Macroscopic tunneling, decoherence and noise-induced activation

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Abstract. We study the effects of the environment at zero temperature on tunneling in an open system described by a static double-well potential. We show that the evolution of the system in an initial Schrödinger cat state, can be summarized in terms of three main physical phenomena, namely decoherence, quantum tunneling and noise-induced activation. Using large-scale numerical simulations, we obtain a detailed picture of the main stages of the evolution and of the relevant dynamical processes.

The tunneling of a particle through a potential barrier is a fundamental effect in quantum mechanics. Macroscopic quantum tunneling can be associated with the tunneling of a many-body wavefunction through a potential barrier, and therefore provides a more stringent test of the validity of quantum mechanics than one particle case. One place where the study of macroscopic quantum tunneling is experimentally accessible is in the tunneling of a Bose-Einstein condensate (BEC) out of an optical trap. These systems have a controllable number of atoms and hence straddle the boundary between microscopic and macroscopic, and hence between quantum and classical systems. Proposals to perform interference experiments using confined atoms \cite{1} rely on the separation and merger of two potential wells to split and recombine atomic wave packets \cite{2}. BECs in a two-well potential have been created in experiment \cite{3}. Atom-atom interactions tend to localize particles in either potential well and reduce the coherence of the splitting and recombination processes \cite{4}, whereas tunneling serves to delocalize the atomic wave packets and keeps a well-defined relative phase between the potential wells.

Macroscopic systems are generally open systems, interacting with an external environment, and in this context quantum tunneling \cite{5, 6} is qualitatively different from its experimentally verified microscopic analogue \cite{7}. The analysis of open systems has led to interesting results, detailing the dynamics of a quantum system coupled to a thermal bath with arbitrary temperature. A closed quantum system described by a state localized around a meta-stable minimum, should tunnel through the potential barrier with a well defined time-scale. This tunneling time can be estimated using standard techniques such as the instaton method \cite{8}. For an open system, on the other hand, it is well known that the environment induces decoherence on the quantum particle, its behavior becoming classical as soon as interference terms are destroyed by the external
noise. This transition from a quantum to a classical behavior is forced by the interaction with a robust environment and takes place at a given time-scale, the decoherence time. This quantity depends on the properties of the system, its environment and their mutual coupling. If the decoherence time is significantly smaller than the tunneling time, one would expect that after classicalization the state should become confined to the meta-stable vacuum (or potential well), with tunneling being suppressed. The particle could still cross the barrier but only if excited by the bath, its energy increasing via thermal activation, for example. This process is distinct from quantum tunneling, is classical in its nature and should be efficient mostly at high environmental temperatures. An interesting question arises: what is the effect on tunneling if the particle is coupled to a reservoir at zero temperature? Though in this case there should be in principle no thermal activation, we know there is decoherence induced by a quantum environment at zero temperature \[9\]. This would lead to classicalization and one could conclude that even at \( T = 0 \), quantum tunneling should be inhibited by the interaction with the external environment \[10\].

The study of the effects of an external environment on tunneling was initiated in Refs. \[5\]. It was shown that dissipation inhibits tunneling. Authors consider a two level limit of a particle in a double-potential well with Hamiltonian \( H = -\frac{1}{2} \hbar \Delta_0 \sigma_x + \frac{1}{2} \epsilon \sigma_z \), where \( \epsilon \) is the detuning frequency. In the case \( \epsilon = 0 \), the eigenstates can be written as combinations of antisymmetric and symmetric states: \( \psi_0 = 1/\sqrt{2}(\psi_R - \psi_L) \) and \( \psi_E = 1/\sqrt{2}(\psi_R + \psi_L) \), respectively. Therefore, the probability to stay on the right or left well is given by an oscillatory function: \( P(t) = P_R - P_L = \cos(\Delta_0 t) \). This result has no classical analog, and this is the genuine expression of the phase coherence between the states (i.e. NH3 inversion coherence). In the case this two level system is coupled to a reservoir (spin-boson model), the tunneling is inhibited by the dissipation in the limit of \( \Delta_0 / \Lambda \ll 1 \) (\( \Lambda \) is the Debye frequency of the environment) and \( k_B T / \hbar \Lambda \ll 1 \) (low temperature limit) \[5\].

In Ref. \[11\] we have studied a general tunneling system described by a static Hamiltonian. Specifically, we have looked in detail at the evolution of a particle in a quantum state localized at one of the minima of a double well potential, when coupled to an external environment at both zero and high temperature. We have presented analytical descriptions of the effects of dissipation and diffusion, and estimated the time-scales associated with the distinct physical processes governing the dynamics of the system: decoherence, quantum tunneling and activation. A very interesting extension of previous analysis is to study superpositions of macroscopic quantum states. This is a crucial aspect when analyzing BECs in double-well traps \[12\]. Therefore, our goal here is to extend our previous considerations about decoherence, tunneling and noise-induced activation to the case of an initial coherent superposition of two Gaussian wave packets. The interactions between atoms in finite size affect the coherence and the relative phase undergoes diffusion due to the presence of a condensate self-interaction and also the interaction between condensate and non-condensate atoms creates decoherence \[13\]. In the experiments on BECs of dilute alkali-metal atomic gases, trapped atoms
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are evaporatively cooled and exchange particles with their environment. Macroscopic quantum coherence of BECs results in coherent quantum tunneling of atoms between the two modes, analogously to the coherent tunneling of Cooper pairs in a Josephson junction. Thus, our motivation is to see how robust is the quantum coherence between condensates confined in each of the different traps.

We will start by considering an anharmonic trap given by $V(x) = -\frac{1}{4} \Omega^2 x^2 + \lambda x^4$. This is a double well potential with two absolute minima at $x_0 = \pm \Omega/\sqrt{8\lambda}$ separated by a potential barrier with height $V_0 = \Omega^4/(64\lambda)$. We will assume that the system (BEC) is open, meaning that it is coupled to an environment composed of an infinite set of harmonic oscillators, by which we model the interaction with the non-condensate atoms.

The dynamics of the non-linear potential can be obtained by tracing over the degrees of freedom of the environment and obtaining a master equation for the reduced density matrix of the system, $\rho_i(t)$. We will assume that the initial states of the system and environment are uncorrelated, with the latter being in thermal equilibrium at zero temperature for $t = 0$. Only when the interaction is turned on the system is allowed to evolve and the initial condition is not an equilibrium state. As we are interested in studying tunneling-like phenomena, we will estimate the tunneling time $\tau$ by looking at the evolution of a state for which the particle is initially localized in one of the sides of the double potential well. Numerically, we found that in general $\tau = 3/(E_0 - E_E)$, where $E_E$ and $E_0$ are the energies of the symmetric/anti-symmetric eigenstates respectively. The energy difference and corresponding tunneling time can be obtained by a straightforward instanton calculation, the final result being $\tau = \frac{3}{E_0 - E_E} = \frac{3}{8 \sqrt{\frac{\Omega}{V_0}}} \exp \left( \frac{16 \sqrt{\Omega}}{3 V_0} \right)$. The expression inside the exponential is the classical action for the instanton, $S_0 = (16/3) \times V_0/\Omega$.

For the open case, we focus on Ohmic environments with spectral density $I(\omega) = \frac{2}{\pi} \gamma_0 \omega \frac{\Lambda^2}{\omega^2 + \Lambda^2}$ at $T = 0$ ($\gamma_0$ is the dissipation constant and $\Lambda$ the frequency cutoff). After a rather lengthy calculation, the master equation at $T = 0$ on the basis of eigenstates of the isolated system can be written as

\[
\dot{\rho}_{\mu\nu} = -i \Delta_{\mu\nu} \rho_{\mu\nu} - \sum_{\alpha\beta} \left\{ D_{\alpha\beta} x_{\mu\alpha} x_{\beta\nu} \rho_{\alpha\beta} - D_{\beta\nu} x_{\mu\alpha} x_{\beta\nu} \rho_{\alpha\beta} - D_{\mu\alpha} x_{\beta\nu} x_{\beta\nu} \rho_{\alpha\beta} + D_{\alpha\beta} x_{\mu\alpha} x_{\beta\nu} \rho_{\alpha\beta} \right\} + i \sum_{\alpha\beta} \left\{ \gamma_{\alpha\beta} x_{\mu\alpha} x_{\beta\nu} \rho_{\alpha\beta} - \gamma_{\alpha\beta} x_{\mu\alpha} x_{\beta\nu} \rho_{\alpha\beta} - \gamma_{\alpha\beta} x_{\mu\alpha} x_{\beta\nu} \rho_{\alpha\beta} + \gamma_{\alpha\beta} x_{\mu\alpha} x_{\beta\nu} \rho_{\alpha\beta} \right\},
\]

(1)

where the time dependent complex coefficients $D_{\alpha\beta} = D_{\alpha\beta}(t)$ and $\gamma_{\alpha\beta} = \gamma_{\alpha\beta}(t)$ are given by $D_{\alpha\beta} = D(\Delta_{\alpha\beta}) + i \Delta_{\alpha\beta} f(\Delta_{\alpha\beta})$ and $\gamma_{\alpha\beta} = -\frac{1}{2} \bar{\Omega}^2 (\Delta_{\alpha\beta}) - i \Delta_{\alpha\beta} (\Delta_{\alpha\beta})$. In this expressions, $\Delta_{\alpha\beta} = \omega_\alpha - \omega_\beta$, is the frequency difference between eigenstates $\alpha$ and $\beta$. The set of coefficients $D_{\alpha\beta}$ encapsulates the effects of diffusion at $T = 0$, with $D(\Delta)$ representing the normal diffusion and $f(\Delta)$ the anomalous one. The others coefficients represent the effect of the environment through the dissipation kernel $\eta$, with $\bar{\Omega}(\Delta)$.
the frequency shift, and $\gamma(\Delta)$ the dissipation coefficient (see analytical expressions in [9, 11]). We have numerically solved equation (1), in the under-damped case, using a standard adaptative step-size fifth order Runge-Kutta method for different parameters of the system and the environment. All results were found to be robust under changes on the parameters of the integration method. From the solution of (1) we will show the Wigner function and the probability distributions of the main system at any time [14].

As an example we have chosen $\Omega = 100$ and $V_0 = 200$ for the system for which the estimated tunneling time scale is $\tau \approx 158.27$. We set the frequency cutoff to $\Lambda = 10V_0 = 2000$. With this set of parameters, the effects of the frequency shift in the initial state can be neglected [11]. The decoherence time $t_D$ has been analytically evaluated in [9], getting a bounded value $t_D \leq 1/8\gamma_0$ for very flat potentials, and $t_D \sim 1/\Lambda$ for large values of $\Omega$.

Fig. 1 shows the Wigner function of the system for the indicated times, both for the isolated and open systems. The initial Schrödinger cat state is depicted in the first picture of each row (left). Black fringes denote the quantum interference terms present in the initial state. Already at very early times, the negative regions of $W(x,p)$ are considerably suppressed for the open case when compared to the closed system, suggesting that decoherence has a crucial role in the evolution. For $t \leq \tau$, $W(x,p)$ becomes positive definite and the open system displays no tunneling interferences [15]. Decoherence inhibits tunneling. Once the interferences are destroyed, the spread of the Wigner function increases as a consequence of diffusion induced by the environment. As expected, decoherence has clearly been effective by the time the Wigner function is strictly positive everywhere. As the tunneling time is reached, though the system is localized on the original wells, the Wigner function explores a large region of the phase space. On the contrary, for the closed system, negative values in the center of the phase space clearly indicate quantum behavior. The isolated system is tunneling from one to the other well.

In Fig. 2 we show the probability distribution $\sigma(x,x)$ for the isolated and open systems for the indicated times, measured in units of the estimated tunneling time $\tau$. It is worthy of note that for the closed case the state keeps its phase coherence and the tunneling effect is present. The state is localized on the original wells and the evolution is clearly unitary. In the open case, even though the system is still localized on the original wells for early times, the probability spreads due to the diffusion induced by the environment. Probability differs from the closed case owing to the noise-induced diffusion. $\sigma$ starts spreading for early times. By $t \sim 0.5\tau$ there is nonzero probability at the position of the barrier; clearly indicating that there is probability crossing the barrier but not by tunnel effect (as we have shown in the Wigner pictures, the system is already classical by the tunneling time). It is expected that the probability over the barrier grows in time, reaching an uniform value asymptotically. This fact suggests that there is a process of energy activation induced by the presence of the environment [11].

When trying to interpret the post-decoherence behaviour of the open system, several features of its dynamics should be kept in mind. Firstly, one should emphasize that the
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Figure 1. Wigner functions for the isolated (row on top) and open (bottom row) systems, for the indicated times. The horizontal axis corresponds to $x$, vertical axis to $p$. The medium grey shade on the background correspond to zero values for the Wigner function, lighter and darker shades, respectively, to positive and negative values of $W(x, p)$. The open system has totally decohered before the tunneling time-scale.

initial condition is clearly not the ground state of the composite system. As soon as the interaction between the main system and the environment is turned on, at $t = 0$, the system will find itself in an excited state. In relation to the new minima of the potential, the environment will have a non-zero amount of energy. From a purely classical point of view, this energy cannot be responsible for the excitation of the particles over the potential barrier. In fact, the height of the potential increases in relation to the new vacuum, in such a way that the total energy of the full system is still lower than the barrier separating regions of positive and negative $x$. Note the fact that there are no fluctuations in the environment classically at T=0, plays a crucial role in this reasoning. Even for small but finite T, the energy of the environment would go as T. By choosing T small enough, this contribution could always be made smaller than the barrier height. As a consequence, and in contrast with the high-T case, we will not be able to describe the evolution of the quantum system after classicalization by simply taking its classical exact equivalent. The quantum fluctuations present in the initial state of the environment must play a role in the “activation”. One should note that these fluctuations are not “vacuum fluctuations” of the full system. The quantum nature of the environment, which could be ignored at high-T, leads in this limit to important non-negligible effects. In terms of the master equation, the quantum fluctuations of the bath oscillators generate non-zero $f(t)$ and $D(t)$ terms, making diffusive phenomena possible. This is particularly true in the case of the anomalous diffusion coefficient $f(t)$ that depends logarithmically on the cutoff $\Lambda$ and thus can be considerably large [9]. Diffusion effects induced by quantum fluctuations are thus responsible for exciting the particles over the potential barrier. The interplay of decoherence and excitation processes in the $T = 0$ case deserves a deeper insight. For both quantities, the value of the environment frequency cutoff $\Lambda$, seems to play an important role, affecting both
the decoherence time, and the excitation process in the same direction. Since we do not have explicit estimates of the “activation” time in terms of $\Lambda$, it is hard to predict whether there is a regime for which decoherence happens fast enough and excitation is considerably delayed. Numerical results presented in Fig. 3 suggests that this is not possible. The figure show the mean energy and its dispersion as a function of time. Also in the inset, we show the energy of the main system for several choices of the cutoff. $\Lambda$ varies from the smallest frequency present in the system; i.e. the difference between the first exited and the ground state energy levels, $E_0 - E_E$; and $\Lambda = 10V_0$. Also shown are two intermediate cutoff values, $\Lambda = V_0/10$ and $\Lambda = V_0$. By lowering $\Lambda$, the “activation” time is indeed postponed, but so is decoherence [9]. In this situation the particles are simply able to tunnel back and forth the two minima for a longer period. Higher values of the cutoff, on the other hand lead to both fast decoherence and fast “activation”. As a result we were never able to localize the particle on one of the wells, with tunneling and “activation” being simultaneously suppressed. The dispersion in the energy distribution $\Delta E(t)$ shows that fluctuations in the environment at $T = 0$ are non-negligible for large values of $\Lambda$. The latter have a faster growth in time and reach a bigger final value than the mean energy of the system. Noise-induced energy activation is a consequence of this fact.

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