CHARACTER OF DISSIPATION IN LARGE AMPLITUDE COLLECTIVE NUCLEAR MOTION

Aurel BULGAC
Department of Physics, University of Washington, P.O. Box 351560, Seattle, WA 98195–1560, USA

Giu DO DANG
Laboratoire de Physique Théorique et Hautes Energies, Université de Paris–Sud, F–91405 Orsay, FRANCE

Dimitri KUSNEZOV
Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520–8120, USA

Within the Feynman–Vernon path integral formalism and in the Markovian limit, we consider the time evolution of a collective subsystem coupled to a "bath" of intrinsic degrees of freedom. We show that dissipation leads to major qualitative and quantitative modifications of the time evolution of the density matrix of the collective subsystem. In either the spatial, momentum or energy representation the density distribution acquires very long tails, and in particular tunneling is greatly enhanced.

1 Introduction

Even though the accumulated knowledge, from both theoretical and experimental sides, about Large Amplitude Collective Motion (LACM) is impressive, one would not be completely off the mark by saying that we are still quite a distance away from understanding it. We definitely lack an *ab initio* approach. Phenomenological models abound, but whether there is a link to the underlining microscopic description is yet an unsolved mystery. LACM is in some generic way slow, however this is not always a very well defined concept and whether the adiabatic approach is appropriate is still an open question. One can find without effort opposite arguments on these issues in the published literature. The slowness of LACM would allow us to resort to a relatively simple Hamiltonian description, where only quadratic terms in the collective velocity are present. There is no doubt however that going beyond the adiabatic approximation is a necessity. One does not need so much to consider higher powers in the collective velocity as to account for the relatively strong coupling to non–collective degrees of freedom. The "irreversible" aspect of this coupling is what is referred to routinely as dissipation.

2 Time evolution of the density matrix

2.1 The path integral approach

The Hamiltonian governing the dynamics of a collective quantum subsystem coupled to a complex intrinsic subsystem has the generic form

$$H(X,x) = H_0(X) + H_1(X,x). \tag{1}$$

Here $H_0(X)$ describes the collective degrees of freedom only and $H_1(X,x)$, which depends parametrically on the "shape" X, describes the internal motion. We refer to X as "shape" variables, since often they indeed stand for actual nuclear shapes. Henceforth we shall not display explicitly the dependence of the Hamiltonian H_1 on the intrinsic variables x. For reasons which we shall not dwell upon here, H_1 is modelled through a parametric banded random matrix[3,4,5]. For the sake of simplicity, we assume, though this is not necessary, that the initial state is a product wave function

$$\Psi(X,x) = \psi(X)\phi(x) \tag{2}$$

and we also introduce the influence functional

$$\begin{aligned} \mathcal{L}(X(t),Y(t),t) &= \langle\phi| \left\{ \mathrm{T}_a \exp\left[\frac{i}{\hbar}\int_0^t dt'' H_1(Y(t''))\right]\right\} \\ &\times \left\{ \mathrm{T}\exp\left[-\frac{i}{\hbar}\int_0^t dt' H_1(X(t'))\right]\right\} |\phi\rangle. \end{aligned} \tag{3}$$

Here T and T_a represent time ordering and anti–ordering operators respectively. When evaluating $\mathcal{L}(X(t),Y(t),t)$ the ensemble average over the appropriate realization of the random Hamiltonian H_1 is implied[5]. According to Feynman and Vernon[1] one obtains the following double path integral representation for the density matrix of the "slow" subsystem

$$\begin{aligned} \rho(X,Y,t) &= \int dX_0 dY_0 \psi(X_0)\psi^*(Y_0) \int_{X(0)=X_0}^{X(t)=X} \mathcal{D}X(t) \int_{Y(0)=Y_0}^{Y(t)=Y} \mathcal{D}Y(t) \\ &\times \exp\left\{\frac{i}{\hbar}\left[S_0(X(t)) - S_0(Y(t))\right]\right\} \mathcal{L}(X(t),Y(t),t). \end{aligned} \tag{4}$$

Here $S_0(X(t))$ stands for the classical action corresponding to the Hamiltonian $H_0(X)$. In the case of an adiabatic evolution of the slow subsystem, $\mathcal{L}(X(t),Y(t),t)$ acquires an extremely simple form[5]

$$\mathcal{L}(X(t),Y(t),t) = \exp\left\{\frac{\Gamma^{\downarrow}}{\hbar}\int_0^t \left[G(X(t'),Y(t')) - 1\right] dt'\right\}, \tag{5}$$

where $G(X,Y)$ (with $|G(X,Y)| \leq 1$ and $G(X,X) = 1$) is related to the correlation function between matrix elements of the intrinsic Hamiltonians $H_1(X)$ and $H_1(Y)$, corresponding to two distinct "shapes" X and Y. The spreading width $\Gamma^{\downarrow}$ appearing here defines also the coupling strength between collective and intrinsic subsystems [3,4,5]. The expression (5) differs qualitatively from the widely used in literature Caldeira and Leggett's form [2], which is quadratic in $X(t)$ and $Y(t)$. One can show now that the density matrix satisfies a Shrödinger like equation of the form [5]

$$i\hbar\partial_t \rho(X,Y,t) = \{H_0(X) - H_0(Y) + i\Gamma^{\downarrow}[G(X,Y) - 1]\}\rho(X,Y,t). \qquad (6)$$

This evolution equation for $\rho(X,Y,t)$ describes a quantum mechanical Markovian process and it also satisfies the conditions of the Lindblad's theorem [6]. This last feature ensures that its solutions can be given a probabilistic interpretation at any times.

2.2 Linear potential

The case when the collective variables evolve in a linear potential

$$H_0(X) = -\frac{\hbar^2}{2m}\partial_X^2 - FX \qquad (7)$$

is particularly instructive. We shall assume furthermore that the "effective potential" is "translation invariant", namely $G(X,Y) = G(X-Y)$. In terms of the difference and average variables $s = X-Y$, $r = (X+Y)/2$, the evolution equation for $\rho(X,Y,t)$ becomes

$$(i\hbar\partial_t + \frac{\hbar^2}{m}\partial_r\partial_s)\rho(r,s,t) = \{-Fs + i\Gamma^{\downarrow}[G(s) - 1]\}\rho(r,s,t). \qquad (8)$$

We look for a solution of the form

$$\rho(r,s,t) = \int \frac{dk}{2\pi\hbar} \exp\left(\frac{ikr}{\hbar}\right) d(k,s,t). \qquad (9)$$

The function $d(s,t,k)$ satisfies the equation

$$\left(\partial_t + \frac{k}{m}\partial_s\right) d(k,s,t) = \left\{\frac{iFs}{\hbar} + \frac{\Gamma^{\downarrow}}{\hbar}[G(s) - 1]\right\} d(k,s,t). \qquad (10)$$

For either $s = 0$ or $k = 0$, $d(k,s,t)$ is the characteristic function [7] for the spatial or momentum distribution of the slow subsystem.

Using the method of characteristics for wave equations [8] Eq. (10) can be solved through quadratures and the density matrix is thus determined to be

$$\begin{aligned}\rho(r,s,t) &= \iint \frac{dr'dk}{2\pi\hbar}\rho_0\left(r', s-\frac{kt}{m}\right)\exp\left\{\frac{ik(r-r')}{\hbar}\right\} \\ &\times \exp\left\{\frac{iFst}{\hbar}-\frac{iFt^2k}{2\hbar m}+\frac{\Gamma^{\downarrow}m}{\hbar k}\int_{s-\frac{kt}{m}}^{s}ds'[G(s')-1]\right\}. \quad (11)\end{aligned}$$

where $\rho_0(r,s)=\rho(r,s,0)$ is the initial density matrix. $D(s,t)=d(0,s,t)$, see Eqs. (9) and (11), is the characteristic function for the momentum distribution

$$D(s,t)=\int dr\rho(r,s,t)=\int dr\rho_0(r,s)\exp\left(\frac{iFst}{\hbar}+\frac{\Gamma^{\downarrow}t}{\hbar}[G(s)-1]\right). \quad (12)$$

One extremely economical and intuitive way to characterize the momentum distribution of the collective subsystem is through its cumulants [7]

$$\langle\langle p^n\rangle\rangle|_t=\left(\frac{\hbar d}{ids}\right)^n \ln D(s,t)\Big|_{s=0} \quad (13)$$

For the case of a Gaussian correlation function $G(X)=\exp[-X^2/2X_0^2]$, one gets thus explicitly

$$\langle\langle p\rangle\rangle|_t = \langle\langle p\rangle\rangle|_{t=0}+Ft, \quad (14)$$

$$\langle\langle p^2\rangle\rangle|_t = \langle\langle p^2\rangle\rangle|_{t=0}+\frac{\Gamma^{\downarrow}\hbar t}{X_0^2}, \quad (15)$$

$$\langle\langle p^{2n}\rangle\rangle|_t = \langle\langle p^{2n}\rangle\rangle|_{t=0}+(2n-1)!!\frac{\Gamma^{\downarrow}t}{\hbar}\left(\frac{\hbar}{X_0}\right)^{2n}. \quad (16)$$

The meaning of the "correlation length" X_0 is that intrinsic shapes separated by $|X-Y|>X_0$ are statistically uncorrelated. Notice that only the first cumulant is affected by the presence of a linear potential in the expected manner, namely a uniform acceleration of the slow subsystem. The "bath" of intrinsic degrees of freedom affects only higher order even cumulants of the momentum distribution and the odd cumulants of order higher than one remain unchanged. This is due to the particular choice for the correlator $G(X)$ we have used here, which is an even function of its argument.

The cumulants of the spatial distribution can be obtained from the characteristic function $d(k,0,t)$. From Eq. (11) it immediately follows that

$$\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{ik}{\hbar}\right)^n\langle\langle r^n\rangle\rangle = \ln d_0(k,0,t)+\left(-\frac{ik}{\hbar}\right)\frac{Ft^2}{2m}$$

$$+ \quad \frac{\Gamma^{\downarrow} m}{\hbar k} \int_{-\frac{kt}{m}}^{0} ds' [G(s') - 1]. \tag{17}$$

The term $\ln d_0(k,0,t)$ gives the contributions to the cumulant expansion arising from the free expansion alone of the initial wave packet, in the absence of both the linear potential and the coupling to the internal degrees of freedom. The linear potential leads to the expected (classical) behaviour of the center of the wave packet (see the second term on the rhs of the above expression). The contribution arising from dissipation alone to the even cumulants is

$$\langle\langle r^{2n} \rangle\rangle|_{diss} = \frac{(2n-1)!!}{2n+1} \frac{\Gamma^{\downarrow} t}{\hbar} \left(\frac{\hbar t}{m X_0} \right)^{2n}. \tag{18}$$

Of particular interest is the second cumulant

$$\langle\langle r^2 \rangle\rangle|_{diss} = \frac{\Gamma^{\downarrow} \hbar t^3}{3 X_0^2 m^2}, \tag{19}$$

which shows that dissipation leads to a very fast expansion of the wave packet. This behaviour is to be contrasted with the free expansion or ballistic propagation, in which case $\langle\langle r^2 \rangle\rangle \propto t^2$ and with normal diffusion, for which $\langle\langle r^2 \rangle\rangle \propto t$. The energy tails of the energy distribution are significantly longer than in traditional phenomenological transport approaches, like Fokker–Planck or Langevin equations. One can show that in the tails the energy distribution has the following behaviour

$$P(\varepsilon) \propto \exp(-\alpha |\varepsilon| \ln^{1/2} |\varepsilon|), \tag{20}$$

where α is some constant and ε stands for the energy of the slow subsystem with respect to its initial value. Similarly, one can show that with logarithmic accuracy for large values of the variable $\theta(r,t) = |r - Ft^2/2m|/t$ (assuming vanishing initial average linear momentum) the spatial distribution behaves as

$$\rho(r,0,t) \propto \exp\left[-\nu \theta(r,t) ln^{1/2} \theta(r,t) \right], \tag{21}$$

where ν is some constant. Thus the role of dissipation is undeniably not only significant, but leads to qualitatively new features.

2.3 Quadratic potential

Another case that is susceptible to an analytical treatment is that of a quadratic potential for the collective subsystem

$$H_0(X) = -\frac{\hbar^2}{2m} \partial_X^2 + \frac{m\omega^2 X^2}{2}. \tag{22}$$

Using the representation for $\rho(r,s,t)$ of Eq. (9), the equation for the transformed density now becomes

$$\left(\partial_t + \frac{k}{m}\partial_s - m\omega^2 s\partial_k\right) d(k,s,t) = \frac{\Gamma^{\downarrow}}{\hbar}[G(s)-1]d(k,s,t). \tag{23}$$

The method of characteristics [8] can again be used to determine its solution

$$\begin{aligned}
\rho(r,s,t) &= \int \frac{dk}{2\pi\hbar}\exp\left\{\frac{ikr}{\hbar}\right\} \\
&\times \quad d_0\left(s\cos\omega t - \frac{k}{m\omega}\sin\omega t, m\omega s\sin\omega t + k\cos\omega t\right) \qquad (24)\\
&\times \quad \exp\left\{\frac{\Gamma^{\downarrow}}{\hbar}\int_0^t dt'[G(s\cos\omega(t-t') - \frac{k}{m\omega}\sin\omega(t-t')) - 1]\right\},
\end{aligned}$$

where $d_0(s,k) = d(s,k,0)$. In a similar manner to the one described in the previous subsection, one can determine various cumulants. For both spatial and momentum distributions only even cumulants are affected by dissipation

$$\langle\langle p^{2n}\rangle\rangle|_{diss} = (2n-1)!!\frac{\Gamma^{\downarrow}}{\hbar\omega}\left(\frac{\hbar}{X_0}\right)^{2n}\int_0^{\omega t} d\tau\cos^{2n}\tau \tag{25}$$

$$\approx \frac{[(2n-1)!!]^2}{2^n n!}\frac{\Gamma^{\downarrow}t}{\hbar}\left(\frac{\hbar}{X_0}\right)^{2n}, \tag{26}$$

$$\langle\langle r^{2n}\rangle\rangle|_{diss} = (2n-1)!!\frac{\Gamma^{\downarrow}}{\hbar\omega}\left(\frac{\hbar}{m\omega X_0}\right)^{2n}\int_0^{\omega t} d\tau\sin^{2n}\tau \tag{27}$$

$$\approx \frac{[(2n-1)!!]^2}{2^n n!}\frac{\Gamma^{\downarrow}t}{\hbar}\left(\frac{\hbar}{m\omega X_0}\right)^{2n}. \tag{28}$$

There is a noticeable difference with the case of a linear potential, in that all cumulants increase now only linearly with time. It looks as if the quadratic potential has a "focusing" effect on the spatial distribution. It is a simpler matter to analytically continue these expression to the case of an inverted parabolic potential or barrier. This rather innocuous procedure, leads however to an entirely different time dependence of the cumulants, all of them increasing exponentially with time in this case (as $\cos\tau$ and $\sin\tau$ become $\cosh\tau$ and $\sinh\tau$ respectively).

2.4 Tunneling

Lack of space prevents us from presenting results on the influence of dissipation on tunneling. We have analysed so far a symmetric double well potential and

solved numerically Eq.(6) for an initial wave packet situated in one of the wells. The tunneling time is increased by orders of magnitude in the presence of dissipation, depending of course on the concrete values of $\Gamma^{\downarrow}$ and X_0 in particular.

3 Concluding remarks

The approach we have chosen, even though not entirely microscopic, incorporates the essential microscopic characteristics of a nucleus [3,4,5], namely: an exponentially increasing level density, GOE spectral fluctuations and loss of correlations between intrinsic states significantly differing in macroscopic properties (e.g. shape and excitation energy). We have focused on the way energy is transferred between the collective and the internal degrees of freedom and determine the main characteristics of the collective energy flow. We have shown that the dynamical evolution of the coupled collective and intrinsic subsystems has a number of unexpected and new qualitative aspects. It is as a rule a non–Gaussian process, which leads to rather long tails in excitation energy, spatial and momentum distributions. There are significant violations of the Einstein form of the fluctuation–dissipation theorem as well, especially for not so slow collective motion [5]. The influence of dissipation on tunneling appears to be major. Many of these features shed doubts on the applicability of a Langevin or Fokker–Planck approach to nuclear dissipative motion, which approaches neglect as well the quantum character of LACM. It is our feeling that the present approach holds a great promise towards modelling and understanding the role of dissipation in LACM. It is a fully quantum mechanical approach, technically it is about as simple or as complicated as a Fokker–Planck approach. However, there is no doubt that this approach has such a great flexibility as to incorporate various microscopic models, memory effects and the information which can be extracted is in principle more detailed than in traditional phenomenological approaches. Moreover, the essentially microscopic nature of the entire framework makes it especially appealing.

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