Environmentally induced shift of the quantum arrival time

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Using a simple model potential, we study the effects of weak Markovian dissipation on the quantum arrival time. The interaction with the environment is incorporated into the dynamics through a Markovian master equation of Lindblad type, which allows us to compare time-of-arrival distributions and approximate crossing probabilities for different dissipation strengths and temperatures. We also establish a connection to an earlier study where quantum tunneling with dissipation was investigated, which leads us to some conclusions concerning the formulation of the continuity equation in the Lindblad theory.

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I. INTRODUCTION

The problem of the quantum arrival time has been intensively studied during the last years [1–15] both because it is a fundamental issue in quantum mechanics and because it can be of practical relevance for the particle detection process. The main difficulties are (i) how to construct a time-of-arrival (TOA) operator in quantum mechanics [16–23], (ii) how to establish a quantum mechanical TOA distribution [24–28], and (iii) how the corresponding observables can be measured [29–33]. In the vast majority of the cases, these questions were studied within the Schrödinger equation, but also a relativistic Dirac equation approach was adopted in some cases [34,35]. A unitary time evolution, however, cannot be used to describe irreversible dissipative processes. In the present work, we do not primarily aim at a further discussion of possible definitions but rather wish to address a different question: how does a dissipative interaction with an environment affect the quantum mechanical arrival time? The TOA problem in the presence of an environment has been studied earlier, e.g., using so-called decoherent histories [36,37], an absorbing potential [38], or a formalism based on quantum canonical transformations [39]. An alternative approach was demonstrated in Ref. [40], where Aoki *et al.* solved the time-dependent Schrödinger equation (TDSE) numerically using the Crank-Nicholson method in order to propagate a wave packet through a square potential barrier and interpret the barrier-induced changes in the wave packet shape and dispersion relation as an environmental effect. Still, such an approach is different from the one adopted here in the sense that the TDSE dynamics is unitary and allows us to compare the arrival times of free and tunneling particles rather than the arrival times for different dissipation strengths. In the present work, instead of considering a potential barrier itself as an environment, we will investigate the arrival times of particles passing through a barrier but being exposed to different coupling strengths and temperatures. For that purpose, we solve a Markovian master equation of Lindblad type [41], which, for the parabolic potential barrier considered here, is possible even analytically. At this point, one should mention that conceptually the problem at hand is related to the well-studied topic of dissipative effects on quantum tunneling [42–51]. This will also be discussed later.

The paper is structured as follows. The model system which is used as a test case for our study is introduced in Sec. II, and the results are presented in Sec. III, where we also establish a connection to earlier work. A brief summary is given in Sec. IV. Atomic units are used throughout the paper.

II. MODEL

We consider the initial wave function to be a one-dimensional Gaussian wave packet of the form

$$\psi(x,t=0) = \frac{1}{(2\pi\Delta_x)^{1/4}}\exp\left(\frac{1}{4\Delta_x}(x-x_0)^2 + \frac{i}{\hbar}p_0 x\right), \quad (1)$$

where p_0 and x_0 are the initial expectation values of position and momentum and Δ_x is the initial spread in position space. We assume that the wave packet is initially centered around $x_0>0$ in position space and $p_0<0$ in momentum space, approaching a parabolic potential barrier which is centered at the origin,

$$\hat{U} = -\frac{m\omega^2\hat{x}^2}{2}. \quad (2)$$

Here, m is the mass of the particle and ω is a parameter describing the barrier steepness. The central questions to be addressed are the following: what is the probability that the particle arrives at the origin within a certain time interval, when is this most likely to happen, and how are the arrival probability and time affected by temperature and dissipation. Trying to answer these questions, we will not propagate the wave packet in time with TDSE; instead, we work with the Lindblad master equation which is convenient if we wish to incorporate environmental effects. This is sufficient to completely cover the dynamics in the given case since it yields the time evolution of the Wigner function W corresponding to the initial wave packet [Eq. (1)] from which all information required for the present study can be extracted. In the following, we denote by $\sigma_A(t)$ the expectation value of an operator $\hat{A}$ and by $\sigma_{AB}(t)=\sigma_{BA}(t)$ the covariance of two op-

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erators $\hat{A}$, $\hat{B}$ (which, for $\hat{A}=\hat{B}$, reduces to the variance $\sigma_{AA}=\langle\hat{A}^2\rangle-\langle\hat{A}\rangle^2$). For the case $\hat{A}=\hat{x}$, $\hat{B}=\hat{p}$ we also define the covariance determinant $\sigma(t)=\sigma_{xx}(t)\sigma_{pp}(t)-\sigma_{px}(t)^2$. With this notation, the initial Wigner function corresponding to the wave packet in Eq. (1) reads

$$W(x,p,t=0)=\frac{1}{2\pi\sqrt{\sigma(0)}}\times\exp\Bigg[-\frac{1}{2\sigma(0)}\{\sigma_{pp}(0)[x-\sigma_x(0)]^2+\sigma_{xx}(0)[p-\sigma_p(0)]^2-2\sigma_{px}(0)[x-\sigma_x(0)]\times[p-\sigma_p(0)]\}\Bigg], \tag{3}$$

where $\sigma_x(0)=x_0$, $\sigma_p(0)=p_0$, $\sigma_{xx}(0)=\Delta_x$, $\sigma_{pp}(0)=\hbar^2/[4\sigma_{xx}(0)]$, and $\sigma_{px}(0)=0$. The advantage of choosing a parabolic potential barrier [Eq. (2)] is that the Hamiltonian,

$$\hat{H}=\frac{\hat{p}^2}{2m}+\hat{U}, \tag{4}$$

is quadratic both in $\hat{x}$ and $\hat{p}$ and hence the Wigner function remains Gaussian for all times. Therefore, it is sufficient to determine the time evolution of the expectation values $\sigma_x(t)$, $\sigma_p(t)$, the variances $\sigma_{xx}(t)$, $\sigma_{pp}(t)$, and the covariance $\sigma_{px}(t)$. The Wigner function at any time t is then given by the same expression as in Eq. (3), where the initial values of the first and second moments are replaced by their value at time t. The equations of motion can be derived from the master equation, which, for an operator $\hat{A}$, in the Heisenberg picture reads

$$\frac{d\hat{A}}{dt}=\frac{i}{\hbar}[\hat{H},\hat{A}]+\frac{1}{2\hbar}\sum_j(\hat{V}_j^\dagger[\hat{A},\hat{V}_j]+[\hat{V}_j^\dagger,\hat{A}]\hat{V}_j). \tag{5}$$

The so-called Lindblad operators $\hat{V}_j$ describe the dissipative interaction of the system with the environment. Convenient choices of the latter are linear superpositions of the position and momentum operators,

$$\hat{V}_j=a_j\hat{p}+b_j\hat{x},\quad \hat{V}_j^\dagger=a_j^*\hat{p}+b_j^*\hat{x},\quad j=1,2, \tag{6}$$

where a_j and b_j are complex numbers. Such operators were initially introduced to study dissipation effects in nuclear physics [52–54] and they were also used in other general quantum mechanical discussions [50,51,55–61]. The advantages are that the number of Lindblad operators is limited by the dimension of the system and that the resulting equations of motion are analytically solvable for a Hamiltonian quadratic in $\hat{x}$ and $\hat{p}$. For the studied case of a Gaussian wave packet in an inverted parabolic potential, the latter were derived and solved elsewhere [50,51], so that we just briefly quote the relevant results. The expectation values evolve as

$$\sigma_x(t)=e^{-\lambda t}\left[\cosh(\omega t)x_0+\frac{1}{m\omega}\sinh(\omega t)p_0\right], \tag{7}$$

$$\sigma_p(t)=e^{-\lambda t}[m\omega\sinh(\omega t)x_0+\cosh(\omega t)p_0]. \tag{8}$$

Here, λ is the environmental coupling strength parameter which is connected to the Lindblad operators [Eq. (6)] as

$$\lambda=-\mathrm{Im}\sum_j a_j^*b_j. \tag{9}$$

The time evolution of the second moments can be written in matrix form as

$$\begin{pmatrix}\sigma_{xx}(t) & \sigma_{px}(t)\\ \sigma_{px}(t) & \sigma_{pp}(t)\end{pmatrix}=\Lambda(t)(\Gamma^0-\Gamma)\Lambda(t)^T+\Gamma, \tag{10}$$

where

$$\Lambda(t)=\exp\left[t\begin{pmatrix}-\lambda & 1/m\\ m\omega^2 & -\lambda\end{pmatrix}\right],\quad \Gamma^0=\begin{pmatrix}\sigma_{xx}(0) & \sigma_{px}(0)\\ \sigma_{x_p}(0) & \sigma_{pp}(0)\end{pmatrix} \tag{11}$$

and the elements of Γ are given by

$$\Gamma_{11}=\frac{1}{2m^2\lambda(\lambda^2-\omega^2)}[m^2(2\lambda^2-\omega^2)D_{xx}+D_{pp}+2m\lambda D_{px}],$$

$$\Gamma_{22}=\frac{1}{2\lambda(\lambda^2-\omega^2)}[(m\omega^2)^2D_{xx}+(2\lambda^2-\omega^2)D_{pp}+2m\omega^2\lambda D_{px}],$$

$$\Gamma_{12}=\frac{1}{2m\lambda(\lambda^2-\omega^2)}[\lambda(m\omega)^2D_{xx}+\lambda D_{pp}+2m\lambda^2D_{px}],$$

$$\Gamma_{21}=\Gamma_{12}. \tag{12}$$

The diffusion coefficients D_{xx}, D_{pp}, and D_{px} that appear in the equations above are connected to the Lindblad operators as

$$D_{xx}=\frac{\hbar}{2}\sum_j|a_j|^2,\quad D_{pp}=\frac{\hbar}{2}\sum_j|b_j|^2,\quad D_{px}=-\frac{\hbar}{2}\mathrm{Re}\sum_j a_j^*b_j. \tag{13}$$

A common choice is [50–52,54,57]

$$D_{xx}=\frac{\hbar\lambda}{2m\omega}\coth\left(\frac{\hbar\omega}{2k_BT}\right),\quad D_{pp}=\frac{\hbar\lambda m\omega}{2}\coth\left(\frac{\hbar\omega}{2k_BT}\right),\quad D_{px}=0 \tag{14}$$

since it allows us to incorporate temperature dependence (k_B denotes the Boltzmann constant) and to satisfy the fundamental constraints [62]

$$D_{xx}>0,\quad D_{pp}>0,\quad D_{xx}D_{pp}-D_{px}^2\geq\lambda^2\hbar^2/4. \tag{15}$$

Thus, from Eqs. (7), (8), and (10) the Wigner function of the system is known for all times,

$$W(x,p,t)=\frac{1}{2\pi\sqrt{\sigma(t)}}\times\exp\Bigg[-\frac{1}{2\sigma(t)}\{\sigma_{pp}(t)[x-\sigma_x(t)]^2+\sigma_{xx}(t)[p-\sigma_p(t)]^2-2\sigma_{px}(t)[x-\sigma_x(t)]\times[p-\sigma_p(t)]\}\Bigg]. \tag{16}$$

In Sec. III, we use this result to study the effects of dissipation and temperature on the arrival time.

III. EFFECTS OF THE ENVIRONMENT ON THE ARRIVAL TIME AND CONNECTION TO TUNNELING PROBABILITY

As already mentioned in Sec. I, choosing an appropriate measure of the TOA is far from trivial. One possible approach is to use the probability density current $j(x,t)$. Here, we follow the derivation given in Appendix A in Ref. [37] and consider a wave packet which is approaching the origin from the right (i.e., $x_0 > 0$, $p_0 < 0$). We define the approximate probability for the particle to cross the origin during the interval $[0, t]$ as

$$P(0,t) = \int_0^t j(0,t')dt' . \tag{17}$$

Although, as extensively discussed in the references listed in Sec. I, this definition still contains some ambiguities, e.g., due to possible backflow, it is nevertheless sufficient for our study. First of all, since we are not primarily interested in tunneling, we will consider a situation where the initial energy of the wave packet is well above the barrier, thus reducing the backflow. Second, since the potential has a maximum at the origin, the backflow at this point should be particularly small. The current at $x=0$ can be obtained from the Wigner function in the following way:

$$j(0,t) = -\int_{-\infty}^{+\infty} dp \frac{p}{m} W(0,p,t). \tag{18}$$

Here we just quoted Eq. (A2) from Ref. [37]. A formal discussion concerning the use of Wigner functions to study the TOA problem can be found in, e.g., Ref. [63]. For the Wigner function derived in Sec. II [Eq. (16)], the above integral can be carried out analytically. The result is

$$j(0,t) = \frac{\sigma_x(t)\sigma_{px}(t) - \sigma_p(t)\sigma_{xx}(t)}{\sqrt{2\pi m^2 \sigma_{xx}(t)^3}} \exp\left[-\frac{\sigma_x(t)^2}{2\sigma_{xx}(t)} \right]. \tag{19}$$

It is interesting to note that while the Wigner function depends also on the spread in momentum $\sigma_{pp}(t)$, the current at the origin does not. The probability density current and the approximate crossing probability are plotted in Fig. 1 for different environmental coupling strengths and temperatures [for convenience, we introduced dimensionless parameters $\xi = \lambda/\omega$ and $\epsilon = \hbar\omega/(k_B T)$].

We observe that for low temperatures, the coupling to the environment hardly influences the TOA distribution and the approximate crossing probability. At this point, it should be stated that this does not necessarily need to hold for the case of strong dissipation where $\lambda \approx \omega$, but such a case cannot be analyzed within the model adopted here since it violates the Markovian condition and is beyond the validity region of the master equation used here [Eq. (5)]. However, in the case $\hbar\omega \ll k_B T$ both quantities become more sensitive even to weak Markovian dissipation, and one clearly observes a shift in the TOA distribution. This emphasizes the crucial role of diffusion processes for particles propagating through interacting environments. Qualitatively, our result for high temperatures agrees with the conclusion obtained in Ref. [40] where it was found that environmental effects, in fact, can

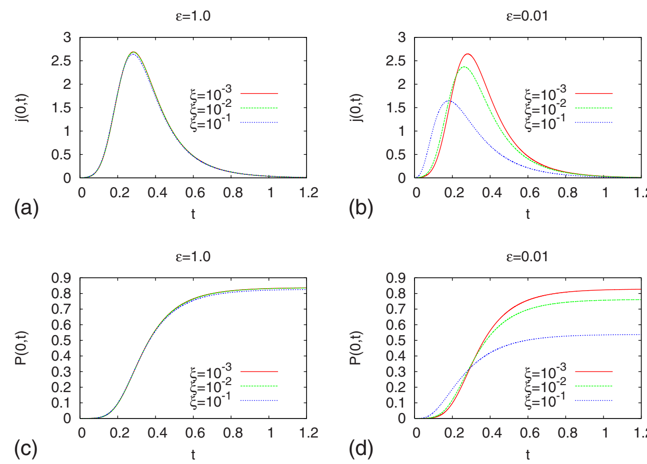

FIG. 1. (Color online) Upper panels: TOA distribution defined in terms of the probability density current for low (left) and high (right) temperatures [$\epsilon = \hbar\omega/(k_B T)$], shown for three different environmental coupling strengths ($\xi = \lambda/\omega$). Lower panels: approximate crossing probabilities in the case of low (left) and high (right) temperatures. The following values were used in the calculations: $\omega = 3.0$, $m=1.0$, $x_0=4.0$, $p_0=-15.0$, and $\Delta_x=1.0$. All quantities are given in atomic units.

lead to an earlier TOA. For the case studied therein, namely, a wave packet either propagating freely or crossing a potential barrier, this behavior was explained by the fact that the barrier filters out slow components while the fast components tunnel through the barrier. In our case, however, it is very important to stress that while the maximum of the TOA distribution is shifted to earlier times, the total asymptotic crossing probability is decreasing with increasing environmental coupling. In other words, the probability of the particle to arrive at the origin decreases, but, in the case it arrives, the arrival is more likely to occur earlier than in the noninteracting case.

Next, we would like to point out a connection between the present study and earlier work where the same model was used to study quantum tunneling with dissipation [50,51]. In Ref. [51], Isar *et al.* considered the same kind of wave packet and potential barrier, with the initial energy expectation value being below the barrier maximum. The tunneling probability was then defined in terms of the probability density ρ as the asymptotic probability of finding the particle beyond the barrier,

$$\mathcal{P}_T = \lim_{t\to\infty} \int_{-\infty}^{0} dx \rho(x,t), \tag{20}$$

for which the following analytical expression was derived:

$$\int_{-\infty}^{0} dx \rho(x,t) = \frac{1}{2}\left(1 + \text{erf}\left[-\frac{\sigma_x(t)}{\sqrt{2\sigma_{xx}(t)}} \right] \right). \tag{21}$$

In both equations, the original notation is modified according to the chosen convention (in Ref. [51] a wave packet with $x_0 < 0$ and $p_0 > 0$ was considered, while we considered $x_0 > 0$ and $p_0 < 0$). The error function is defined as

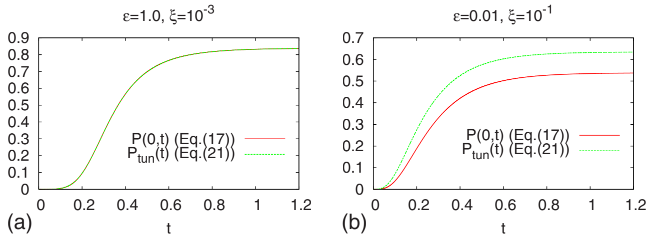

FIG. 2. (Color online) Comparison of the probabilities from Eqs. (17) and (21) for the case of low temperatures with a weak dissipation (left panel) and high temperatures with a stronger dissipation (right panel). Note that the two curves overlap in the former case. The values used in the calculations are as stated in the caption of Fig. 1, with $\epsilon = \hbar\omega/(k_B T)$ and $\xi = \lambda/\omega$. All quantities are given in atomic units.

$$\mathrm{erf}(u) = \frac{2}{\sqrt{\pi}} \int_0^u e^{-s^2} ds. \tag{22}$$

A natural question to ask is whether the definitions in Eqs. (17) and (21) are related. In fact, in case of unitary dynamics they are the same, which directly follows from the integration of the one-dimensional continuity equation

$$\frac{\partial \rho(x,t')}{\partial t'} + \frac{\partial j(x,t')}{\partial x} = 0 \tag{23}$$

in space and time, provided the initial condition

$$\int_{-\infty}^{0} |\psi(x,t=0)|^2 dx \approx 0 \tag{24}$$

is satisfied and bearing in mind that the current always vanishes at $x \to -\infty$. Although both conditions hold for the set of parameters we used in our calculations, we found that the two quantities [Eqs. (17) and (21)] are equal only in the limit of weak dissipation and/or low temperatures, while for higher temperatures and increasing dissipation they differ, as demonstrated in Fig. 2.

This may seem unphysical, but the behavior can be understood if one recalls that the probability density in the continuity equation [Eq. (23)] can be expressed as the position representation of the density operator ($\rho(x,t) = \langle x|\hat{\rho}(t)|x\rangle$), which in the case of unitary time evolution satisfies the von-Neumann equation

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}]. \tag{25}$$

The master equation we used in the present work, on the other hand, contains an additional term that accounts for the environmental effects,

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \frac{1}{2\hbar}\sum_j ([\hat{V}_j\hat{\rho},\hat{V}_j^\dagger] + [\hat{V}_j,\hat{\rho}\hat{V}_j^\dagger]), \tag{26}$$

and as a direct consequence of that the continuity equation acquires an additional term as well. This term is negligible if the magnitude of the coefficients a_j, b_j in the Lindblad operators [Eq. (6)] is small, i.e., in the case of weak dissipation, but it grows as the dissipation increases, which explains the behavior displayed in Fig. 2. As a conclusion, we may, in fact, say that in order for the probability density current defined in terms of the Wigner function as in Eq. (18) and the probability density, which is connected to the Wigner function via

$$\rho(x,t) = \int_{-\infty}^{+\infty} dp W(x,p,t), \tag{27}$$

to satisfy the continuity equation in the framework of the Lindblad theory, the additional term arising from the Lindblad operators needs to be incorporated into Eq. (23). This result is not obvious since one may expect that the effects of the environment are already accounted for in the time evolution of the Wigner function from which both the probability density and the current are derived; the considered example, however, clearly demonstrates that this alone is not sufficient and the additional term in the continuity equation is indeed necessary. At the same time, we emphasize that the reformulation of the latter does not imply a violation of the norm conservation since the total probability remains constant, i.e., the relation

$$\int_{-\infty}^{+\infty} dx \rho(x,t) = 1 \tag{28}$$

is still valid for all times. This is a consequence of the crucial property of the Lindblad equation to preserve the trace of the density matrix, which is well known.

As the last topic to be addressed here, we investigate how the previously discussed environmental effects on the TOA vary at different energies. In Table I, we present the asymptotic crossing probability $P(0,t\to\infty) = P_\infty$ [Eq. (17)] and the asymptotic tunneling probability $\mathcal{P}_T$ [Eq. (20)] for different dissipation strengths and initial energy expectation values. The latter can be tuned via the initial momentum expectation value p_0 and is given by

$$E_0 = \frac{1}{2m}\left(p_0^2 + \frac{\hbar^2}{4\Delta_x}\right) - \frac{m\omega^2}{2}(x_0^2 + \Delta_x). \tag{29}$$

Essentially, we observe the following behavior: at energies well below the barrier, the asymptotic tunneling probability increases with increasing dissipation, in accordance with the conclusion obtained in Ref. [51], while at high energies increasing dissipation has a suppressing effect. The asymptotic crossing probability shows qualitatively the same behavior at high energies. However, the enhancement through growing dissipation emerges only at very low energies and is much weaker than it is the case for the tunneling probability. This illustrates, once again, the non-negligibility of the additional Lindbladian term in the continuity equation which is responsible for the observed deviation.

IV. SUMMARY

We studied the effects of weak Markovian dissipation on the quantum arrival time using a parabolic potential barrier as a test case. In the framework of the Lindblad master equa-

TABLE I. The asymptotic crossing probabilities $P_\infty = P(0, t \to \infty)$ [Eq. (17)] and the asymptotic tunneling probability $\mathcal{P}_T$ [Eq. (20)] given for different dissipation strengths and initial momentum and energy expectation values. The latter are given with respect to the barrier peak at $E=0$. Positive energies imply that the particle is classically allowed to cross the barrier while for negative energies the opposite holds. All other parameters are as given in caption of Fig. 1, with $\epsilon = 0.01$.

p_0	−15.0		−14.0		−12.5		−12.0		−11.0		−10.0	
E_0	36.125		21.625		1.750		−4.375		−15.875		−26.375	
	P_∞	$\mathcal{P}_T$	P_∞	$\mathcal{P}_T$	P_∞	$\mathcal{P}_T$	P_∞	$\mathcal{P}_T$	P_∞	$\mathcal{P}_T$	P_∞	$\mathcal{P}_T$
$\xi = 10^{-3}$	0.829	0.830	0.736	0.738	0.560	0.563	0.497	0.500	0.372	0.375	0.259	0.262
$\xi = 10^{-2}$	0.762	0.778	0.675	0.695	0.526	0.551	0.474	0.500	0.372	0.399	0.278	0.305
$\xi = 10^{-1}$	0.538	0.635	0.486	0.591	0.407	0.523	0.381	0.500	0.330	0.454	0.281	0.409

tion, we derived an analytical expression for the probability density current in terms of the Wigner function from which a time-dependent expression for the approximate crossing probability was obtained. We also compared the results to earlier work devoted to quantum tunneling with dissipation, in particular the approximate crossing probability derived here in terms of the current with the tunneling probability defined in terms of the probability density. Also the influence of dissipation and initial energy on both these quantities was examined. We found the following:

(a) While for energies well above the barrier the total approximate crossing probability decreases, the peak of the TOA distribution is shifted to earlier times with increasing dissipation. This effect becomes more and more negligible as the temperature decreases.

(b) In the limit of vanishing dissipation and temperature, the approximate crossing probability and the tunneling probability approach the same value, which is reasonable since both should be identical in the case of unitary dynamics as a direct consequence of the continuity equation. However, for sufficiently large coefficients in front of the Lindblad operators, the additional term in the continuity equation that is emerging from the latter causes a noticeable deviation between the two probabilities.

(c) In the latter case, the probabilities differ not only in the absolute value but also in their dependence on the initial energy and dissipation. While the tunneling probability is suppressed by dissipation at high energies and enhanced at low energies, the latter aspect for the approximate crossing probability is much less pronounced and emerges only at very low energies.

We would like to conclude by pointing out some limits of the model adopted here, which should be considered when interpreting the results. The Markovian condition limits the range of dissipation strengths that can be chosen. Thus, we cannot draw a conclusion whether the results listed above also apply in case of strong dissipation. Furthermore, the choice of Lindblad operators and diffusion coefficients adopted here is mostly used to describe a damped harmonic oscillator, while in the present work the potential is not bounded from below. Still, in the vicinity of the origin one may hope that the physical effects of the environment are still represented sufficiently well, although, to the best of our knowledge, no rigorous proof of the validity of such an approach is known so far. Finally, it should be stressed that for more complicated potentials also the qualitative dependence of the TOA on the environment can be far more complex; the simple case studied here, however, should at least roughly reflect the main physical aspects.

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