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Quantum Dissipation

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Abstract

We address the question of the microscopic origin of dissipation in collective motion of a quantum many-body system in the framework of a parametric random matrix approach to the intrinsic dynamics. We show that the fluctuation-dissipation theorem is generally violated and, moreover, energy diffusion has a markedly non-Gaussian character and the corresponding distribution has very long tails. Such features do not support a Langevin or Fokker–Planck approach to dissipation in collective nuclear motion.

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While theory and experiment have gone a long way in the study of the collective nature of large amplitude nuclear motion, the theoretical understanding of the coupling between the collective and the intrinsic degrees of freedom is still in its infancy. Most of the approaches are more or less phenomenological in nature. Hill and Wheeler [1] suggested almost forty years ago that Landau–Zener transitions are at the origin of nuclear dissipation. Over the years there have been a relatively large number of studies of this particular mechanism [2] and the range of results is equally diverse. Implicit in this interpretation is the presumption that irreversibility is of quantum origin. Even though there exist quantum approaches (the linear response model [3], the hopping model [4], path integral method [5] and others), many formulations are basically classical, e.g. the so called "wall formula" [6]. These include the more pragmatic phenomenological models, such as the Langevin equation or Fokker–Planck equation [7], Maxwell's model for friction with memory effects [8], and to a certain extent kinetic approaches, e.g. two-body dissipation mechanism [6]. In an analysis of a generic problem of coupled slow and fast degrees of freedom, Berry and Robbins 9 obtained friction for the slow subsystem only by treating the entire system classically, attributing it to "a clash between the essence of quantization, namely the discrete spectrum of frequencies, and the essence of chaos, namely mixing and a continuous spectrum extending to zero frequency" [9]. The present status of our understanding of the microscopic origin of dissipation in many-body quantum systems is thus rather unsatisfactory. In this letter we explore the nature of dissipation in a many-body system, using parametric random matrix theory, which allows for direct solution in many cases of the quantum dynamics of the system.

The physical systems we explore are many-body systems which exhibit excitations on two distinct time scales, described by collective (slow) and intrinsic (fast) degrees of freedom. In order to address how energy is transferred from the slow (X, P) to the fast (x, p) modes, we will assume that the slow modes evolve classically at constant velocity V_0 according to $X(t) = V_0 t$. (Although we do not consider it here, this restriction can be lifted, and the more general problem solved using the results and methods presented here.) As a consequence of this assumption, we can solve for the quantum dynamics of the fast subsystem, and even obtain analytic results for situations which are analogous to the conventional adiabatic and diabatic limits. The intrinsic system is defined by its matrix elements, and is taken as complex, described by its average level density, $\rho(E)$, and its spectral fluctuations, in the form

$$H(X) = H_0 + H_1(X).$$
 (1)

Here H_0 is chosen to be a diagonal $N \times N$ matrix, defining the average density of states, with $\langle k|H_0|l\rangle = [H_0]_{kl} = \varepsilon_k \delta_{kl}$. In the basis of the eigenstates of H_0 , we define $H_1(X)$ as a parameter dependent, $N \times N$ real Gaussian random matrix, which is completely specified by its first two moments

$$\overline{[H_1(X)]_{ij}[H_1(Y)]_{kl}} = [\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}]\mathcal{F}_{ij}(X - Y),$$

$$\overline{[H_1(X)]_{kl}} = 0.$$
(2)

 $\mathcal{F}_{ij}(X-Y)$ is a "bell-shaped" correlation function with a characteristic width X_0 , and the overline stands for the ensemble average. The dependence on i, j allows for the description of banded matrices, where an effective number of states $N_0 \leq N$ can be coupled by $H_1(X)$. Such a parametrization implies that correlations between different instantaneous spectra corresponding to different 'shapes' X are effective only within a distance $\approx X_0$. The average level density for each fixed shape X is given by H_0 , while its spectral fluctuation properties (in this case GOE, but all our formalism applies to GUE as well) are determined by $H_1(X)$. We use a convenient parametrization of the correlator $\mathcal{F}_{ij}(X)$ introduced in Refs. [5]

$$\mathcal{F}_{ij}(X) = \frac{W_0}{\sqrt{\rho(\varepsilon_i)\rho(\varepsilon_j)}} \exp\left[-\frac{(\varepsilon_i - \varepsilon_j)^2}{2\kappa_0^2}\right] F\left(\frac{X}{X_0}\right).$$
(3)

Here $F(x) = F(-x) = F^*(x) \leq 1$, F(0) = 1 and W_0 , κ_0 $(N_0 \approx \kappa_0 \rho(\varepsilon))$ and X_0 are characteristic to the given system. The instantaneous spectra of a Hamiltonian H(X)with constant average level density, $[H_0]_{kl} = k\delta_{kl}$, is shown in Fig. 1 for gaussian $F(x) = \exp(-x^2/2)$ (top) and exponential $F(x) = \exp(-|x|)$ (bottom) correlations. Notice that a conventional adiabatic limit does not exist for the exponential, as the individual energy levels undergo Brownian motion, and are not smooth on any time scale.

The time evolution of this system is found by solving the time-dependent Schrödinger equation:

$$\psi(t) = \operatorname{Texp}\left[-\frac{i}{\hbar} \int_0^t ds H(X(s))\right] \psi(0) = \mathcal{U}(t)\psi(0).$$
(4)

where T is the time-ordering operator, and $\mathcal{U}(t)$ the propagator. (We assume that the initial state $\psi(0)$ is uncorrelated with the Hamiltonian H(X(t)) at later times.) The average propagator $U(t) = \overline{\mathcal{U}(t)}$, found by using Eqs. (2) and resumming all leading order diagrams in perturbation expansion of $\mathcal{U}(t)$ in the limit $N_0 \gg 1$, satisfies the system of integral equations [11]:

$$U_{k}(t) = U_{0 k}(t) - \frac{1}{\hbar^{2}} \int_{0}^{t} ds_{1} \int_{0}^{s_{1}} ds_{2} U_{0 k}(s_{2}) U_{k}(t - s_{1}) \\ \times \sum_{n=1}^{N} \mathcal{F}_{kn}(X(s_{1}) - X(s_{2})) U_{n}(s_{1} - s_{2}),$$
(5)

where $U_{0k}(\tau) = \exp(-i\varepsilon_k t/\hbar)$. In order to compute averages of observables, we introduce the set of generalized occupation number probabilities

$$\mathcal{N}_{k}(t_{1}, t_{2}) = \overline{\langle \psi(t_{1}) | k \rangle \langle k | \psi(t_{2}) \rangle} \\ = \sum_{l} \overline{\langle l | \mathcal{U}^{\dagger}(t_{1}) | k \rangle \langle k | \mathcal{U}(t_{2}) | l \rangle} n_{l}(0), \qquad (6)$$

where $n_l(t) \equiv \mathcal{N}_l(t,t)$ is the occupation probability of the state $|l\rangle$. $\mathcal{N}_k(t_1,t_2)$ satisfy the following set of integral equations

$$\mathcal{N}_{k}(t_{1}, t_{2}) = U_{k}^{*}(t_{1})U_{k}(t_{2})n_{k}(0) + \frac{1}{\hbar^{2}} \int_{0}^{t_{1}} ds_{1} \int_{0}^{t_{2}} ds_{2} \sum_{l} \mathcal{N}_{l}(s_{1}, s_{2})\mathcal{F}_{lk}(s_{1} - s_{2}) \times U_{k}^{*}(t_{1} - s_{1})U_{k}(t_{2} - s_{2}).$$
(7)

These equations specify the time evolution of the system, and we will consider (i) the numerical solutions of (5)-(7) and the velocity dependence of the diffusion constant, and (ii) the extension of the formalism to the regime $1 \ll N_0 < N = \infty$, where we find analytic limits and a great simplification of the formalism as well.

The first situation we study is that of constant average level density $([H_0]_{kl} = k\delta_{kl})$, as in a stadium billiard. Eqs. (5)-(7) have been solved numerically for N = 101 levels, a bandwidth $N_0 = 21$, a gaussian correlation $F(x) = \exp(-x^2/2)$ with $X_0 = 1$, and initial conditions $n_k(0) = \delta_{k,51}$. The resulting occupation numbers $n_k(t)$ are shown in Fig. 2 for the cases of fast ($V_0 = 4$, top) and slow ($V_0 = 1/16$, bottom) driving velocities. As the results are symmetric with respect to the index k, $n_k(t) = n_{102-k}(t)$, only k = 1 - 51are shown, counting from the bottom of the figure. One might expect that even a small driving velocity would result in a complicated time evolution, as the Hamiltonian is timedependent, and has many small gaps in the instantaneous spectrum, where Landau-Zener transitions might occur and thus induce "irreversibility" [1]. Actually, as we have discussed at length in Ref. [10], this mechanism, which has been advocated in many previous treatments [2], is valid only for isolated level crossings and thus is unrealistic when there are many non-isolated ones as shown in Fig.1.

In Fig. 2, one can clearly distinguish two time scales: a relatively rapid initial transient evolution, followed by a much slower one. While the initial transient behaviour is almost identical in both cases, governed by the same spreading width Γ^{\downarrow} , the long time behaviour is strikingly different. For small driving velocities, the time evolution rapidly equilibrates, and can be understood in terms of the $V_0 \rightarrow 0$ limit, corresponding to constant random matrix theory [11]. For large velocities there is a steady evolution to a different probability distribution. The initial transient behaviour arises only because our initial occupation probabilities $n_k(0)$ did not originate from an instantaneous eigenstate of H(0) (detailed discussion on initial conditions will be presented elsewhere[10]). The subsequent long time behaviour is due to the explicit time dependence of the Hamiltonian H(t) and would be absent for a time independent one.

The diffusion process associated with these time evolutions can be characterized by the energy variance, $\Delta_E(t)$, and the energy diffusion constant $D(V_0^2)$, defined by

$$\Delta_E(t) = \overline{\langle \psi(t) | [H(t) - E(t)]^2 | \psi(t) \rangle} \approx \operatorname{const} + 2D(V_0^2)t.$$

$$t \to \infty$$
(8)

In Fig. 3, $D(V_0^2)$ can be seen to exhibit quadratic velocity dependence, in contradiction to previous claims [2]. In the case we consider here of a symmetrical initial distribution $n_k(0)$ and constant level density, the average energy $E(t) = \overline{\langle \psi(t) | H(t) | \psi(t) \rangle}$ is constant, hence the reaction force on the slow system, in particular the friction force, exactly vanishes. This is consistent with a fluctuation-dissipation theorem in the following sense. Expressed as $\gamma = \beta D$, where γ is the "friction" coefficient and $\beta = 1/T = d \ln \rho(e)/de \equiv 0$ is the inverse thermodynamic temperature, we have the expected result $dE(t)/dt = \gamma \equiv 0$. We shall outline briefly a further extension and simplification of the formalism in the limit $N \to \infty$, i.e. in the spirit of the standard constant random matrix theory, by introducing the characteristic functional [11]

$$\mathcal{N}(t_1, t_2, \tau) = \overline{\langle \psi(t_1) | \exp\left[\frac{iH_0(\tau - t_1 + t_2)}{\hbar}\right] | \psi(t_2) \rangle},$$

$$\mathcal{N}_k(t_1, t_2) = \frac{1}{2\pi \hbar \rho(\varepsilon_k)} \int d\tau \mathcal{N}(t_1, t_2, \tau)$$

$$\times \exp\left[-\frac{i\varepsilon_k(\tau - t_1 + t_2)}{\hbar}\right],$$
(9)

$$\mathcal{N}(t,t,\tau) = \exp\left[\sum_{n} \overline{\langle\!\langle \psi(t) | H_0^n | \psi(t) \rangle\!\rangle} \frac{(i\tau)^n}{\hbar^n n!}\right],\tag{10}$$

where $\overline{\langle\!\langle \psi(t) | H_0^n | \psi(t) \rangle\!\rangle}$ are cumulants. $\mathcal{N}(t_1, t_2, \tau)$ satisfies the evolution equation

$$\mathcal{N}(t_{1}, t_{2}, \tau) = \sigma^{*}(t_{1})\sigma(t_{2}) + \frac{\sqrt{2\pi\kappa_{0}W_{0}}}{\hbar^{2}} \int_{0}^{t_{1}} ds_{1} \int_{0}^{t_{2}} ds_{2} \\ \times \mathcal{N}(s_{1}, s_{2}, \tau) \exp\left[\frac{\kappa_{0}^{2}}{2} \left(\frac{\beta}{2} + i\frac{s_{1} - s_{2} - \tau}{\hbar}\right)^{2}\right] \\ \times F\left(\frac{(s_{1} - s_{2})V_{0}}{X_{0}}\right) \sigma^{*}(t_{1} - s_{1})\sigma(t_{2} - s_{2}),$$
(11)

where $\sigma(t) = \exp(i\varepsilon_k t/\hbar)U_k(t)$ (note $\sigma(t)$ is state independent), for which an equation similar to Eq. (5) can be derived. In this case, there is only one equation to be solved, instead of *N*-coupled equations (cf. Eq. (7)), which results in a significant simplification of the entire formalism. Moreover, various analytic solutions can be obtained, as we exemplify below, by analyzing the adiabatic and the diabatic evolutions of the occupation numbers for a system with a realistic level density of the form $\rho(\varepsilon) = \rho_0 \exp(\beta\varepsilon)$. $\beta = 0$ corresponds to the case we have just described, of constant average level density, while the case of finite β approximates fairly well a many-fermion system.

The *adiabatic limit* corresponds to $\kappa_0 X_0 / \hbar V_0 \gg 1$ (and also $\kappa_0 \beta \ll 1$), from which we find

$$\mathcal{N}(t,t,\tau) = \exp\left\{\frac{2\pi W_0}{\hbar} \left[F\left(\frac{\tau V_0}{X_0}\right) - 1\right]t - \frac{2\pi W_0|\tau|}{\hbar}\right\}.$$
(12)

All odd moments of H_0 vanish identically (since F(x) = F(-x)), and in the limit $t \to \infty$, all even cumulants of H_0 increase linearly in time. If $F(x) = \exp(-x^2/2)$ (we shall use this form hereafter for illustrative purposes) then

$$\overline{\langle\!\langle \psi(t) | H_0^{2n} | \psi(t) \rangle\!\rangle} = \frac{2\pi W_0 t}{\hbar} \left(\frac{\hbar V_0}{X_0}\right)^{2n} \frac{(2n)!}{2^n n!},$$
$$D(V_0^2) = \frac{\pi \hbar W_0 V_0^2}{X_0^2} = \frac{\hbar \Gamma^{\downarrow} V_0^2}{2X_0^2},$$
(13)

 $(\Gamma^{\downarrow} = 2\pi W_0)$ resulting in a non-Gaussian distribution.

In the *diabatic limit*, $\kappa_0 X_0 / \hbar V_0 \ll 1$, we find

$$\mathcal{N}(t,t,\tau) = \exp\left\{\frac{2\pi X_0 W_0 \kappa_0}{\hbar^2 V_0} \left[\exp\left(\frac{\kappa_0^2}{2} \left(\frac{\beta}{2} + \frac{i\tau}{\hbar}\right)^2\right) - \exp\left(\frac{\kappa_0^2 \beta^2}{8}\right)\right] t\right\}.$$
 (14)

In this case again all the cumulants of H_0 increase linearly in time

$$\overline{\langle\!\langle \psi(t) | H_0^n | \psi(t) \rangle\!\rangle} = \left[\frac{2\pi X_0 W_0 \kappa_0}{\hbar^2 V_0} \exp\left(\frac{\beta^2 \kappa_0^2}{8}\right) \left(\frac{i\kappa_0}{\sqrt{2}}\right)^n \mathcal{H}_n\left(-\frac{i\kappa_0\beta}{2\sqrt{2}}\right) \right] t, \tag{15}$$

where $H_n(x)$ are Hermite polynomials. From the explicit expressions for the first and second cumulants we thus obtain that

$$\beta D = \gamma \left(1 + \frac{\beta^2 \kappa_0^2}{4} \right),\tag{16}$$

which shows that the Einstein fluctuation-dissipation theorem is generally violated.

The most salient feature of the solutions (12) and (14) becomes evident when one considers the asymptotic behaviour of the cummulants. Since cumulants of higher than second order are nonvanishing, Gaussian processes are not obtained in any of these limiting cases for the energy diffusion. $\langle \langle \psi(t) | H_0^n | \psi(t) \rangle \rangle$ either increase indefinitely with nor increase subsequently after an initial decrease, depending on the values of parameters. As a result the energy distribution has very long tails. In particular for $V_0 \equiv 0$ the distribution corresponding to Eq. (12) has a Lorentzian shape. These features imply that a Langevin or Fokker–Planck approach to energy dissipation is at least questionable. As we have discussed in Ref. [10] the present results apply equally to the GUE case.

The present approach treats the fast subsystem quantum mechanically and the slow subsystem classically, as has been done often in the past [2]. The energy diffusion process is described in terms of some intrinsic characteristics of the many-body system (thermodynamic temperature, spreading width Γ^{\downarrow} , κ_0 and X_0) and V_0 . It is not clear yet whether these characteristics have a meaningful classical limit separately or only in a given combination, and this seemingly points to an apparent lack of a classical limit for the fast degrees of freedom ($\hbar \rightarrow 0$) of the solutions (13), (15). In Ref. [9], friction was obtained only in a classical treatment of both fast and slow system, while in Ref. [5], dissipation and friction appear only in a explicit quantum treatment (path integral) of the entire system and the presence of quantum fluctuations in the slow subsystem was essential. The wall formula [6] leads to a diffusion constant $D \propto V_0^2$ as we have obtained here (see Fig. 3 and Eq. (13)), but is essentially a classical result, which does not depend in any significant way on \hbar , and apparently reflects a different underlying mechanism. It will be highly desirable to identify the classical limit of the present approach.

In conclusion, we have presented numerical and analytical solutions of the time dependent evolution of a driven complex quantum system, such as a nucleus, under the assumption that the number of levels is large. The parametric random matrix approach chosen here incorporates the essential attributes of the intrinsic dynamics, namely: an exponentially increasing level density, GOE spectral fluctuations and loss of correlations during large amplitude collective motion. We have shown that the resulting energy diffusion process is highly non–Gaussian in character, that the energy distribution has very long tails and also that the energy diffusion constant is proportional to the square of the collective velocity.

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Figure 1: Instantaneous eigenvalue spectrum $E_n(X)$ as a function of the "shape" (X), for a Hamiltonian of the ensemble defined by Eqs. (1–3), with $[H_0]_{jk} = k\delta_{jk}$, using the correlator $F(x) = \exp(-x^2/2)$ (top) and $F(x) = \exp(-|x|)$ (bottom).

Figure 2: The time dependence of the occupation probabilities $n_k(t)$, for k = 1, ..., 51(in this case $n_k(t) = n_{102-k}(t)$), where k counts from bottom to top in the figure, for the case of fast, $V_0 = 4$ (top), and slow, $V_0 = 1/16$ (bottom), driving velocities.

Figure 3: The time dependence of the energy variance $\Delta_E(t)$ for a range of velocities $V_0 = 4, 2, 1, 0.5, 0.25, 0.125$ and 0.0625. The highest curve corresponds to the larger velocity. The insert shows the diffusion constant $D(V_0^2)$ as a function of V_0^2 , indicating $D \propto V_0^2$.