DYNAMICS OF A SIMPLE QUANTUM SYSTEM IN A COMPLEX ENVIRONMENT Aurel BULGAC

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We present a theory for the dynamical evolution of a quantum system coupled to a complex many–body intrinsic system/environment. By modelling the intrinsic many–body system with parametric random matrices, we study the types of effective stochastic models which emerge from random matrix theory. Using the Feynman–Vernon path integral formalism, we derive the influence functional and obtain either analytical or numerical solutions for the time evolution of the entire quantum system. The form of our influence functional is qualitatively different from the Caldeira–Leggett model, which leads to observable effects. We discuss thoroughly the structure of the solutions for some representative cases and make connections to well known limiting results, particularly to the Brownian motion and the Kramers classical limit.

Quantum dissipation is a problem with such a long history and such a multitude of results that even a cursory review will not make justice to the numerous contributions of a large number of authors over several decades, see Refs. [1, 2, 3, 4, 5] and the references therein. Here we present a short review of our continuing effort to understand the character of energy flow between the slow degrees of freedom and the intrinsic degrees of freedom in many–body systems. Even though the whole system is finite and in a strict sense there is no irreversible behaviour in this case, for all practical purposes the time evolution of the collective or slow quantum system has the character of quantum dissipative dynamics. The central question is: can one describe the dynamical behaviour of the simple system using for example an equation of the form

$$M\frac{d^2X}{dt^2} = -\frac{dU(X)}{dX} - M\gamma\frac{dX}{dt} + f(X,t) \tag{1}$$

as in the case of a Brownian particle, if in the absence of the interaction the Hamil-

tonian of the system is

$$H_0(X) = \frac{P^2}{2M} + U(X) \tag{2}$$

and where γ is a friction coefficient and $f(X,t)$ is a Langevin–like force? The force $f(X,t)$ can in principle depend not only on time but on position as well, and in this way one can describe a large variety of physical situations, ranging from diffusion to localization [5]. If one were to start from a description of the entire system (reservoir plus simple system) with a Hamiltonian

$$H(X,x) = H_0(X) + H_1(X,x), \tag{3}$$

where $H_1(X,x,p)$ describes the reservoir and its interaction with our system, under what circumstances can one derive an equation of motion like Eq.(1)? Moreover, does the fluctuating force have Gaussian character or not?

We address this problem using a well known approach based on the double path integral formulation of Feynman and Vernon [1]. Our original input is in the functional form of the influence functional, which originates from a parametric random matrix description of the "environment". This has been attempted earlier in Ref. [3]. The functional form for the influence functional we determine is qualitatively different from the popular Caldeira–Leggett type derived by Feynman and Vernon [1]. It comes as no surprise than that under such circumstances the dynamical evolution of a quantum dissipative system in our case has new features as well, as we shall exemplify here. Here we restrict our attention to the Markovian limit only. In spite of its physical limitations (high temperature limit for the intrinsic system) this limit shows already the qualitative differences with the previously known approaches.

The basic assumption concerning the intrinsic states is that there are no governing constants of the motion, so that the dynamics is chaotic. This has been seen to be the general situation in studies of many–body systems, from nuclei to molecules, so it is reasonable to approach the modeling of these degrees of freedom with random matrices, suitably tailored to the problem. We shall refer to X as "shape" variables, since in large amplitude collective nuclear motion it represents the collective coordinates which characterize the nuclear mean field.

The part of the total Hamiltonian Eq. (3) which depends on the intrinsic coordinates $H_1(X,x)$ is defined as a matrix, whose matrix elements depend parametrically on the "slow" coordinate X

$$[H_1(X)]_{ij} = [h_0]_{ij} + [h_1(X)]_{ij}. \tag{4}$$

h_0 is taken to be diagonal and defines the average density of states, with $\langle k|h_0|l\rangle = [h_0]_{kl} = \varepsilon_k \delta_{kl}$. We refer in the main text to these eigenstates as "typical states" of the

intrinsic system with an energy ε. One can think of h_0 as a Hamiltonian describing a "bath" or a "reservoir" and of $h_1(X)$ as a Hamiltonian describing the interaction between the "bath/reservoir" and the "slow" system. Whereas in statistical physics the interaction between the thermostat and the system under consideration is assumed to be negligible, we shall not make such an approximation here. As a matter of fact, for the physically interesting situations we envision, this coupling term can be large.

In Refs. [4] we discussed the reasons why one chooses this specific form of the Hamiltonian. 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 aas follows [3]

$$\begin{aligned} \overline{[h_1(X)]_{kl}} &= 0, \\ \overline{[h_1(X)]_{ij}[h_1(Y)]_{kl}} &= \frac{[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}]\Gamma^{\downarrow}}{2\pi\sqrt{\rho(\varepsilon_i)\rho(\varepsilon_j)}} \exp\left[-\frac{(\varepsilon_i-\varepsilon_j)^2}{2\kappa_0^2}\right] G\left(\frac{X}{X_0}\right). \end{aligned} \tag{5}$$

The overline stands for statistical averages over the ensemble of random Gaussian matrices from the Gaussian Orthogonal Ensemble (GOE). Here $G(x) = G(-x) = G^*(x) \leq 1$, $G(0) = 1$, and the spreading width $\Gamma^{\downarrow}$, κ_0 (linked with the effective band width $N_0 \approx \kappa_0\rho(\varepsilon)$) and X_0 are characteristic of the intrinsic system. Even though it is not necessary, we shall consider a particular from for $G(x)$, namely $G(x) = \exp(-x^2/2)$.

For an intrinsic subsystem with a large number of degrees of freedom, the average density of states $\rho(\varepsilon) = \overline{\mathrm{Tr}\delta(H_1(X)-\varepsilon)}$, for each given shape X increases sharply with energy. The overline denotes here a procedure for extracting the smooth part of $\rho(\varepsilon)$ as a function of energy, which amounts essentially to an ensemble average. For a many Fermion system, $\rho(\varepsilon)$ has a roughly exponential behaviour and $\ln\rho(\varepsilon)$ is approximately proportional to the thermodynamic entropy of the intrinsic system, which is an extensive quantity. Therefore is equivalent to stating that the intrinsic subsystem has a large heat capacity and thus can play the role of a "reservoir", although not necessarily ideal. In principle $\rho(\varepsilon)$ can be X–dependent as well, but we shall ignore this aspect here. Without an X–dependence of the average density of states, mechanical work cannot be performed on or by the model environment we study here, and only heat exchange is allowed.

The quantum description of our coupled system will be treated through the path integral construction of the density matrix. According to Feynman and Vernon [1], one can write the following double path integral representation for the density

matrix of the entire system

$$\mathcal{R}(X,x,Y,y,t) = \int dX_0 dY_0 \psi(X_0)\psi^*(Y_0) \int_{X(0)=X_0}^{X(t)=X} \mathcal{D}X(t) \int_{Y(0)=Y_0}^{Y(t)=Y} \mathcal{D}Y(t)$$
$$\times \exp\left\{\frac{i}{\hbar}\left[S_0(X(t)) - S_0(Y(t))\right]\right\}$$
$$\langle x|\mathrm{T}\exp\left[-\frac{i}{\hbar}\int_0^t dt' H_1(X(t'))\right]|\phi\rangle\langle\phi|\mathrm{T}_a \exp\left[\frac{i}{\hbar}\int_0^t dt'' H_1(Y(t''))\right]|y\rangle, \qquad (6)$$

where T and T_a represent the time ordering and time anti–ordering operators respectively. In this representation, we have used a particular form for the initial state wave function $\Psi(X,x) = \psi(X)\phi(x)$. Other choices are equally possible, such as an initial density matrix.

In the adiabatic approximation (in this case this amounts to treating everything to first order in the inverse temperature $\beta = 1/T$) one can show that the density matrix satisfies the following Schrödinger like equation (for similar examples see Refs. [2])

$$i\hbar\partial_t \rho(X,Y,t) = \left\{\frac{P_X^2}{2M} - \frac{P_Y^2}{2M} + U(X) - U(Y)\right. \qquad (7)$$
$$\left. - \frac{\beta\Gamma^{\downarrow}\hbar}{4X_0 M} G'\left(\frac{X-Y}{X_0}\right)(P_X - P_Y) + i\Gamma^{\downarrow}\left[G\left(\frac{X-Y}{X_0}\right) - 1\right]\right\}\rho(X,Y,t)$$

with an arbitrary initial condition $\rho(X,Y,0) = \rho_0(X,Y)$. It can be shown that the classical limit of this equation is well known Kramers equation [4].

In the remaining part of this short review we will consider solutions to the evolution equations (7). For certain forms of the potential, one can readily obtain explicit solutions to the time evolution of the density matrix, while for others we solve the evolution equation numerically see last two Refs. [4].

Let us consider the case when there is a linear potential acting on the slow variables

$$H_0(X) = -\frac{\hbar^2}{2M}\partial_X^2 - FX. \qquad (8)$$

In the limit $t \to \infty$ the slow system reaches a steady state characterized by a time independent momentum distribution and a time dependent spatial distribution. The salient features of this solution can be more easily appreciated by considering various cumulants. In particular the first and second momentum cumulants acquire the expected thermal values:

$$\langle\langle p\rangle\rangle = \frac{2MFX_0^2}{\beta\Gamma^{\downarrow}\hbar} = \frac{F}{\gamma}, \qquad \langle\langle p^2\rangle\rangle = \frac{M}{\beta} = MT. \qquad (9)$$

What is notable, however, is that the momentum distribution has higher than second order cumulants, which increase exponentially with the order of the cumulant:

$$\langle\langle p^{2n}\rangle\rangle (-1)^{n-1}\frac{(2n-1)!!}{n}\frac{MX_0^2}{\hbar^2\beta}\left(\frac{\hbar}{X_0}\right)^{2n}, \tag{10}$$

$$\langle\langle p^{2n-1}\rangle\rangle = (-1)^{n-1}(2n-3)!!\frac{F}{\gamma}\left(\frac{\hbar}{X_0}\right)^{2n-1} \tag{11}$$

All higher than second order cumulants vanish in the strict classical limit $\hbar \to 0$. These cumulants also vanish in the limit $X_0 \to \infty$, which should be interpreted as a weak coupling limit to the thermostat. Naively, one would have expected that the coupling to the thermostat is controlled mainly by the magnitude of $\Gamma^{\downarrow}$. As one can easily convince oneself however, the coupling between the two systems is also controlled by the correlation length X_0. In the limit $X_0 \to \infty$ there is no energy exchange between the two subsystems, irrespective of the value of the "coupling constant" $\Gamma^{\downarrow}$. The first two spatial cumulants are:

$$\langle\langle r\rangle\rangle = \frac{2FX_0^2}{\beta\Gamma^{\downarrow}\hbar}\,t\frac{Ft}{M\gamma} = \frac{\langle\langle p\rangle\rangle t}{M}, \qquad \langle\langle r^2\rangle\rangle = \frac{4X_0^2}{\beta^2\Gamma^{\downarrow}\hbar}\,t = 2Dt. \tag{12}$$

The particle position grows linearly with time as expected and the average position displays diffusion consistent with Brownian motion, which can be used to define the diffusion constant D. As with the momentum distribution, the coordinate distribution in not Gaussian, and has longer tails. One can see from the expressions for the cumulants that if the limits

$$\frac{\hbar}{X_0} \to 0, \qquad \frac{X_0}{\Gamma^{\downarrow}} \to 0 \tag{13}$$

are taken, with the friction coefficient γ remaining finite, one obtains the case of pure classical Brownian motion. All but the first two cumulants for coordinate and momenta vanish, and one is left with a Gaussian process. These limits can be achieved also by keeping $\hbar$ finite and thus obtaining the case of a quantum Brownian particle.

For a particle in a harmonic oscillator potential one can determine analytically cumulants of the the momentum and spatial distributions as well. In the $t \to \infty$ limit one obtains that

$$\frac{\langle\langle p^2\rangle\rangle}{2M} = \frac{\langle\langle M\omega^2 r^2\rangle\rangle}{2} = \frac{1}{2\beta} = \frac{T}{2}, \tag{14}$$

as one might have expected. However, as in the case of a linear potential the momentum and spatial distributions show the presence of significant higher then

second order cumulants. Except for a "trivial" overall factor, the shape of this function is controlled by a single parameter, the "characteristic action" $2M\omega X_0^2$, which depends on the "roughness" of the coupling to the "reservoir".

The tunneling through a potential having the shape of an inverted parabo-la can be studied by performing the formal replacement $\omega = i\Omega_0$ in the corresponding equations of the previous section. Kramers showed that dissipation leads to a reduction of the flux through an inverted parabolic barrier, as the unperturbed attempt frequency in the transition state theory should be replaced with the renormalized one [2].

$$\Omega_0 \to \Omega_+ = -\frac{\gamma}{2} + \sqrt{\Omega_0^2 + \frac{\gamma^2}{4}} \leq \Omega \tag{15}$$

One basic assumption in Kramers approach was the fact that the friction coefficient is momentum independent. The present approach can be interpreted as a theory with a momentum dependent friction coefficient, which in the zero velocity limit reduces to the classical value. For finite velocities however, the effective friction coefficient in our approach is smaller than the one for zero velocity (see the above approximate solution for the trajectory for the case of small friction). One can thus expect two effects: *i*) the effective or average attempt frequency in our approach is in between the Kramers value and the value corresponding to no friction, i.e. $\Omega_+ < \Omega_{eff} < \Omega_0$; *ii*) the spatial density distribution is also modified. Overall the effect of an effective momentum dependent friction coefficient it is likely to lead to an enhancement of the tunneling probability when compared with the classical Kramers result. It can be shown also that all cumulants increase exponentially both with the order and with time.

We have developed a dynamical theory of simple quantum systems coupled to complex quantum environments, where the environment is a general "chaotic" bath of intrinsic excitations. The model Hamiltonian we introduce for the intrinsic subsystem incorporates the generic properties of finite many–body systems. This includes an average level density of states sharply increasing with energy, the presence of universal spectral (or random matrix) fluctuations for the intrinsic system and the variation of these properties while changing the "shape" of the intrinsic system modeled with parametric banded random matrices. In this way, the intrinsic system is capable to easily absorb energy due to its large heat capacity. We did not yet allow the intrinsic system to perform mechanical work, but this feature can be readily implemented.

The evolution equation is surprisingly easy to manipulate and in many instances one can construct full solutions by quadratures, for cases when the corresponding

path integral can be computed only by brute force. The entire treatment is performed at the quantum level. We showed on the other hand that at the classical limit, the evolution equation reduces to the Kramers form. The quantum evolution equation we have derived for the density matrix is not more complicated than a classical Fokker–Planck equation. However, this evolution equation describes processes which first of all are quantum in nature and moreover have manifestly non–Gaussian features. The spatial and momentum distributions are characterized by high order cumulants, which increase exponentially with the order. As we have discussed earlier [4], this is indicative of the fact that the corresponding distributions have longer tails than previously expected.

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