Quantum tunneling with dissipation in smoothly joined parabolic potentials

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Abstract. This paper is devoted to the study of quantum dissipation in cluster decay phenomena in the frame of the Lindblad approach to quantum open systems. The tunneling of a metastable state across a piecewise quadratic potential is envisaged for two cases: one and two harmonic wells smoothly joined to an inverted parabola which simulates the barrier. The width and depth of the second harmonic oscillator well was varied over a wide range of values in order to encompass particular cases of tunneling such as the double well potential and the cluster decay. The evolution of the averages and covariances of the quantum sub-system is studied in both under- and overdamped regimes. For a gaussian initial wave-packet we compute the tunneling probability for different values of the friction coefficient and fixed values of the diffusion coefficients. The ansatz used for these coefficients corresponds to the case with temperature $T = 0$ as happens in the cold fission and cluster decay phenomena.

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1. Introduction

The question of how collective energy is dissipated in various decaying phenomena occurring in solid-state and nuclear physics is a topic of major interest. A particular case is represented by the decay of a metastable state through quantum tunneling at very small or zero temperatures. Such cold decay phenomena are well known at the microscopic level for nuclei undergoing cold fission or emission of heavy clusters [1, 2] but also for macroscopic systems like Josephson junctions [3] or SQUID’s [4].

Twenty years ago Caldeira and Legget proposed a model of tunneling of a metastable quantum state at $T = 0$ based on the Feynman path integral technique [5]. Assuming a linear dependence on the tunneling coordinate $q$ for the friction term entering the Lagrangian, they showed that the dissipation decreases the tunneling probability. Since that time a new formalism for studying quantum dissipative systems emerged. In this approach the system is opened, i.e. it is regarded as a subsystem
interacting with a larger system, referred to as the reservoir or the bath \[3\]. The dissipation arises as a consequence of this interaction.

The Lindblad’s axiomatic way \[4\] of introducing dissipation in quantum mechanics consists in replacing the one-parameter group action

\[
U_t(\rho) = \exp \left( -\frac{i}{\hbar}Ht \right) \rho(t) \exp \left( \frac{i}{\hbar}Ht \right),
\]

of a closed physical system with Hamiltonian \(H\), by a new one, \(\Phi_t(\rho)\) which describes the evolution of the corresponding open subsystem. Like \(U_t\), this operator should satisfy the conditions of self-adjointness \((\Phi_t^*(\rho) = \Phi_t(\rho))\), positivity \((\Phi_t(\rho) > 0)\) and unitary trace \((\text{Tr}(\Phi_t(\rho)) = 1)\). Moreover \(\Phi_t(\rho) \to \rho\) when \(t \to 0\).

Using the above mentioned approach the quantum mechanics of one and two coupled harmonic oscillators has been extensively studied \[8, 9, 10\]. Based on these results, very recently, the tunneling probability with dissipation was computed exactly for the inverted parabolic potential and approximately for the cubic one \[11, 12\]. It was found that there might be cases when friction favours the penetration. However the inverted parabola is not a good candidate to describe a real tunneling process because no metastable state could be conceived in it. The cubic potential is more likely to describe the decay of a metastable state but in this case the authors faced the problem of dealing with a system of equations in averages and higher momenta which is not closed. Therefore all cubic and higher momenta have been dropped off providing thus an approximate solution.

In this paper we consider that the quantum decay process, characterized by the coordinate \(q\) is modelled by the tunneling of a one-dimensional potential barrier whose explicite form is given by joining first two parabolic segments as in the Kramers problem \[13\], and next we add a third parabolic well beyond the barrier. The description of tunneling phenomena accompanied by dissipation in Josephson junctions \[14\] or fission of heavy compound nuclei \[15\] offenly employs such barriers. Besides computing the averages and covariances of the decay coordinates we are mainly interested to investigate the dependence of the tunneling probability on the friction.

2. Lindblad approach to open one-dimensional quantum systems

According to the original paper of Lindblad \[7\] the time evolution of an observable \(A(q,p)\) belonging to a system undergoing a non-equilibrium process is written in the Heisenberg picture as follows

\[
\frac{dA}{dt} = \frac{i}{\hbar}[H,A] + \frac{i\lambda}{2\hbar} (q[A,p] + [A,p]q - [A,q]p - p[A,q])
- \frac{D_{qq}}{\hbar^2} [p, [p, A]] - \frac{D_{pp}}{\hbar^2} [q, [q, A]] + \frac{D_{qp}}{\hbar^2} ([q, [p, A]] + [p, [q, A]])
\]

where \(\lambda\) is the friction constant whereas \(D_{qq}, D_{pp}\) and \(D_{pq}\) are the quantum diffusion coefficients. The Hamiltonian \(H\) of the one-dimensional subsystem with mass \(m\),
corresponding to the above equation of motion, has the general form in coordinate \( q \) and momentum \( p \)

\[
H = \frac{p^2}{2m} + V(q)
\]  

(3)

Note that eq.(2) was derived under the assumption of a weak coupling of the subsystem with its environment [16].

Since the dynamics of the subsystem is described in terms of averages and covariances, for two self-adjoint operators \( A \) and \( B \) the following notations are introduced:

\[
\sigma_A(t) = \text{Tr}(\rho(t)A), \quad \sigma_{AB}(t) = \text{Tr} \left( \rho(t) \frac{AB + BA}{2} \right) - \sigma_A(t)\sigma_B(t)
\]  

(4)

If \( A = q \) or \( p \) the equations of motion derived from eq.(2) looks like

\[
\begin{align*}
\frac{d\sigma_q(t)}{dt} &= -\lambda\sigma_q(t) + \frac{1}{m}\sigma_p(t) \\
\frac{d\sigma_p(t)}{dt} &= -\text{Tr} \left( \rho(t) \frac{dV(q)}{dq} \right) - \lambda\sigma_p(t)
\end{align*}
\]  

(5)

and

\[
\begin{align*}
\frac{d\sigma_{qq}(t)}{dt} &= -2\lambda\sigma_{qq}(t) + \frac{2}{m}\sigma_{pq}(t) + 2D_{qq} \\
\frac{d\sigma_{pp}(t)}{dt} &= -2\lambda\sigma_{pp}(t) - \text{Tr} \left( \rho(t) \frac{dV(q)}{dq} \right) p + h.c. \\
&\quad + 2\text{Tr} \left( \rho(t) \frac{dV(q)}{dq} \right) \sigma_p(t) + 2D_{pp} \\
\frac{d\sigma_{pq}(t)}{dt} &= -2\lambda\sigma_{pq}(t) + \frac{1}{m}\sigma_{pp}(t) + \sigma_q(t) \text{Tr} \left( \rho(t) \frac{dV(q)}{dq} \right) \\
&\quad - \text{Tr} \left( \rho(t) \frac{dV(q)}{dq} \right) q + 2D_{pq}
\end{align*}
\]  

(6)

The above set of first-order o.d.e. has been solved exactly for the harmonic oscillator, \( V = m\omega^2q^2/2 \), and the inverted parabolic potential (\( \omega \rightarrow i\omega \))[8, 12].

3. Quantum tunneling across quadratic potentials

We formulate the decay problem as the tunneling of an initial gaussian wave packet, confined in a harmonic oscillator well (potential pocket), located at the left of the barrier, with given values of the position average \( \sigma_q(0) \) and covariance \( \sigma_{qq}(0) \):

\[
\psi(q) = \frac{1}{(2\pi\sigma_{qq}(0))^{1/4}} \exp \left[ -\frac{1}{4\sigma_{qq}(0)} (q - \sigma_q(0))^2 + \frac{i}{\hbar} \sigma_p(0)q \right]
\]  

(7)

According to [17], the transition probability for an irreversible process described by the set (5,6) reads

\[
W(q, p, t) = (2\pi)^{-1}(\text{Det } \sigma)^{-1/2} \exp \left\{ -\frac{1}{2} \left[ \sigma^{-1}(t) \right]_{qq} (q - \sigma_q(t))^2 \\
- \left[ \sigma^{-1}(t) \right]_{pq} (q - \sigma_q(t))(p - \sigma_p(t)) - \frac{1}{2} \left[ \sigma^{-1}(t) \right]_{pp} (p - \sigma_p(t))^2 \right\}
\]  

(8)
where $\sigma$ is the $2 \times 2$ matrix of the covariances defined in eq. (4). The probability to find the wave-packet to the right of the barrier is [18]:

$$P(q_b; t) = \int_{q_b}^{+\infty} dq \int_{-\infty}^{+\infty} dp \ W(q, p; t) = \frac{1}{2} \text{erfc} \left( \frac{\sigma_q(t) - q_b}{\sqrt{2} \sigma_{qq}(t)} \right)$$

(9)

The decay rate, or fission width, is given by the ratio between the diffusion current across the barrier, $J(q_b; t) = \int_{-\infty}^{+\infty} dp \ W(q_b, p; t)$ and the tunneling probability

$$\Gamma_f(t) = J(q_b; t) P(q_b; t)$$

$$= \frac{1}{\sqrt{2\pi \sigma_{qq}(t)^3}} \left( \sigma_q(t) \sigma_{pp}(t) + \sigma_{pq}(t)(q_b - \sigma_q(t)) \right) \frac{\exp \left[ -\frac{(\sigma_q(t) - q_b)^2}{2\sigma_{qq}(t)} \right]}{\text{erfc} \left( \frac{\sigma_q(t) - q_b}{\sqrt{2} \sigma_{qq}(t)} \right)}$$

(10)

The purpose of the next two subsections is to develop the above formalism for two case studies, namely the tunneling of a metastable state from a parabolic pocket to a quadratic unbound potential and next the tunneling between two quadratic wells with finite depths, separated by an inverted parabola.

### 3.1. Two smoothly joined parabolic potentials

In this case the potential is given by joining at $q_t$, an inverted oscillator to an upright ground-state oscillator (see Fig.1):

$$V(q) = V(q_a) + \frac{1}{2} \Omega_a^2 (q - q_a)^2, \quad q \leq q_t$$

$$= V(q_b) - \frac{1}{2} \Omega_b^2 (q_b - q)^2, \quad q \geq q_t$$

(11)

In the above expression one suppose that the height of the barrier $B = V(q_b) - V(q_a)$, and the frequency $\Omega_b$ of the inverted oscillator are known. In the case of nuclear reactions this means to know the barrier from the heavy-ion interaction of the two clusters or the dependence of the total energy on deformation [19, 20]. Assigning a decay energy $E_0$ to the particle of mass $m$ we suppose that the minimum of the first harmonic oscillator well $q_a$ coincides with the first turning point. Naturally, since we deal with smoothly joined segments, the continuity of $V$ and its derivative $dV/dq$ is required at $q = q_t$. From here we get the frequency of the well’s bottom:

$$\Omega_a^2 = \frac{2\Omega_b^2 B}{\Omega_b^2 (q_b - q_a)^2 - 2B}$$

(12)

and the position of the joining point:

$$q_t = \frac{q_a \Omega_a^2 + q_b \Omega_b^2}{\Omega_a^2 + \Omega_b^2}$$

(13)

In order to integrate the systems (3,6) we need to establish the initial conditions. The initial wave-packet will be confined inside the harmonic oscillator well centered at $\sigma_q(0)$. In our calculation, motivated by specific examples from nuclear fission we chose $\sigma_q(0) = q_a$, i.e. the gaussian wave-packet is centered at the minimum of the
potential pocket. In order to overcome the barrier the initial momentum should satisfy the inequality $\sigma_p(0) > \sqrt{2mB}$ for a vanishing friction coefficient $\lambda$. The initial value of the coordinate covariance $\sigma_{qq}(0)$ is chosen in such a way that its time derivative vanishes. Assuming that $\sigma_{pq}(0)$ vanishes too, we then get from eq. (13)

$$\sigma_{qq}(0) = \frac{D_{qq}}{\lambda}$$

Since we deal with a gaussian wave packet, the momentum and the coordinate covariances are simply related by means of the following relation [12]

$$\sigma_{pp}(0) = \frac{\hbar^2}{4\sigma_{qq}(0)}$$

For the diffusion coefficients we take the rotating-wave approximation [21]

$$D_{qq} = \frac{\lambda\hbar}{2\sqrt{m}\Omega^2_a} D_{pp} = m\Omega^2_a D_{qq}, \quad D_{pq} = 0$$

These values were obtained from eq.(13) by assuming that the initial Gaussian metastable state is a Gibbs state at $T = 0$.

In Figs.2 and 3 we represented the averages and covariances of the coordinate and momentum taking four choices of the friction coefficient $\lambda$. We assumed that the initial momentum is the same, i.e. $\sigma_p(0) = 1200$ MeV. The general trend is a damping of the motion due to friction. Above a critical value $\lambda_{cr}$ of the friction coefficient all the momenta tends to infinity, faster if $\lambda = 0$ and slower if $\lambda \nearrow \lambda_{cr}$. Below this critical value the gaussian wave packet will perform damped oscillation around the potential minimum. From the inspection of Figure 2 it is obvious that the wave-packet is spending a longer time in the barrier if $\lambda$ is approaching its critical value. The decreasing of the tunneling probability (see eq.(9)) with $\lambda$ is shown in Fig.4. After a certain transition time ($\approx 5 \times 10^{-22}$ s) the tunneling probability will reach a non-vanishing asymptotic value for $\lambda < \lambda_{cr}$. Looking on the first panel of Fig.2 one sees that after this lapse of time the centroid of the gaussian is located on the other side of the barrier. Consequently, in the present approach, the tunneling time, a different quantity from the metastable state life-time, is assigned to the time necessary to attain an asymptotic value $P(q_b; \infty)$. For a discussion of this subject in the frame of the WKB-approximation and time dependent approach to Schrödinger equation, see [22, 23].

For $\lambda > \lambda_{cr}$ the tunneling probability eventually tends to zero but at the beginning of the motion, between certain lapses of time, the right tail of the wave function is found inside the barrier. If the initial momentum $\sigma_p(0)$ would be increased then the barrier is once again overcomed. However in tunneling phenomena like cluster decay the initial average momentum of the wavefunction should not exceed certain limits and thus upon comparison with the penetrabilities deduced from experiment, the range of possible values of the friction coefficient could be deduced.

Thus, for two smoothly joined parabolas, the friction reduces the tunnelling probability of the metastable state in the frame of Lindblad’s axiomatic approach.
3.2. Three smoothly joined parabolic potential

The case studied below suffers from the deficiency that the right tail of the potential falls to \(-\infty\). In usual applications we deal with tails which tend to \(+\infty\) or to 0. We thus join a third parabolic segment at a second turning point, \(q_{t2}\), centered at \(q_c\) (see fig.5):

\[
V(q) = V(q_a) + \frac{1}{2} \Omega_a^2 (q - q_a)^2, \quad q \leq q_{t1}
\]

\[
= V(q_b) - \frac{1}{2} \Omega_b^2 (q_b - q)^2, \quad q_{t1} \leq q \leq q_{t2}
\]

\[
= V(q_c) + \frac{1}{2} \Omega_c^2 (q - q_c)^2, \quad q \geq q_{t2}
\]

(17)

Imposing the same condition of continuity of \(V\) and its derivative \(dV/dq\) at \(q = q_{t2}\) one gets

\[
\Omega_c^2 = \frac{2 \Omega_b^2 \Delta V_{bc}}{\Omega_b^2 (q_c - q_b)^2 - 2 \Delta V_{bc}}
\]

(18)

and

\[
q_{t2} = \frac{q_c \Omega_c^2 + q_b \Omega_b^2}{\Omega_c^2 + \Omega_b^2}
\]

(19)

where \(\Delta V_{bc} = V(q_b) - V(q_c)\) is the difference between the top of the barrier and the bottom of the second well.

In Fig.6 the evolution of averages were represented for two harmonic wells with equal bottoms, i.e. \(V(q_b) = V(q_c)\) (a) and \(V(q_c) = 0\) (b). For the location of the second well minima several values were selected. The first one \((q_c = 16.5\ \text{fm})\) corresponds almost to the symmetric double-well problem. In the absence of friction the tendency of \(\sigma_q(t)\) is to oscillate indefinitely between these two wells with amplitude and period determined by the location of the second minimum \(q_c\). Like in the case examined in the preceding subsection, a critical value of \(\lambda\) will occur. Above this value the wave-packet will never cross the barrier and will perform damped vibrations inside the first well. If \(\lambda \leq \lambda_{cr}\) then the gaussian will pass in the second well and will not return in the first well due to the kinetic energy loose by friction. In this last case the centroid of the wave packet will tend asymptotically to the center of the second well \(q_c\). As one sees from Fig.6 there are no qualitative difference between the motions in the potential with \(V(q_b) = V(q_c)\) and \(V(q_c) = 0\).

In terms of tunneling probability, the results obtained for the three smoothly joined parabolas are displayed in Fig.7. If friction is absent the tunneling probability will tend to 0.5, i.e. half of the wave-packet is found at the right of the barrier’s top, \(q_b\), and half to its left. If friction is switched on, but up to \(\lambda_{cr}\), then asymptotically the wave-packet tunnels 100\% in the second well after a certain lapse of time. This lapse of time will be shortened if the minima of the second well is shifted towards higher values. When \(\lambda_{cr}\) is exceeded the tunneling probability goes to zero since the wave packet is constrained by the high friction to not leave the first harmonic well.
Contrary to the preceding case, for the double-well problem the value of the friction constant, below a threshold, favours the tunneling. Above this threshold the tunneling is totally hindered.

4. Conclusions

In this paper the study of tunneling, in a one-dimensional piecewise potential built-up from two and three parabolic segments, was carried out in the frame of the Lindblad approach to quantum systems for a gaussian wave-packet. In this way the interaction of the system with the environment was taken into account and the effect of dissipation incorporated in the equation of motion for the averages and the covariances. In view of the applications in cold fission and cluster decay only the case with temperature $T=0$ was considered. This amounts to admit a linear dependence of the diffusion coefficients on the friction constant for an initial metastable state.

For the two-smoothly joined parabolic potentials, if the friction constant is below a certain critical value, the gaussian wave-packet cross just one time the barrier and afterwards it moves to infinity with a high or a low momentum, depending on how large is the friction. The computation of the tunneling probability in this case confirms older results which claimed that the effect of linear friction decreases the chance to find the wave-packet beyond the barrier.

In the case of three-smoothly joined parabolas the situation is different. If the motion is unviscous then the wave packet will oscillate unhindered between the infinite walls of the two wells. Therefore, the probability current flowing from the left to the right of the barrier will be compensated by the one flowing in the opposite direction. If the friction is present in the system, although below a certain limit, the tunneling is stimulated, in the sense that asymptotically all the wave-function is located in the right well. This happens no matter how large or deep is this second well. Only the time necessary to establish the equilibrium will depend on the features of the employed potential.

It would be interesting to extend the calculations presented in this paper to other one-dimensional potentials which are more likely to simulate the behaviour of systems undergoing decay by quantum tunneling. One of the limitations of the present approach is that the potential needs to be provided in analytical form, preferably as a polynomial of lower degree. Already for a cubic polynomial complications occur because the system of first order differential equations describing the time evolution of averages and higher momenta is non-linear and is not closed. A solution would be to consider the realistic one-dimensional potential as a smooth piecewise curve given by cubic splines. Otherwise, the exact treatment of the problem would be to solve directly the time-dependent Schrödinger equation, which unfortunately is non-local and non-linear.
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**Figure 1.** Gaussian wave-packet with average initial momentum $\sigma_p(0)$ centered at $q_a$ undergoing tunneling across a barrier of height $B$ built-up from two smoothly joined parabolas.

**Figure 2.** The time dependence of the average values of the coordinate $\sigma_q(t)$ and momentum $\sigma_p(t)$ for two smoothly joined parabolas. Four different values of the friction constant $\lambda$ are taken.

**Figure 3.** The evolution of $\sigma_{qq}(t)$, $\sigma_{pp}(t)$ and $\sigma_{pq}(t)$ for friction constants taken as in Fig. 2.

**Figure 4.** The decrease of the tunneling probability in time with the friction constant in the two smoothly joined parabolas case.

**Figure 5.** Same as in Fig.1 but for three smoothly joined parabolas. The location $q_c$ and depth of the second well minima are varied over a wide range.

**Figure 6.** The evolution of $\sigma_q(t)$ for three smoothly joined parabolas. Three different values are taken for the friction constant $\lambda$ and four choices for $q_c$. In (a) the depth of the two harmonic wells are equal, i.e. $V(q_a) = V(q_b)$, whereas in (b) $V(q_c) = 0$.

**Figure 7.** The tunneling probability in the three smoothly joined parabolas case for (a) $V(q_a) = V(q_b)$ and (b) $V(q_c) = 0$. 

\[ \sigma_q(t) \text{ (fm)} \]

\[ \sigma_p(t) \text{ (MeV)} \]

\( \lambda = 0. \text{ MeV} \)

\( \lambda = 0.50 \text{ MeV} \)

\( \lambda = 0.85 \text{ MeV} \)

\( \lambda = 1.50 \text{ MeV} \)

Time \( (0.3(3) \times 10^{-23} \text{ s}) \)
\[ P(q_b; t) \]

- $\lambda = 0. \text{ MeV}$
- $\lambda = 0.5 \text{ MeV}$
- $\lambda = 0.85 \text{ MeV}$
- $\lambda = 1.5 \text{ MeV}$

$q_b = 15.08 \text{ fm}$

\[ \text{time (0.3(3)x} \ 10^{-23} \text{s)} \]
\( \sigma_q(t) \) (fm)

- \( q_c = 16.5 \text{ fm} \)
- \( q_c = 20 \text{ fm} \)
- \( q_c = 25 \text{ fm} \)
- \( q_c = 50 \text{ fm} \)

\( \lambda = 0. \text{ MeV} \)
\( \lambda = 0.50 \text{ MeV} \)
\( \lambda = 1. \text{ MeV} \)

Time \((0.3(3) \times 10^{-23} \text{ s})\)
\begin{align*}
P(q_b; t) &= P(q_a; t) \\
\text{time (0.3(3) x } 10^{-23} \text{s})
\end{align*}

\begin{align*}
q_c &= 16.5 \text{ fm} \\
q_c &= 20 \text{ fm} \\
q_c &= 25 \text{ fm} \\
q_c &= 50 \text{ fm}
\end{align*}

\begin{align*}
\lambda &= 0 \text{ MeV} \\
\lambda &= 0.5 \text{ MeV} \\
\lambda &= 1 \text{ MeV} \\
V(q_c) &= V(q_a)
\end{align*}
$P(q; t)$

$q_c = 20 \text{ fm}$

$q_c = 50 \text{ fm}$

$q_c = 100 \text{ fm}$

$q_c = 500 \text{ fm}$

\[ V(q_c) = 0 \]

\[ \lambda = 0 \text{ MeV} \]

\[ \lambda = 0.5 \text{ MeV} \]

\[ \lambda = 1 \text{ MeV} \]

\[ \text{time} (0.3(3) \times 10^{-23} \text{s}) \]

\[ \text{time} (0.3(3) \times 10^{-23} \text{s}) \]