Characteristic times for thermal wave packets in dissipative Bohmian mechanics: the parabolic repeller

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Thermal wave packets are used to analyze transmission probabilities and characteristic times through a parabolic repeller within the dissipative Bohmian mechanics. Thermal arrival, dwelling, transmission and reflection times are defined and calculated by using a Maxwell-Boltzmann distribution for the initial velocities of the incident particles. The dissipation is considered within the Caldirola-Kanai and Kostin approaches where a linear and nonlinear framework is used, respectively. The initial parameters are chosen to have only a dissipative tunnelling dynamics at zero temperature; at any nonzero temperature, transmission proceeds not only via tunnelling.

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I. INTRODUCTION

Time in quantum mechanics is a permanent and important issue subject to many definitions depending on the process studied, leading to very interesting and endless debates for conservative problems \cite{1-3}. This is due mainly to the fact that time is usually considered as a parameter (external parameter) and not as an observable in the non-relativistic framework. Thus, we usually talk about phase, tunnelling, transmission, resident, dwelling, arrival, etc. times. In general, we could globally name them as characteristic times. Calculations of these characteristic times are usually extracted from some time distributions. For example, the so-called transition path time distribution which gives the probability distribution of transition times between two spatial points has been proposed in the context of the transition state theory and rate coefficients \cite{4}. This distribution defined in terms of a symmetrized thermal density correlation function has been successfully used by Pollak to calculate tunnelling times in presence of (Ohmic) friction following the Caldeira-Leggett Hamiltonian in the Langevin formalism \cite{5-8}.

On the other hand, Ford, Lewis and O’Connell \cite{9-13} studied decoherence in the quantum Brownian motion at high temperatures in the absence of dissipation and a zero temperature with dissipation starting from the quantum Langevin equation for Ohmic friction and for thermal wave packets. In particular, in Ref. \cite{9} they studied tunnelling through a parabolic potential in the presence of dissipation.

Within the framework of Bohmian mechanics \cite{14}, where particle trajectories are calculated, time quantities like arrival time, transmission and reflection times are unambiguously defined and widely used for conservative dynamics \cite{15, 16}. In continuation of our study of dissipative tunnelling through a parabolic repeller \cite{17, 18} through scaled trajectories, we extend this study here by introducing temperature through the Maxwell-Boltzmann distribution of velocities for an incoming wave packet and analyzing some typical characteristic times. Our system represents thus an ensemble of non-interacting particles with a thermal distribution of initial velocities. The initial state is taken to be a mixed ensemble of Gaussian wave packets with weights given by the Maxwell-Boltzmann distribution as Ford et al. \cite{12} and also in the study of time-of-flight distribution for a cloud of cold atoms falling freely under gravity \cite{19}. Thermal arrival, dwelling, transmission and reflection times are defined and calculated through dissipative Bohmian trajectories. Dissipation is considered within the Caldirola-Kanai and Schrödinger-Langevin or Kostin approaches \cite{20}, within a linear and nonlinear theoretical framework, respectively. Leavens \cite{21} has also shown that arrival time distributions are given by the modulus of the probability current density. Due to the non-crossing property of Bohmian trajectories, in a scattering (transmission) problem there is a critical trajectory which bifurcates transmitted trajectories from the reflected ones. This provides a way to split dwelling time into transmission and reflections times \cite{15}. In this way, the computation of characteristic times reduces to the computation of the single critical trajectory. However, it is also proved \cite{22} that there is even no need to compute this single trajectory.

The paper is organized as follows. In Section \textsuperscript{11} thermal wave packets are built for an ensemble of non-interacting
particles, each one being described by a Gaussian wave packet whose central velocity is distributed according to the Maxwell-Boltzmann distribution function. In section [III] the effect of the dissipation on the evolution of the thermal wave packet is considered within the Bohmian mechanics framework. Finally, Section [IV] presents and discusses transmission through a parabolic repeller by considering different characteristic times such arrival, dwelling and reflection times.

II. CONSTRUCTING THERMAL WAVE PACKETS

Consider an ensemble of noninteracting particles where each particle is initially described by the state \( |\psi_{v_0}(0)\rangle \) with \( v_0 \) being the central velocity of the corresponding wave packet

\[
\psi_{v_0}(x,0) = \frac{1}{(2\pi \sigma_0^2)^{1/4}} \exp \left[ -\frac{(x - x_0)^2}{4\sigma_0^2} + i \frac{mv_0}{\hbar} x \right].
\]

Particles are assumed to have a Maxwell-Boltzmann distribution of initial velocities given by

\[
f_T(v_0) = \frac{m}{2\pi k_B T} \exp \left[ -\frac{mv_0^2}{2k_B T} \right],
\]

\( m \) being the mass of the particles, \( k_B \) the Boltzman constant and \( T \) the temperature.

According to Eq. (A9) of Appendix A, our mixed ensemble is described by [12]

\[
|\rho_T(0)\rangle = \int_{-\infty}^{\infty} dv_0 \ f_T(v_0) |\psi_{v_0}(0)\rangle \langle \psi_{v_0}(0)|
\]

whose time evolution is given by the von-Neumann equation of motion (A1) and expressed as

\[
\hat{\rho}_T(t) = e^{-i\hat{H}t/\hbar} \hat{\rho}_T(0) e^{i\hat{H}t/\hbar} = \int_{-\infty}^{\infty} dv_0 \ f_T(v_0) |\psi_{v_0}(t)\rangle \langle \psi_{v_0}(t)|
\]

where \( |\psi_{v_0}(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi_{v_0}(0)\rangle \), \( \hat{H} \) being the Hamiltonian of the system.

Matrix elements of the thermal density operator (1) in the coordinate representation are given by

\[
\rho_T(x,x',t) = \int_{-\infty}^{\infty} dv_0 \ f_T(v_0) \psi_{v_0}(x,t) \psi_{v_0}^*(x',t).
\]

In the following, we will separately consider propagation in the force-free field, propagation in a constant force field and in a linear force field where the propagators are known to have analytic expressions. We find that, in all cases considered, the diagonal elements of the density matrix, which are interpreted as a probability distribution, has the Gaussian form

\[
\rho_T(x,t) = \rho_T(x,x',t)|_{x'=x} = \frac{1}{\sqrt{2\pi \sigma_T(t)}} \exp \left[ -\frac{(x - X(t))^2}{2\sigma_T(t)^2} \right]
\]

where the center of the packet follows the thermal-averaged trajectory \( X(t) = \langle x_t \rangle \), \( x_t \) being the center of the wave packet \( |\psi_{v_0}(x,0)|^2 \); and its width has a temperature contribution. From (A2), we have that

\[
\langle \hat{A} \rangle_T(t) = \int_{-\infty}^{\infty} dv_0 \ f_T(v_0) \int_{-\infty}^{\infty} dx \ \psi_{v_0}^*(x,t) A(x, -i\hbar \partial / \partial x) \psi_{v_0}(x,t)
\]

for the expectation value of an observable \( \hat{A} = \hat{A}(\hat{x}, \hat{p}) \). As a special case, the expectation value of space coordinate \( \hat{x} \) is given by

\[
\langle \hat{x} \rangle_T(t) = \int_{-\infty}^{\infty} dv_0 \ f_T(v_0) \int_{-\infty}^{\infty} dx \ \psi_{v_0}^*(x,t) x \psi_{v_0}(x,t)
\]

\[
= \int_{-\infty}^{\infty} dx \ x \ \rho_T(x,t)
\]

This relation confirms the interpretation of the diagonal matrix elements of the density operator as the probability density.
A. Free particles

The propagator of the free particle, $\hat{H} = \frac{\hat{p}^2}{2m}$, is given by

$$\langle x|e^{-i\hat{H}t/\hbar}|x'\rangle = \sqrt{\frac{m}{2\pi it}} \exp\left[im\frac{x-x'}{2ht}\right]$$

(9)

and the wave function with initial velocity $v_0$ is then

$$\psi_{v_0}(x, t) = \int_{-\infty}^{\infty} dx' \langle x|e^{-i\hat{H}t/\hbar}|x'\rangle \psi_{v_0}(x', t)$$

$$= \frac{1}{(2\pi)^{1/4}} \sqrt{\frac{1}{st}} \exp\left[im\frac{x^2 + i\hbar t \sigma_0^2}{2m\sigma_0^2} - \sigma_0 \left(x - x_0 - v_0 t + \frac{s_t}{\sigma_0} x_0\right)^2\right]$$

(10)

where the complex width is

$$s_t = \sigma_0 \left(1 + i\frac{\hbar t}{2m\sigma_0^2}\right).$$

(11)

From (11), the Gaussian shape $B$ for the diagonal elements of density matrix with

$$X(t) = x_0$$

$$\sigma_T(t) = \sigma_0 \sqrt{1 + \left(\frac{\hbar^2}{4m^2\sigma_0^2} + \frac{k_B T}{m\sigma_0^2}\right) t^2}$$

(13)

is obtained.

As one clearly sees there is a temperature-dependence contribution to the width. For a given time, the width increases with temperature. Now, from Eq. (17), the first two momenta of the momentum distribution for a given temperature are

$$\langle \hat{p}\rangle_T(t) = 0$$

$$\langle \hat{p}^2\rangle_T(t) = \frac{\hbar^2}{4\sigma_0^2} + mk_B T$$

(15)

and the uncertainty is then given by

$$\Sigma_T = \sqrt{\langle \hat{p}^2\rangle_T(t) - \langle \hat{p}\rangle_T^2(t)} = \sqrt{\frac{\hbar^2}{4\sigma_0^2} + mk_B T}$$

(16)

which is time-independent but has a temperature-dependence contribution. By using (A7) or (A14), the thermal probability current density can be expressed as

$$j_T(x, t) = \left[\frac{\Sigma_T}{m \sigma_T(t)}\right]^2 (x - x_0) t \cdot \rho_T(x, t)$$

(17)

As a consistency check, the thermal Wigner distribution function which is defined by

$$W_T(x, p, t) = \frac{1}{\pi \hbar} \int_{-\infty}^{\infty} dy \langle x + y|\hat{\rho}(t)|x-y\rangle e^{i2p_y/\hbar}$$

$$= \frac{1}{\pi \hbar} \int_{-\infty}^{\infty} dv \int_{-\infty}^{\infty} dy \psi_0(x + y, t) \psi^*_0(x - y, t) e^{i2p_y/\hbar}$$

(18)

can be calculated for the free case reaching

$$W_T(x, p, t) = \frac{1}{\sqrt{\pi (\hbar^2 + 4m\sigma_0^2 k_B T)}} \exp\left[-\frac{2\sigma_0^2 p^2}{\hbar^2 + 4m\sigma_0^2 k_B T} \left(\frac{m(x - x_0) + pt}{2m^2\sigma_0^2}\right)^2\right].$$

(19)

By integrating over the spatial coordinate $x$, it leads to the momentum distribution

$$\Pi_T(p) = \frac{1}{\sqrt{2\pi \Sigma_T}} \exp\left[-\frac{p^2}{2\Sigma_T^2}\right]$$

(20)

with $\Sigma_T$ given by Eq. (16).
B. Linear potential

The propagator for the linear potential $V(x) = Kx$ is

$$\langle x | e^{-i\hat{H}t/\hbar} | x' \rangle = \sqrt{\frac{m}{2\pi i \hbar t}} \exp \left[ \frac{im}{2\hbar t} (x - x')^2 - i \frac{Kt}{\hbar} (x + x') - i \frac{K^2}{24\hbar^2} t^3 \right]$$  \hspace{1cm} (21)

From this, one obtains the Gaussian function $0$ with a width given by $13$ and the center of the thermal packet follows the trajectory

$$X(t) = x_0 - \frac{Kt^2}{2m}.$$  \hspace{1cm} (22)

Again, the first two moments of the momentum distribution are

$$\langle \hat{p} \rangle_T(t) = -Kt$$  \hspace{1cm} (23)

$$\langle \hat{p}^2 \rangle_T(t) = \frac{\hbar^2}{4\sigma_0^2} + mk_B T + K^2 t^2$$  \hspace{1cm} (24)

and, thus, the corresponding uncertainty takes again the form of Eq. 16.

C. Parabolic repeller potential

The propagator for the inverted parabolic potential $V(x) = -\frac{1}{2}m\omega^2x^2$ is

$$\langle x | e^{-i\hat{H}t/\hbar} | x' \rangle = \sqrt{\frac{m\omega}{2\pi i \sinh \omega t}} \exp \left[ \frac{im\omega}{2\hbar \sinh \omega t} ((x - x')^2 \cosh \omega t - 2xx') \right]$$  \hspace{1cm} (25)

and the center of the thermal Gaussian function $0$ ans its width are in this case

$$X(t) = x_0 \cosh(\omega t)$$  \hspace{1cm} (26)

$$\sigma_T(t) = \sigma_0 \sqrt{\cosh^2(\omega t) + \left( \frac{\hbar^2}{4\sigma_0^2} + \frac{k_B T}{m\sigma_0^2} \right) \frac{\sinh^2(\omega t)}{\omega^2}}.$$  \hspace{1cm} (27)

Again, from the first two moments of the momentum distribution

$$\langle \hat{p} \rangle_T(t) = m\omega x_0 \sinh(\omega t)$$  \hspace{1cm} (28)

$$\langle \hat{p}^2 \rangle_T(t) = \left( \frac{\hbar^2}{4\sigma_0^2} + mk_B T \right) \cosh^2(\omega t) + m^2(x_0^2 + \sigma_0^2) \omega^2 \sinh^2(\omega t)$$  \hspace{1cm} (29)

the uncertainty is written as

$$\Sigma_T(t) = \sqrt{\left( \frac{\hbar^2}{4\sigma_0^2} + mk_B T \right) \cosh^2(\omega t) + m^2 \sigma_0^2 \omega^2 \sinh^2(\omega t)}$$  \hspace{1cm} (30)

which is time-independent but temperature dependent. Finally, the thermal probability current density is

$$j_T(x, t) = \omega \sinh(\omega t) \frac{x \left( \frac{\hbar^2}{4\sigma_0^2} + mk_B T + m^2 \omega^2 \sigma_0^2 \right) \cosh(\omega t) - x_0 \left( \frac{\hbar^2}{4\sigma_0^2} + mk_B T \right)}{m^2 \sigma_0^2 \cosh^2(\omega t) + \left( \frac{\hbar^2}{4\sigma_0^2} + mk_B T \right) \sinh^2(\omega t)} \rho_T(x, t)$$  \hspace{1cm} (31)

III. DISSIPATION IN BOHMIAN MECHANICS

We are going to consider dissipation through two different approaches, the linear Schrödinger equation coming from the so-called Caldirola-Kanai (CK) Hamiltonian $23, 24$ and the nonlinear, logarithmic Schrödinger-Langevin (or Kostin) equation $20, 25$, both of them without noise. These equations have been used in our previous works $17, 18$. 
A. Wave equation in the CK and Kostin approaches

In our context, the Schrödinger equation within the CK approach reads as

\[
\frac{i\hbar}{\partial t} \psi_{\nu_0,\gamma}(x,t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + e^{\gamma t} V(x) \right] \psi_{\nu_0,\gamma}(x,t), \tag{32}
\]

being \( \gamma \) the friction. For the quadratic potential

\[
V(x) = Kx - \frac{1}{2} m \omega^2 x^2,
\tag{33}
\]

writing the wave function in polar form and assuming a Gaussian ansatz for the probability density

\[
|\psi_{\nu_0,\gamma}(x,t)|^2 = \frac{1}{\sqrt{2\pi}\sigma_\gamma(t)} \exp \left[ -\frac{(x - x_\gamma(t))^2}{2\sigma_\gamma(t)^2} \right],
\tag{34}
\]

the center of the wave packet and its width are expressed as

\[
x_\gamma(t) = -\frac{K}{m\omega^2} + \left( x_0 + \frac{K}{m\omega^2} \right) \left[ \cosh \Omega t + \frac{\gamma}{2} \frac{\sinh \Omega t}{\Omega} \right] e^{-\gamma t/2} + v_0 \frac{\sinh \Omega t}{\Omega} e^{-\gamma t/2}, \tag{35}
\]

\[
\sigma_\gamma(t) = \sigma_0 e^{-\gamma t/2} \sqrt{\left( \cosh \Omega t + \frac{\gamma}{2} \frac{\sinh \Omega t}{\Omega} \right)^2 + \frac{\hbar^2}{4m^2\sigma_0^2} \frac{\sinh^2 \Omega t}{\Omega^2}}, \tag{36}
\]

where the frequency \( \Omega \) is defined by

\[
\Omega = \sqrt{\omega^2 + \gamma^2/4}. \tag{37}
\]

On the other hand, the so-called Schrödinger-Langevin or Kostin nonlinear (logarithmic) equation for the Ohmic case is written as

\[
\frac{i\hbar}{\partial t} \psi_{\nu_0,\gamma}(x,t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + \frac{\hbar}{2i} \left( \ln \frac{\psi_{\nu_0,\gamma}}{\psi_{\nu_0,\gamma}^*} \cdot \left( \ln \frac{\psi_{\nu_0,\gamma}}{\psi_{\nu_0,\gamma}^*} \right) \right) \right] \psi_{\nu_0,\gamma}(x,t), \tag{38}
\]

and following the same procedure as before, \( x_\gamma(t) \) has the same expression given by Eq. (35) while the width is the solution of the generalized Pinney equation \([20, 26]\)

\[
\ddot{\sigma}_\gamma(t) + \gamma \dot{\sigma}_\gamma(t) - \frac{\hbar^2}{4m^2\sigma_\gamma(t)^3} - \omega^2 \sigma_\gamma(t) = 0 \tag{39}
\]

which has no analytical solution.

Thus, the discrepancy between both approaches relies on the behavior of the width of the thermal distribution. As discussed previously \([18]\), when the interaction with an environment is considered, linear quantum mechanics is no longer applicable. This linear CK approach is seen more like an effective approach to dissipation. The Kostin approach comes from the standard Langevin equation which is also issued from the Caldeira-Leggett Hamiltonian.

B. Effect of dissipation on the width of the thermal Gaussian wave packet

As we have already mentioned, the diagonal elements of the density operator have the interpretation of probability distribution. In a dissipative medium, the time evolution of the state \([34]\) yields to

\[
\rho_{\gamma,T}(x,t) = \langle x | \rho_{\gamma,T}(t) | x \rangle = \frac{1}{\sqrt{2\pi} \sigma_{\gamma,T}(t)} \exp \left[ -\frac{(x - X_{\gamma}(t))^2}{2\sigma_{\gamma,T}(t)^2} \right], \tag{40}
\]

for the thermal probability density, where

\[
X_{\gamma}(t) = -\frac{K}{m\omega^2} + \left( x_0 + \frac{K}{m\omega^2} \right) \left[ \cosh \Omega t + \frac{\gamma}{2} \frac{\sinh \Omega t}{\Omega} \right] e^{-\gamma t/2} \tag{41}
\]

\[
\sigma_{\gamma,T}(t) = \sqrt{\sigma_{\gamma}(t)^2 + e^{-\gamma t} \frac{\kappa B T}{m\Omega^2} \sinh^2(\Omega t)} \tag{42}
\]
It is clear from the previous equations that the temperature-dependence of the wave packet is independent of the approach we use for taking into account the dissipation. For the free case, $\Omega = \gamma/2$ and the explicit form of the variance of the thermal wave packet in the CK framework reads as

$$\sigma^2_x(t) = \sigma^2_0 + \frac{\hbar^2}{4m^2\sigma^2_0\gamma^2} (1 - e^{-\gamma t})^2 + e^{-\gamma t} \frac{4k_B T}{m^2\gamma^2} \sinh^2 \left( \frac{\gamma t}{2} \right). \quad (43)$$

In the study of decoherence, Ford and O’Connell [13] obtained

$$w^2(t) = \sigma^2_0 - \frac{[\hat{x}(0), \hat{x}(t)]^2}{4\sigma^2_0} + (\langle \dot{x}(t) \rangle) \quad (44)$$

for the variance of the the probability distribution at time $t$, taking the initial state as a Gaussian wave packet. The last term which is the mean square displacement is temperature-dependent, while the second term is not. One has that $[\hat{x}(0), \hat{x}(t)] = i\hbar(1 - e^{-\gamma t})/m\gamma$ and $\langle (\dot{x}(t) - \dot{x}(0))^2 \rangle = \frac{2k_B T}{m\gamma} \left(t - \frac{1 - e^{-\gamma t}}{\gamma} \right)$ for high temperatures, $k_B T \gg \hbar\gamma$. Apart from different physical contexts, the comparison of Eqs. (43) and (44) shows that the first two terms of them are exactly the same.

IV. TRANSMISSION THROUGH A PARABOLIC REPELLER

A. Thermal transmission probability with dissipation

Now consider transmission of our ensemble of particles through the parabolic repeller $V(x) = -\frac{1}{2}m\omega^2x^2$. The transmission probability for each element of our ensemble $\psi_{v_0,\gamma}(x,t)$ is given by [27–29]

$$P_{\text{tr}}(t; v_0, \gamma) = \frac{\text{erf}(x_\gamma(t)/\sqrt{2}\sigma_\gamma(t)) - \text{erf}(x_0/\sqrt{2}\sigma_0)}{\text{erfc}(x_0/\sqrt{2}\sigma_0)} \quad (45)$$

where $x_\gamma(t)$ is given by Eq. 55 with $K = 0$ and $\sigma_\gamma(t)$ by Eq. 30 in the CK framework or by the solution of the generalized Pinney equation (39) in the Kostin one. It should be noted that in a transmission process, the incoming wave packet is initially well-localized on the left, $x_0 < 0$, of the barrier. In such a case, $\sigma_0 \ll |x_0|$, one has

$$\text{erf}(x_0/\sqrt{2}\sigma_0) \approx -1, \quad \text{erfc}(x_0/\sqrt{2}\sigma_0) \approx 2$$

from which Eq. (45) can be rewritten as

$$P_{\text{tr}}(t; v_0, \gamma) \approx \frac{1}{2} \text{erfc} \left( - \frac{x_\gamma(t)}{\sqrt{2}\sigma_\gamma(t)} \right). \quad (46)$$

Now, due to the Maxwell-Boltzmann distribution function [2] for the initial velocities, the time dependent thermal transmission probability under the presence of dissipation is given by

$$P_{\text{tr}}(t; \gamma, T) = \int_{-\infty}^{\infty} dv_0 \ f_T(v_0) \ P_{\text{tr}}(t; v_0, \gamma) \quad (47)$$

and from the integral representation of the complementary error function [50]

$$\text{erfc}(z) = \frac{2}{\sqrt{\pi}} e^{-z^2} \int_{0}^{\infty} dy \ e^{-(y^2 + 2zy)}, \quad (48)$$

one can express the corresponding transmission probability as

$$P_{\text{tr}}(t; \gamma, T) = \frac{1}{\pi} \sqrt{\frac{m}{2k_B T}} \int_{0}^{\infty} dy \ e^{-y^2} \int_{-\infty}^{\infty} dv_0 \ \exp \left[ - \frac{mv_0^2}{2k_B T} - \frac{x_\gamma(t)^2}{2\sigma_\gamma(t)} + \sqrt{2} \frac{x_\gamma(t)}{\sigma_\gamma(t)} y \right]$$

$$= \frac{1}{2} \text{erfc} \left( - \frac{X_\gamma(t)}{\sqrt{2}\sigma_\gamma(t)} \right) \quad (49)$$
where \( X_\gamma(t) \) is given by Eq. (41) with \( K = 0 \) and \( \sigma_{\gamma,T}(t) \) by Eq. (42).

An alternative way to compute the thermal transmission probability is to make use of \( \rho_T(x, t) \). Thus, the thermal transmission probability should be given now by

\[
P_{tr}(t; \gamma, T) = \int_0^\infty dx \, \rho_{\gamma,T}(x, t) = \frac{1}{2} \text{erfc} \left( -\frac{X_\gamma(t)}{\sqrt{2} \sigma_{\gamma,T}(t)} \right)
\]

as should be. The stationary value of the thermal transmission probability is reached when

\[
P_{tr}(\gamma, T) = \left. P_{tr}(t; \gamma, T) \right|_{t \to \infty}
\]

which in the CK approach reduces to

\[
P_{tr}(\gamma, T)_{\text{CK}} = \frac{1}{2} \text{erfc} \left( \frac{-x_0(1 + \frac{\gamma}{2\Omega})}{\sqrt{2} \sigma_0 \sqrt{(1 + \frac{\gamma^2}{2\Omega})^2 + \frac{\hbar^2}{4m^2\sigma_0^2\Omega^2} + \frac{k_B T}{m\sigma_0^2\Omega^2}}} \right)
\]

B. Thermal characteristic times with dissipation

In the context of Bohmian mechanics, the complete description of a system is given by its wave function and its position in configuration space. As usual, the evolution of the wave function is given by the Schrödinger equation but particle trajectories are specified through the so-called guidance equation

\[
\frac{dx}{dt} = \frac{\hbar}{m} \text{Im} \left\{ \frac{\partial_x \psi(x, t)}{\psi(x, t)} \right\} \bigg|_{x=x(t)}
\]

where \( \partial_x = \partial/\partial x \) and \( x(t) \) is the Bohmian or quantum trajectory. To be clear, in the following, Bohmian trajectories will be labelled by \( x(x^{(0)}, t; v_0, \gamma) \) when considering a Gaussian ansatz where the center of the corresponding wave packet moves with the initial velocity \( v_0 \) in a viscous medium with friction \( \gamma \) and \( x^{(0)} \) is the initial position of the Bohmian particle. The general expression for this Bohmian trajectory assuming the Gaussian ansatz and for potentials up to second order is written as \[20\]

\[
x(x^{(0)}, t; v_0, \gamma) = x_\gamma(t) + (x^{(0)} - x_0) \frac{\sigma_\gamma(t)}{\sigma_\gamma(0)}
\]

1. Arrival times

In this context, it was proved by Leavens \[16\] from the non-crossing property of Bohmian trajectories that the arrival time distribution for those particles that actually reach the detector is proportional to the modulus of the probability current density. For \( \psi_{v_0,\gamma}(x, t) \), the arrival time distribution at the detector location \( x_d \) is given by

\[
\Pi_A(x_d, t; v_0, \gamma) = \left| \frac{j_{v_0,\gamma}(x_d, t)}{\int_0^\infty dt' |j_{v_0,\gamma}(x_d, t')|} \right|
\]

and therefore for a pure ensemble described by the wave function \( \psi_{v_0,\gamma}(x, t) \), the mean arrival time at the detector location can be written as

\[
\tau_A(x_d; v_0, \gamma) = \int_0^\infty dt' \, \tau_A(x_d, t; v_0, \gamma).
\]

By averaging now over the Maxwell-Boltzmann distribution, one can calculate thermal mean arrival times when the system is described by Eq. \[5\] as

\[
\tau_A(x_d; \gamma, T) = \int dv_0 \, f_T(v_0) \, \tau_A(x_d; v_0, \gamma)
\]

\[
= \int_0^\infty dt' \, \int dv_0 \, f_T(v_0) \, \Pi_A(x_d, t'; v_0, \gamma)
\]
from which one obtains

\[
\Pi_A(x_d, t; \gamma, T) = \int_0^\infty dt \int_0^\infty dv f_T(v_0) \Pi_A(x_d, t; v_0, \gamma) \Pi_A(x_d, t'; v_0, \gamma).
\]  

(59)

for the thermal arrival time distribution with dissipation.

2. Thermal dwelling, transmission and reflection times

In the Bohm trajectory context, characteristic times are also important issues [13]. Here, we would like to generalize this discussion when dealing with a mixed ensemble which is described by the the density matrix, Eq. [1]. The time that a particle, with initial position \(x(0)\), spends in a given space interval \([x_1, x_2]\) can be expressed as

\[
t(x_1, x_2; x(0), v_0, \gamma) = \int_0^\infty dt \theta(x(x(0), t; v_0, \gamma) - x_1) \theta(x_2 - x(x(0), t; v_0, \gamma))
\]  

(60)

\[
= \int_0^\infty dt \int_{x_1}^{x_2} dx \delta(x(x(0), t; v_0, \gamma) - x)
\]  

(61)

where the \(\theta(x)\) is the step function. Then, the mean dwelling time is readily calculated as

\[
\tau_D(x_1, x_2; v_0, \gamma) = \int_{-\infty}^{\infty} dx [\psi_{v_0, \gamma}(x, 0)]^2 t(x_1, x_2; x(0), v_0, \gamma) = \int_0^\infty dt \int_{x_1}^{x_2} dx |\psi_{v_0, \gamma}(x, t)|^2,
\]  

(62)

where, in the second equality, we have used the fact that \(|\psi_{v_0, \gamma}(x, t)|^2 = \int dx \psi_{v_0, \gamma}(x, t)|^2 \delta(x(x(0), t; v_0, \gamma) - x)\). For a one-dimensional motion, due to the non-crossing property of Bohmian trajectories, there is always a critical trajectory \(x_c(t; v_0, \gamma)\) which separates transmitted from reflected trajectories in a scattering problem [31]. Thus, for the stationary transmission probability one can always write

\[
P_{tr}(v_0, \gamma) = \int_{x_c(t; v_0, \gamma)}^\infty dx |\psi_{v_0, \gamma}(x, t)|^2.
\]  

(63)

By introducing now

\[1 = \theta(x - x_c(t; v_0, \gamma)) + \theta(x_c(t; v_0, \gamma) - x)\]

(64)

in Eq. (62), the dwelling time can be split as

\[
\tau_D(x_1, x_2; v_0, \gamma) = P_{tr}(v_0, \gamma) \tau_{tr}(x_1, x_2; v_0, \gamma) + P_{ref}(v_0, \gamma) \tau_{ref}(x_1, x_2; v_0, \gamma)
\]  

(65)

where the transmission and reflection times are defined respectively as follows

\[
\tau_{tr}(x_1, x_2; v_0, \gamma) = \frac{1}{P_{tr}(v_0, \gamma)} \int_0^\infty dt \int_{x_1}^{x_2} dx |\psi_{v_0, \gamma}(x, t)|^2 \theta(x - x_c(t; v_0, \gamma))
\]  

(66)

\[
\tau_{ref}(x_1, x_2; v_0, \gamma) = \frac{1}{P_{ref}(v_0, \gamma)} \int_0^\infty dt \int_{x_1}^{x_2} dx |\psi_{v_0, \gamma}(x, t)|^2 \theta(x_c(t; v_0, \gamma) - x)
\]  

(67)

in terms of the reflection and transmission probabilities with \(P_{ref}(v_0, \gamma) = 1 - P_{tr}(v_0, \gamma)\). These relations show that the calculation of characteristic times within the Bohmian mechanics just requires the knowledge of the critical trajectory \(x_c(t; v_0, \gamma)\). However, it has been proved that there is no need to compute this single trajectory. One can always write

\[
\tau_D(x_1, x_2; v_0, \gamma) = \int_0^\infty dt [Q(x_1, t; v_0, \gamma) - Q(x_2, t; v_0, \gamma)]
\]  

(68)

\[
\tau_{tr}(x_1, x_2; v_0, \gamma) = \frac{1}{P_{tr}(v_0, \gamma)} \int_0^\infty dt \left[ \min(Q(x_1, t; v_0, \gamma), P_{tr}(v_0, \gamma)) - \min(Q(x_2, t; v_0, \gamma), P_{tr}(v_0, \gamma)) \right]
\]  

(69)

\[
\tau_{ref}(x_1, x_2; v_0, \gamma) = \frac{1}{P_{ref}(v_0, \gamma)} \int_0^\infty dt \left[ \max(Q(x_1, t; v_0, \gamma), P_{tr}(v_0, \gamma)) - \max(Q(x_2, t; v_0, \gamma), P_{tr}(v_0, \gamma)) \right]
\]  

(70)
where
\[ Q(x, t; v_0, \gamma) = \int_x^\infty dx' |\psi_{v_0, \gamma}(x', t)|^2 = \int_0^t dt' j_{v_0, \gamma}(x, t') \quad (71) \]
\[ = \frac{1}{2} \text{erfc} \left( \frac{x - x_\gamma(t)}{\sqrt{2} \sigma_\gamma(t)} \right) \quad (72) \]
is the probability of being the particle beyond the point \( x \). For a mixed ensemble of non-interacting particles, which is initially described by the density operator \( \mathbf{1} \), the thermal averaging of Eq. (62) over the Maxwell-Boltzmann distribution yields
\[ \tau_D(x_1, x_2; \gamma, T) = \int_0^\infty dt P_{\gamma, T}(x_1, x_2, t) \quad (73) \]
where
\[ P_{\gamma, T}(x_1, x_2, t) = \int_{x_1}^{x_2} dx \rho_{\gamma, T}(x_1, x_2, t) \quad (74) \]
gives the probability for being the particle in the space interval \([x_1, x_2]\) at time \( t \) and at the temperature \( T \).

By averaging Eq. (63), one has that
\[ \tau_D(x_1, x_2; \gamma, T) = \int_0^\infty dt \left[ Q_{\gamma, T}(x_1, t) - Q_{\gamma, T}(x_2, t) \right] \quad (75) \]
an alternative expression for the dwelling time with
\[ Q_{\gamma, T}(x, t) = \int_{-\infty}^{\infty} dv_0 f_T(v_0) Q(x, t; v_0, \gamma) \quad (76) \]
Again, by using Eq. (48) for the integral representation of the complementary error function, Eq. (76) can be rewritten as
\[ Q_{\gamma, T}(x, t) = \frac{1}{2} \text{erfc} \left( \frac{x - x_0 \cosh(\omega t)}{\sqrt{2} \sigma_{\gamma, T}(t)} \right) \quad (77) \]
One can easily check that the long-time limit of \( Q_{\gamma, T}(x, t) \) for a given \( x \) is just the stationary value for the thermal transmission probability \( 51 \).

The thermal transmission and reflection times in presence of dissipation are respectively given by
\[ \begin{align*}
\tau_{\text{tr}}(x_1, x_2; \gamma, T) &= \int dv_0 f_T(v_0) \tau_{\text{tr}}(x_1, x_2; v_0, \gamma) \quad (78) \\
\tau_{\text{ref}}(x_1, x_2; \gamma, T) &= \int dv_0 f_T(v_0) \tau_{\text{ref}}(x_1, x_2; v_0, \gamma). \quad (79)
\end{align*} \]
It should be noted that at zero temperature, the Maxwell-Boltzmann distribution is just the Dirac delta function centered at \( v_0 = 0 \),
\[ f_T(v_0) \bigg|_{T=0} = \delta(v_0) \quad (80) \]
meaning that instead of a mixed ensemble we have a pure ensemble where all elements of the ensemble are described by the same wave function \( \psi_{v_0=0, \gamma}(x, t) \). In this case, thermal quantities are equivalent to those obtained for the pure ensemble with \( v_0 = 0 \).

V. RESULTS AND DISCUSSION

In order to simplify our calculations, we are going to work on dimensionless quantities. Thus, we use the following reference values: \( \hat{t} = \frac{2m\sigma_0^2}{\hbar}, \hat{\omega} = \frac{1}{\hat{t}} \) and \( \hat{T} = \frac{\hbar^2}{4m\sigma_0^2k_B} \) for times, frequencies and temperatures, respectively. Then,
we have that \( \tilde{\gamma} = \frac{\gamma}{\tilde{\omega}} \), \( \tilde{\Omega} = \frac{\Omega}{\tilde{\omega}} \), \( \tilde{T} = \frac{T}{\tilde{\omega}} \). Moreover, lengths are also dimensionless when dividing by \( \sigma_0 \) and denoted by a bar symbol. In this way, Eq. (52) for the stationary transmission probability for the CK approach takes the simple form

\[
P_{tr}(\tilde{\gamma}, \tilde{T}) = \frac{1}{2} \text{erfc} \left( \frac{-\tilde{x}_0 \left( 1 + \frac{\tilde{\gamma}}{2\tilde{\Omega}} \right)}{\sqrt{2} \left( 1 + \frac{\tilde{\gamma}}{2\tilde{\Omega}} \right)^2 + \frac{1 + \tilde{T}}{\tilde{\Omega}^2}} \right)
\]  

where \( \tilde{x}_0 = x_0/\sigma_0 \). After the behavior of the complementary error function, Eq. (81) shows that the thermal transmission probability increases with temperature for a given friction \( \gamma \) and barrier’s strength \( \omega \) and finally takes a stationary value of 0.5. By taking the partial derivative of the argument of the complementary error function with respect to the barrier’s strength and friction and noting the negative value of \( x_0 \), it is seen that the argument is an increasing function of \( \omega \) (for a given temperature and friction) and also of \( \gamma \) (for a given temperature and barrier’s strength). Thus, the transmission probability also decreases with both \( \omega \) and \( \gamma \). These results are understandable because when one increases \( \omega \), the parabolic barrier becomes more repulsive; whereas, when the friction increases, the interaction between particles and the environment also increases leading to more energy dissipation.

For numerical calculations, we use the mass of electron and the width of the initial wave packet to be \( \sigma_0 = 0.4 \, \text{Å} \). Other parameters chosen are: \( \tilde{x}_0 = -20 \) for the center of the wave packet, \( \omega = 0.05 \) and \( \omega = 0.1 \) for the strengths of the barrier, and \( \tilde{x}_d = 20 \) for the detector location when computing the arrival times. For computing the thermal characteristic times, the interval \([\tilde{x}_1 = -1, \tilde{x}_2 = 1]\) is chosen. To obtain thermal quantities one should integrate over all initial velocities with the Maxwell-Boltzmann distribution for a given temperature. In principle, any velocity should be included, even large negative values. However, due to the decomposition of the dwelling time into transmission and reflection times, Eq. (65), this makes sense only when the transmission probability is not negligible. Thus, from a numerical point of view, the lower limit in the integration equals to a velocity for which this transmission probability is greater than or equal to 0.01. For the frictionless case, this requirement leads to \( \tilde{v}_{0,\min} \approx -1.304 \) for \( \omega = 0.05 \) and \( \tilde{v}_{0,\min} \approx -0.3111 \) for \( \omega = 0.1 \), where \( \tilde{v}_0 = \frac{v_0}{\tilde{v}_0} \) with \( \tilde{v}_0 = \frac{\sigma_0}{\tilde{T}} \) is the dimensionless velocity.

In Figure 1 arrival time distributions for \( \omega = 0.05 \) (left top panel) and \( \omega = 0.1 \) (left bottom panel) with \( \gamma = 0 \)
and different values of temperature: $\bar{T} = 0$ (black curve), $\bar{T} = 1$ (red curve) and $\bar{T} = 5$ (green curve) are plotted. In the right panel of the same figure, it is also displayed mean arrival times at the detector location as a function of the temperature for the two values of $\bar{\omega}$. The maximum of the arrival time distribution moves to shorter times as temperature increases. For a given temperature, this distribution becomes narrower with $\bar{\omega}$. As an expected result, the mean arrival time decreases with temperature and the strength of the barrier in this frictionless case.

For comparison, the transmission probability (top row), dwelling time (middle row) and transmission time (bottom row) versus friction for $\bar{\omega} = 0.05$ (left column) and $\bar{\omega} = 0.1$ (right column) at zero temperature in the CK (black curves) and Kostin (red curves) approaches are displayed in Figure 2. The discrepancies between both approaches are rather important although the global behavior is the same. As commented above, the Kostin values are more reliable than the CK ones. As is known, the transmission probability decreases with friction. With $v_0 = 0$, the only contribution to the kinetic energy comes from the initial width of the Gaussian wave packet which is $\hbar^2/8m\sigma_0^2$. For the values chosen for $\bar{\omega}$, the expectation value of total energy is initially negative. Thus, the dissipative dynamics develops only via tunnelling. Notice that this value is also important because the transmission probabilities are one order of magnitude higher for $\bar{\omega} = 0.05$. The dwelling time also changes dramatically with the strength of the barrier, whereas the transmission time is smoother for both frequencies and of the same order. In Figure 3 the probability of being the particle in the interval $[\bar{x}_1, \bar{x}_2]$ versus time is shown for four different frictions $\bar{\gamma} = 0$ (black curves), $\bar{\gamma} = 0.025$ (red curves), $\bar{\gamma} = 0.04$ (magenta curves) and $\bar{\gamma} = 0.1$ (green curves) at zero temperature in the CK (left column) and Kostin (right column) approach and two parabolic barriers with frequencies $\bar{\omega} = 0.05$ (top row) and $\bar{\omega} = 0.1$ (bottom row). As this figure shows, for a given $\gamma$, probability increases with time, gets its maximum value in a time which depends on $\gamma$ and decreases afterwards. This dynamics describes the entrance of the Gaussian wave packet inside the interval $[\bar{x}_1, \bar{x}_2]$ and then its leakage from this interval during the time. For $\bar{\omega} = 0.1$ (bottom panels) curves with higher values of friction locate inside the curve for the frictionless one. Thus, the surface under the curves decreases with friction meaning dwelling time decreases with friction as the right middle panel of Figure 2 shows. But, this is not true for $\bar{\omega} = 0.05$. In this case, dwelling time increases with friction at first, reaches its maximum value at $\bar{\gamma} \approx 0.025$ for CK and $\bar{\gamma} \approx 0.04$ for Kostin.

Finally, in Figure 4, the thermal dwelling (left column) and transmission (right column) times versus temperature are plotted for three different frequencies $\bar{\omega}$ and two different frictions $\bar{\gamma}$ for the Kostin approach. This dissipative dynamics develops not only via tunnelling. As again expected, both dwelling and transmission times decrease smoothly.
FIG. 3: (Color online) Probability of being the particle in the interval \([\bar{x}_1, \bar{x}_2]\) versus time for three different frictions \(\bar{\gamma} = 0\) (black curves), \(\bar{\gamma} = 0.025\) (red curves), \(\bar{\gamma} = 0.04\) (magenta curves) and \(\bar{\gamma} = 0.1\) (green curves) at zero temperature in the CK (left column) and Kostin (right column) approach and two parabolic barriers \(\bar{\omega} = 0.05\) (top row) and \(\bar{\omega} = 0.1\) (bottom row).

with \(\bar{\omega}\) and temperature but increase with friction. The special case is for the bottom left panel where the thermal dwelling time displays a maximum at low temperatures for a friction of 0.1; that is, the dwelling time is favoured at low temperatures. At these temperatures, the small velocities in both directions maintain the particle inside the barrier more time.

In conclusion, along this work, we have presented and discussed thermal characteristic times for the dissipative dynamics under the presence of a parabolic repeller in terms of Bohmian trajectories. These thermal times as well as transmission probabilities have been defined and analyzed for several values of the frequency of the parabolic barrier and the CK and Kostin approaches within a linear and nonlinear framework, respectively. The thermal average in this work has been considered in a different way to that employed in the study of time-of-flight distributions for cold trapped atoms [19] which for the probability current distribution is defined as

\[
j_{\gamma,T}(x,t) = \int dv_0 f_T(v_0) j_{v_0,\gamma}(x,t)
\]

which is less convenient for a trajectory description. Similar results to previous works have been obtained. This work can be seen as the first step to deal with quantum stochastic dynamics within the Bohmian mechanics where the noise (thermal fluctuations) of the environment is present. Work in this direction is now in progress.

Appendix A: The continuity equation for a mixed ensemble

In the most general formulation of quantum systems, a quantum system is described by a density matrix \(\hat{\rho}\) instead of a state vector \(|\psi\rangle\). In this context, the von Neumann equation

\[
i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]
\]

has to be applied for the evolution of the system, where \(\hat{H}\) is the Hamiltonian of the system.
FIG. 4: (Color online) Thermal dwelling time (left column) and transmission time (right column) versus temperature for different values of parabolic repeller strength: $\bar{\omega} = 0.01$ (black curves), $\bar{\omega} = 0.0125$ (red curves) and $\bar{\omega} = 0.015$ (green curves) and for $\tilde{\gamma} = 0$ (top row) and $\tilde{\gamma} = 0.1$ (bottom row) in the Kostin model.

The expectation value of an observable $\hat{A}$ is computed as follows

$$\langle \hat{A}(t) \rangle = \text{Tr}(\hat{A}\hat{\rho}(t))$$  \hspace{1cm} (A2)$$

where Tr means the trace operation. In one dimension, the coordinate representation of Eq. (A1) can be recast as

$$i\hbar \frac{\partial \rho(x,x',t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \rho}{\partial x^2} - \frac{\partial^2 \rho}{\partial x'^2} \right) + V(x,t) - V(x',t) \right] \rho(x,x',t)$$  \hspace{1cm} (A3)$$

with $\rho(x,x',t) = \langle x|\hat{\rho}|x' \rangle$ and $V$ is the interaction potential. From [32], the current density matrix is

$$j(x,x',t) = \frac{\hbar}{m} \frac{1}{2i} \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right) \rho(x,x',t)$$  \hspace{1cm} (A4)$$

and the equation of motion [A3] can be expressed in the coordinate representation as

$$\frac{\partial \rho(x,x',t)}{\partial t} + \frac{\partial j(x,x',t)}{\partial x} + \frac{\partial j(x,x',t)}{\partial x'} + \frac{i}{\hbar} (V(x,t) - V(x',t))\rho(x,x',t) = 0.$$  \hspace{1cm} (A5)$$

One notes that

$$\frac{\partial j}{\partial x} + \frac{\partial j}{\partial x'} = \frac{\hbar}{m} \frac{1}{2i} \left( \frac{\partial^2 \rho}{\partial x'^2} - \frac{\partial^2 \rho}{\partial x^2} \right) = \frac{\hbar}{m} \frac{1}{2i} \left( \frac{\partial^2 \rho}{\partial x^2} - \frac{\partial^2 \rho^*}{\partial x'^2} \right) \bigg|_{x'=x}$$

where in the second equality we have used the fact that $\rho(x,x',t) = \rho^*(x',x,t)$. Thus, for $x' = x$ we have that

$$\left( \frac{\partial j}{\partial x} + \frac{\partial j}{\partial x'} \right) \bigg|_{x'=x} = \frac{\partial}{\partial x} \text{Im} \left[ \frac{\hbar}{m} \frac{\partial \rho}{\partial x} \bigg|_{x'=x} \right]$$

Now, from (A5) for $x' = x$, we have that

$$\frac{\partial \rho(x,x',t)}{\partial t} \bigg|_{x'=x} + \frac{\partial}{\partial x} \text{Im} \left[ \frac{\hbar}{m} \frac{\partial \rho}{\partial x} \bigg|_{x'=x} \right] = 0.$$
with
\[ \rho(x, t) = \rho(x', t) \bigg|_{x' = x} \]  
\[ j(x, t) = j(x', t) \bigg|_{x' = x} \]  
being the probability density function and probability current density, respectively. In the more familiar form, we have the continuity equation
\[ \frac{\partial \rho(x, t)}{\partial t} + \frac{\partial j(x, t)}{\partial x} = 0 \]  
(A8)

In a statistical mixture of states, the density operator is initially given by
\[ \hat{\rho}(0) = \sum_i w_i |\psi_i(0)\rangle \langle \psi_i(0)|, \quad \sum_i w_i = 1. \]  
(A9)

where the coefficient \( w_i \) gives the weight of the \( |\psi_i(0)\rangle \) state. By using the evolution equation (A1), the density matrix at time \( t \) is then written as
\[ \hat{\rho}(t) = \sum_i w_i |\psi_i(t)\rangle \langle \psi_i(t)|, \]  
(A10)

where \( |\psi_i(t)\rangle = e^{-i\hat{H}/\hbar}|\psi_i(0)\rangle \). Now, due to the continuity equation for the component \( \psi_i(x, t) \)
\[ \frac{\partial}{\partial t} |\psi_i(x, t)|^2 + \frac{\partial}{\partial x} \left( \frac{\hbar}{m} \text{Im} \left[ \psi_i^*(x, t) \frac{\partial}{\partial x} \psi_i(x, t) \right] \right) = 0, \]  
(A11)
oned, one has that
\[ \frac{\partial}{\partial t} \sum_i w_i |\psi_i(x, t)|^2 + \frac{\partial}{\partial x} \left( \frac{\hbar}{m} \text{Im} \left[ \sum_i w_i \psi_i^*(x, t) \frac{\partial}{\partial x} \psi_i(x, t) \right] \right) = 0. \]  
(A12)

with
\[ \rho(x, t) = \sum_i w_i |\psi_i(x, t)|^2 \]  
(A13)

and
\[ j(x, t) = \frac{\hbar}{m} \sum_i w_i \text{Im} \left[ \psi_i^*(x, t) \frac{\partial}{\partial x} \psi_i(x, t) \right], \]  
(A14)

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