of a complete evaluation with all the poles of the ICF results in a short-time expansion of $C(t)$.

Given that it is very difficult to analytically or even numerically calculate Δ_ν's for most interacting dynamical systems, not enough is known about how the Δ_ν's grow with ν in most systems as a function of temperature. It turns out that if one considers an infinite harmonic oscillator chain, the velocity autocorrelation of any particle decays in time as a Bessel function and the corresponding $\Delta_\nu = \text{const}$ for $\nu > 1$ [6]. This result is true at any temperature. Thus, in this case $\alpha = 0$. Given what is known at the present time, the $\alpha = 0$ case is realized in harmonic oscillator systems [6], in electron gas problems [7] and in certain spin problems as well [8]. If one probes the relaxation function in a $s = \frac{1}{2} XY$ chain at $T = \infty$, one finds that the transverse relaxation function at any site j, $\langle S_j^x(t) S_j^x(0)\rangle/\langle S_j^{x2}\rangle$, relaxes as a Gaussian function in time [9]. In this case one finds, $\Delta_\nu/\nu = \text{const}$, i.e., $\alpha = 1$ [9]. There are many other many body physical systems that have been probed and in most of the cases studied it has been found that $\alpha \leqslant 2$ [10].

However, there are systems, such as particles in anharmonic wells and such as spins in certain spin clusters where one finds $\alpha > 2$ [11,12]. As mentioned above, the ICFs in these cases cannot be solved perturbatively . There are two important points to be noted here. First, the nonperturbative nature of the ICFs in the Mori–Lee formalism does not necessarily forbid one from solving these problems via different approaches. Second, the fast growth in Δ_ν's implies that even if one anharmonic well is present in one site in a system where the remainder of the system is such that $\alpha < 2$, the systems relaxation is going to be completely dominated by this anharmonic well [12]. Let us call these relaxation processes "sensitive". We contend that they belong to a special category of dynamical problems, which may be fairly ubiquitous. In what follows, we discuss these sensitive relaxation processes in some detail.

2. Mori–Lee formalism

In this formalism one constructs a complete orthogonal set of d time-independent basis vectors f_ν and a complete set of d time-dependent coefficients (which can be later identified with various fundamental dynamical correlations) $a_\nu(t)$ to write

$$A(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu \ , \tag{3}$$

such that $A(t)$ is a solution to the Liouville equation (Eq. (1)). To define orthogonal f_ν's it is necessary to choose a scalar product. One simple choice for instance turns out to be the fluctuation formula [2]

$$(f_\nu, f_\nu) = (\langle f_\nu f_\mu \rangle - \langle f_\nu \rangle \langle f_\mu \rangle)\delta_{\nu\mu} \ , \tag{4}$$

where $\langle \rangle$ defines a canonical ensemble average. One can now select the first basis vector, a common choice to make the connection with linear response theory being $f_0 = A(t=0)$ and hence $a_0(t=0) = C(t=0) = 1$, a condition that excludes exponential relaxation as a rigorous result for $C(t)$ in hermitian systems [2]. Gram–Schmidt orthogonalization using Eq. (4) yields [2]

$$f_1 = \mathrm{L} f_0 \ , \tag{5a}$$

$$f_{\nu_{+1}} = \mathrm{L} f_\nu + \Delta_\nu f_{\nu_{-1}} \ , \tag{5b}$$

where

$$\Delta_\nu \equiv (f_\nu, f_\nu)/(f_{\nu_{-1}}, f_{\nu_{-1}}) \ . \tag{5c}$$

Using the $\{f_\nu\}$, and Eq. (3) in Eq. (1) one finds a second recurrence relation for the $a_\nu(t)s$.

$$\Delta_1 a_1(t) = -\mathrm{d}a_0/\mathrm{d}t \ , \tag{6a}$$

$$\Delta_{\nu+1} a_{\nu_{+1}}(t) = -\mathrm{d}a_\nu/\mathrm{d}t + a_{\nu_{-1}}(t) \ . \tag{6b}$$

It is usually difficult to solve Eq. (6) directly. Laplace transform of both sides of Eq. (6) yields the CF in Eq. (2). Thus, complete solution for $A(t)$ requires construction of $\{f_\nu\}$ and $\{a_\nu\}$. However, construction of $C(t)$ is less laborious and requires construction of $\{\Delta_\nu\}$, and hence the solution of an equilibrium problem.

3. Sensitive relaxation processes

We recall that in a number of simple many body systems such as the harmonic oscillator chains, the spin $\frac{1}{2}XY$ and Heisenberg systems, in electron gas problems and

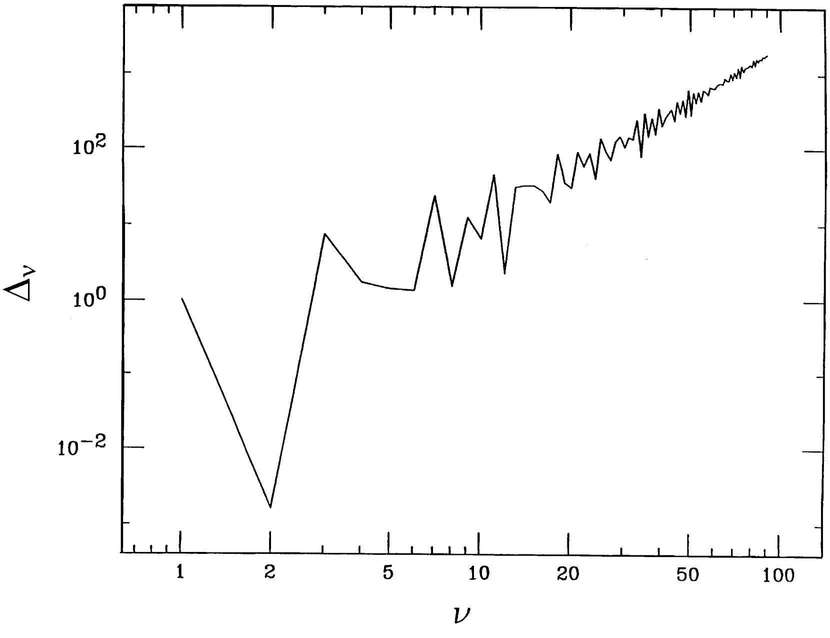

Fig. 1. Plot of Δ_ν versus ν for $\beta = 100$ in a system with $V(x) = (x^2/2) + (x^4/4)$. In the case shown below $\Delta_\nu = \nu^{2.5}$.

in mean-field spin models [6–10], the growth of $\Delta_\nu \sim \nu^\alpha$, where α is typically 0 or 1 as $\nu \to \infty$. Presumably there are many other systems where similar structure is obtained for Δ_ν's. In all of these systems, Eq. (2) can be obtained perturbatively, i.e., by replacing the ICFs by finite CFs with a large number of levels, where by large one means thousands or more levels [5].

However, this is not the case for some systems where $\alpha \geqslant 2$. There is no known physical case where $\alpha = 2$ has been rigorously realized [13]. There are, however, several instances where $\alpha > 2$ has been obtained. The simplest of these cases is the case where a single particle is placed in an anharmonic potential with $V(x) = (a/4)x^4$, where a is some constant. In this problem, regardless of whether one considers a single quartic well or a double well, $\alpha \approx 2.5$ [12] (see Fig. 1). Very similar results have been obtained for cases where the lowest order anharmonic term is an even number that is greater than 4 [12]. In those cases higher values of α than 2.5 have been realized. These ICFs cannot be evaluated perturbatively and all the poles must somehow be taken into account to solve Eq. (2) [5]. These ICFs are reminiscent of a familiar scenario in the study of the phase transitions, where all the poles of a partition function must be taken into account to construct a description of phase transition phenomena [14]. Given the special nonperturbative nature of Δ_ν's in certain physical systems, one can perhaps categorize such systems as special and deserving of exclusive attention. We refer to these systems, where $\alpha \geqslant 2$, as systems that exhibit sensitive relaxation processes. We discuss below the typical behavior of sensitive relaxation processes.

One realization of a sensitive relaxation process is the case where one places an anharmonic on-site potential in an infinite system of harmonically connected particles [12]. If one calculates any relaxation function (e.g., the velocity autocorrelation function) for the particle in the anharmonic site or at a site in its vicinity it turns out that the behavior of the Δ_v's would pick up a contribution with $\alpha \sim 0$ from the harmonic interactions and a contribution with $\alpha \approx 2.5$ from the on-site anharmonic potential [12]. While the detailed relaxation process would differ from that of the single anharmonic oscillator, the asymptotic behavior of the Δ_v's in the many body system of harmonically coupled particles with a single on-site anharmonic potential will be largely controlled by the single on-site potential itself.

When an interacting many body system undergoes a phase transition, the system becomes highly correlated (e.g., see Ref. [14, Chapter 7]). Intuitively speaking, during such a phase, every particle in the system somehow becomes cognizant of interactions that transpire between every other particle to an extent. Although actual calculations of asymptotic behavior of Δ_v's remain a challenge at this time for systems undergoing phase transitions, it is possible that many systems might exhibit values of $\alpha > 2$. Indeed, in the Landau–Ginzburg mean-field picture of a phase transition, where one describes the free energy as a double-well function in the order parameter with quartic anharmonicity, the relaxation of the order-parameter itself turns out to be a sensitive relaxation process [15].

4. Summary and conclusions

In this work, we have focused on the physical meaning of superlinear growth rates in Δ_v's that enter into the ICF representation of the Laplace transformed relaxation function of some dynamical variable in any system described by a hermitian Hamiltonian. We have pointed out that in case of superlinear growth, the ICFs cannot be evaluated in perturbative fashion and that such a property may be typical in nonlinear systems and/or in highly correlated systems where a single site or a few sites may dictate the physical behavior of a many body system. We have suggested that such sensitive systems with nonperturbative structures in their ICFs deserve special categorization and need to be exclusively probed.

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