# **Semiclassical theory of energy diffusive escape in a Duffing oscillator**

Alvise Verso and Joachim Ankerhold

*Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany* (Received 14 August 2010; published 12 November 2010)

Motivated by recent experimental progress to readout quantum bits implemented in superconducting circuits via the phenomenon of dynamical bifurcation, transitions between steady orbits in a driven anharmonic oscillator, the Duffing oscillator, are analyzed. In the regime of weak dissipation a consistent diffusion equation in the semiclassical limit is derived to capture the intimate relation between finite tunneling and reflection and bath induced quantum fluctuations. From the corresponding steady-state distribution an analytical expression for the switching probability is obtained. It is shown that a reduction of the transition rate due to finite reflection at the phase-space barrier is overcompensated by an increase due to environmental quantum fluctuations that are specific for diffusion processes over dynamical barriers. The scaling behavior of the rate is discussed and it is revealed that close to the bifurcation threshold the escape dynamics enters an overdamped domain such that the quantum-mechanical energy scale associated with friction even exceeds the thermal energy scale.

DOI: [10.1103/PhysRevE.82.051116](http://dx.doi.org/10.1103/PhysRevE.82.051116)

PACS number(s): 05.70.Ln, 82.20.Xr, 03.65.Sq, 03.67.-a

### **I. INTRODUCTION**

The prospect to tailor devices for quantum information processing has stimulated major experimental research in the past years. Several different technologies have been explored to assess the possibility to realize quantum bits, such as ion traps  $[1]$  $[1]$  $[1]$ , liquid state magnetic resonance, linear optics, electrons in liquid helium, and superconducting Josephson Junction (JJ) devices  $[2-4]$  $[2-4]$  $[2-4]$ . Particularly for the latter ones the insulation of the circuitry from its surrounding is of substantial relevance to suppress decoherence. This issue also includes the readout device of the qubit state which must be designed such as to minimize its back-action prior to the measurement on the one hand, but to efficiently gather the required information during the measurement on the other hand.

A powerful readout scheme is based on the phenomenon of dynamical bifurcation, realized in form of the Josephson bifurcation amplifier  $\lceil 5.6 \rceil$  $\lceil 5.6 \rceil$  $\lceil 5.6 \rceil$  and the cavity bifurcation amplifier  $[2]$  $[2]$  $[2]$ . A big JJ is placed in parallel to a Cooper-pair box and driven by an external microwave source. Accordingly, close to the first bifurcation threshold determined by the frequency and the amplitude of the drive, two stable oscillations appear in the big JJ with thermal fluctuations inducing transitions between them. The sensitivity of this process to the shape of the Josephson potential is used to retrieve information about the qubit state. However, the possibility to tune parameters over wide ranges makes these systems interesting on their own as devices to study fundamental aspects of driving, nonlinearity, and dissipation. In particular, the question about the impact of quantum fluctuations on transitions between two stable basins of attraction in phase space goes far beyond the standard situation for escape over static energy barriers.

Theoretically, within the relevant range the driven big JJ can be described as a Duffing oscillator  $[7]$  $[7]$  $[7]$ . This system is particularly important because it represents the simplest model to analyze phenomena such as bifurcation, period doubling, and dynamical tunneling. Its classical dynamics is well known. Transitions between the two stable states, induced by thermal fluctuations, have been investigated in detail  $[8,9]$  $[8,9]$  $[8,9]$  $[8,9]$ . With lowering temperature quantum-mechanical effects appear in basically three ways. First, the transmission probability through and the reflection probability from the phase space barrier become finite; second, zero-point fluctuations appear in the basins of attractions; and third, quantum fluctuations of the environment become relevant. For escape over static barriers, it turns out that for weak dissipation reflection from the barrier for energies above the transition energy may lead to a reduction of the escape rate as compared to the classical situation  $\lceil 10,11 \rceil$  $\lceil 10,11 \rceil$  $\lceil 10,11 \rceil$  $\lceil 10,11 \rceil$ . Thus, the question arises whether the same is true for transitions over dynamical barriers. Moreover, it has to be explored how a consistent semiclassical description for driven dissipative anharmonic systems must be formulated. To solve both issues is the purpose of this paper.

A powerful procedure for analytical investigations is to describe driven oscillators in a frame rotating with a frequency equal to the response frequency of the system  $[9,12]$  $[9,12]$  $[9,12]$  $[9,12]$ . Using this approach Dykman and Smelyanski analyzed the diffusive escape for the Duffing oscillator  $[13]$  $[13]$  $[13]$  and for other periodically driven systems  $\lceil 14 \rceil$  $\lceil 14 \rceil$  $\lceil 14 \rceil$ . The focus there has been on reservoir induced quantum effects. Complementary, in [[15](#page-9-8)] macroscopic quantum tunneling has been addressed in the deep quantum regime without accounting for environmental influences. A numerical description of the problem based on master equations in the intermediate regime, where the density of states in the stable basins appears still to be discrete, has been given in  $[16]$  $[16]$  $[16]$  and taking into account multiphoton resonances in  $[17]$  $[17]$  $[17]$ . In the present work we focus on the semiclassical regime with an almost dense spectrum in the basins and treat consistently all quantum processes starting from a properly derived diffusion equation. In contrast to  $[13-15]$  $[13-15]$  $[13-15]$  the impact of finite barrier reflection or tunneling and the whole structure of the quantum dissipative dynamics in the rotating frame  $\lceil 18 \rceil$  $\lceil 18 \rceil$  $\lceil 18 \rceil$  are included in this formulation. The corresponding analytical expressions for the escape rate apply to the range of weak damping and moderate temperatures. We note that in this domain a direct numerical evaluation of the escape process within a quantum-mechanical master equation as in  $[16]$  $[16]$  $[16]$  requires a very large basis set of system eigenstates and is thus not feasible for long times.

The paper is organized as follows. In Sec. [II](#page-1-0) we introduce the model and the basic notation including the mapping to the rotating frame. This description is extended in Sec. [III](#page-1-1) to explicitly include also the bath degrees of freedom. This formulation provides the basis to derive in Sec. [IV](#page-3-0) a semiclassical expansion of the master equation the steady-state distributions of which are used to derive the escape rates in Sec. [V.](#page-4-0) In Sec. [IV](#page-3-0) this quantum diffusion equation is discussed and the quantum corrections to the classical escape rate are obtained.

### <span id="page-1-0"></span>**II. SYSTEM AND MAPPING ON A ROTATING FRAME**

We consider a system with a weakly anharmonic potential driven by an external time-periodic force Duffing oscillator), namely,

<span id="page-1-4"></span>
$$
H_S(t) = \frac{1}{2M}p^2 + \frac{1}{2}M\omega_0^2 q^2 - \frac{1}{4}\Gamma q^4 + Fq\cos(\omega_d t). \tag{1}
$$

Accordingly, for the anharmonic coefficient, we assume  $\Gamma \langle q^2 \rangle \ll M \omega_0^2$  so that driving is almost resonant for

$$
\delta\omega = \omega_0 - \omega_d \leq \omega_d. \tag{2}
$$

Classically, when damping is taken into account, two stable oscillations with different amplitudes and phases appear beyond a bifurcation threshold. The latter one depends on external parameters such as driving amplitude *F* and frequency mismatch  $\delta \omega$ . In phase space, these two stable states correspond to stable basins of attraction which are separated by an unstable domain. Thermal fluctuations may induce transitions between these basins that in turn carry information about the global shape of the phase space barrier and the environment.

Theoretically, the difficulty for a rate description in this kind of system is that the Hamiltonian of the isolated system  $H<sub>S</sub>(t)$  is time dependent and, therefore, energy is not conserved. However, the dissipative system approaches a steadystate situation such that the reduced density matrix takes the form  $\rho(t) \sim \bar{\rho}(t) \cos(\omega_d t)$  with an only weakly time-dependent  $\overline{\rho}$ . For further analysis it is thus convenient to switch to a rotating frame, given by the unitary operator,

$$
U_S(t) = e^{-i\hat{a}^\dagger \hat{a}\omega_d t},\tag{3}
$$

where  $\hat{a} = \sqrt{2M/\hbar \omega_d} (\omega_d q + \frac{i}{M}p)$  and  $\hat{a}^\dagger = \sqrt{2M/\hbar \omega_d} (\omega_d q)$  $-\frac{i}{M}p$  are the annihilation and creation operators for *harmonic* oscillators in the system, respectively. The transformation  $U<sub>S</sub>(t)$  applied to the coordinate *q* and momentum *p* give

$$
U_S^{\dagger} q U_S = Q \cos(\omega_d t) + \frac{1}{\omega_d M} P \sin(\omega_d t), \tag{4}
$$

$$
U_S^{\dagger} p U_S = -\omega_d M Q \sin(\omega_d t) + P \cos(\omega_d t), \qquad (5)
$$

with  $Q$  and  $P$  as new (slowly varying) coordinates. From these equations it is clear that the unitary transformation is

<span id="page-1-2"></span>

FIG. 1. (Color online) The Hamiltonian function [from Eq. ([6](#page-1-3))] in the rotating frame for  $\alpha = 1/27$ . The energy is scaled with  $\omega_d M \delta \omega L^2$ . The minimum (m) and the maximum (a) in the figure are the stable sates with low and high amplitudes, respectively, separated by a marginal state (b).

the equivalent to a rotation of the classical phase space. In the rotating frame determined by  $U<sub>S</sub>(t)$  the Hamiltonian reads

<span id="page-1-3"></span>
$$
\tilde{H}_{S} = U_{S}^{\dagger} \left[ H - i\hbar \frac{\partial}{\partial t} \right] U_{S}
$$
\n
$$
= M \omega_{d} \delta \omega L^{2} \left[ -\frac{1}{4} \left( \frac{Q^{2}}{L^{2}} + \frac{P^{2}}{(L \omega_{d} M)^{2}} - 1 \right)^{2} + \frac{\sqrt{\alpha}}{L} Q \right] (6)
$$

with a length scale  $L = \sqrt{8\omega_d \delta \omega M/3\Gamma}$  and the bifurcation parameter

$$
\alpha = \frac{3F^2 \Gamma}{32(\omega_0 \delta \omega M)^3}.
$$
 (7)

Moreover following a rotating wave approximation fast oscillating terms  $\exp(\pm in \omega_d t)$ ,  $n \ge 1$ , are neglected such that a time independent Hamiltonian  $\tilde{H}_S$  is obtained. For  $0 < \alpha$  $\leq$  4/27 the rotating-frame system exhibits three extrema, whereas the two stable ones correspond in the laboratory frame to oscillations with low and high amplitudes, respectively. They are separated by a phase-space barrier associated with an unstable extremum (see Figs. [1](#page-1-2) and [2](#page-2-0)). For  $\alpha < 0$ only the low amplitude states exist and for  $\alpha$  > 4/27 only the high amplitude state remains.

### <span id="page-1-1"></span>**III. SYSTEM AND BATH: MICROSCOPIC DESCRIPTION**

In order to describe quantum dissipation, we explicitly introduce a bath coupled to the system, so that the total Hamiltonian in the rest frame is given by

<span id="page-2-0"></span>

FIG. 2. The energies  $E_m$  (solid),  $E_b$  (dotted), and  $E_a$  (dashed) of the minimum, of the marginal state, and of the maximum as functions of  $\alpha$ . The barrier height  $V_b \equiv E_b - E_m$  is maximal for  $\alpha = 0$  and vanishes for  $\alpha = 4/27$ . The energies are scaled with  $L^2 \omega_d M \delta \omega$ .

$$
H = H_S + H_R + H_I,\tag{8}
$$

<span id="page-2-2"></span>with a system part as in Eq.  $(1)$  $(1)$  $(1)$ , a reservoir part  $H_R$  and an interaction  $H_I$ , i.e.,  $[19,20]$  $[19,20]$  $[19,20]$  $[19,20]$ 

$$
H_R + H_I = \sum_{\alpha} \frac{p_{\alpha}^2}{2m_{\alpha}} + \frac{m_{\alpha}\omega_{\alpha}^2}{2} \left(x_{\alpha} - \frac{c_i}{m_{\alpha}\omega_{\alpha}^2} q\right)^2.
$$
 (9)

In order to systematically account for the interaction with the reservoir in the perturbative treatment discussed below, we switch to the rotating frame for the composite system  $[15,18]$  $[15,18]$  $[15,18]$  $[15,18]$ , i.e.,

<span id="page-2-1"></span>
$$
U(t) \equiv U_S(t)U_R(t) = \exp(-i\hat{a}^\dagger \hat{a}\omega_d t - i\sum_n^N \hat{b}_n^\dagger \hat{b}_n \omega_d t),
$$
\n(10)

whereas  $\hat{b}_n$  and  $\hat{b}_n^{\dagger}$  are annihilation and creation operators for harmonic oscillators in the bath. In the rotating frame the total Hamiltonian reads

$$
\widetilde{H} = \widetilde{H}_S + \widetilde{H}_R + \widetilde{H}_I, \tag{11}
$$

<span id="page-2-3"></span>with  $\widetilde{H}_S$  as in Eq. ([6](#page-1-3)) and

$$
\widetilde{H}_{R} = \sum_{n=1}^{N} \frac{p_n^2}{2\widetilde{m}_n} + \frac{\widetilde{m}_n}{2} \widetilde{\omega}_n^2 x_n^2,
$$
\n
$$
\widetilde{H}_{I} = -\sum_{n=1}^{N} \widetilde{c}_n \left( x_n Q + \frac{p_n}{\widetilde{\omega}_n \widetilde{m}_n} \frac{P}{\omega_d M} \right)
$$
\n
$$
+ \left( Q^2 + \frac{P^2}{(\omega_d M)^2} \right) \sum_{n=1}^{N} \frac{c_n^2}{4m_n \omega_n^2}, \tag{12}
$$

where the new bath parameters read as

$$
\widetilde{m}_n = \frac{m_n}{1 - \omega_d/\omega_n}, \quad \widetilde{\omega}_n = \omega_n - \omega_d, \quad \widetilde{c}_n = \frac{c_n}{2}.
$$
 (13)

With the unitary transformation  $(10)$  $(10)$  $(10)$  the total Hamiltonian *H* in the laboratory frame [Eq.  $(8)$  $(8)$  $(8)$ ] is mapped onto a new Hamiltonian  $\tilde{H}$  in the moving frame, composed of the system part [Eq.  $(6)$  $(6)$  $(6)$ ], a reservoir part [Eq.  $(12)$  $(12)$  $(12)$ ] with new parameters, and an interaction part  $[Eq. (12)]$  $[Eq. (12)]$  $[Eq. (12)]$ . The mapped composite system can now be described by techniques applied for undriven escape problems with the notable difference, though, which the interaction between system and environment becomes more complex containing in addition to the conventional position-position coupling, also momentummomentum contributions. However, as shown in  $\lceil 18 \rceil$  $\lceil 18 \rceil$  $\lceil 18 \rceil$ , following the standard procedure all bath properties can be captured by a spectral density and by temperature. Consequently, in the rotating frame we can adapt the ap-proach developed in [[11](#page-9-4)] for transition rates over energy barriers in the energy diffusive limit (weak dissipation).

One starts from the time evolution of the density matrix of the full compound  $W(t)$  obeying the Liouville–von Neumann equation  $i\hbar dW(t)/dt = [\tilde{H}, W(t)]$  with an initial state  $W(0)$ . The relevant operator is the reduced density  $\rho(t) = \text{tr}_B\{W(t)\}$ after eliminating the bath degrees of freedom for which a simple equation of motion does, in general, not exist. In case of weak friction and sufficiently fast bath modes, however, progress is made within a Born-Markov approximation. One then obtains a master equation which for the present case can be cast in the form  $\lceil 18 \rceil$  $\lceil 18 \rceil$  $\lceil 18 \rceil$ 

<span id="page-2-4"></span>
$$
i\hbar \frac{d\rho}{dt} = [\widetilde{H}_S, \rho] + \left( \mathcal{L}_{QQ} + \frac{\mathcal{L}_{QP}}{\omega_d M} + \frac{\mathcal{L}_{PQ}}{\omega_d M} + \frac{\mathcal{L}_{PP}}{(\omega_d M)^2} \right) [\rho].
$$
\n(14)

Here operators  $\mathcal{L}_{xy}$  are defined according to

$$
\mathcal{L}_{xy}[\rho] = \int_0^\infty ds K'_{xy}(s)[x,[y(-s),\rho(t)]]
$$

$$
+ \int_0^\infty ds i K''_{xy}(s)[x,\{y(-s),\rho(t)\}], \qquad (15)
$$

with operators  $y(s)$  in the Heisenberg representation and  $\{\}$ denoting the anticommutator. In the rotating frame the forceforce correlators are defined by

<span id="page-2-5"></span>
$$
K_{xy} = K'_{xy} + iK''_{xy} = \frac{1}{\hbar} \langle F_x(t) F_y(0) \rangle_{\beta}, \quad x, y = Q, P, \quad (16)
$$

<span id="page-2-6"></span>where the bath forces read according to Eq.  $(12)$  $(12)$  $(12)$ ,

$$
F_Q = \sum \tilde{c}_n x_n, \quad F_P = \sum \tilde{c}_n \frac{p_n}{\tilde{\omega}_n \tilde{m}_n}.
$$
 (17)

Our goal is now to derive from the above master equation  $[Eq. (14)]$  $[Eq. (14)]$  $[Eq. (14)]$  a semiclassical equation in the energy diffusive limit to determine the leading quantum corrections (order  $\hbar$ ) to the transition rates between the two phase-space basins. In case of no external driving the analysis in  $[11]$  $[11]$  $[11]$  revealed that a conventional position-position interaction between bath and system produces in the corresponding diffusion equation only quantum corrections of order  $\hbar^2$ . The leading impact of quantum mechanics is thus due to finite transmission through the barrier, i.e., tunneling and reflection. Here, however, we will see that while the contribution  $\mathcal{L}_{PP}$  has a behavior similar to  $\mathcal{L}_{OO}$ , the unconventional bath contributions  $\mathcal{L}_{OP}$  and  $\mathcal{L}_{PQ}$  yield a supplementary correction of order  $\hbar$  that dominates.

## **IV. SEMICLASSICAL MASTER EQUATION**

<span id="page-3-0"></span>As shown in  $\lceil 11 \rceil$  $\lceil 11 \rceil$  $\lceil 11 \rceil$  a semiclassical energy diffusion operator can be derived starting from a continuous occupation probability of a well state with energy *E* via

$$
P(E,t) = \sum_{n=0} \delta(E - E_n) p_n(t).
$$
 (18)

Here  $p_n$  is the occupation probability of a well eigenstate with quasienergy  $E_n$  and identical to the diagonal part of the reduced density matrix in the energy representation. The explicit construction of these states follows a type of WKB recipe as shown below. The time evolution  $[Eq. (14)]$  $[Eq. (14)]$  $[Eq. (14)]$  can now be represented (for details see  $[11]$  $[11]$  $[11]$ ) as

<span id="page-3-1"></span>
$$
\dot{P}(E,t) = \int dE' \left[ W_{E,E'} \frac{R(E')P(E',t)}{n(E')} - W_{E',E} \frac{R(E)P(E,t)}{n(E)} \right] - T(E) \frac{\omega(E)}{2\pi} P(E,t),
$$
\n(19)

with  $\omega(E)$  being the frequency of a classical oscillation at energy  $E$  and  $n(E)$  being the density of states. Equation ([19](#page-3-1)) captures the incoming probability flux to and outgoing probability flux from the state *E* according to intrawell transition rates  $[21]$  $[21]$  $[21]$ ,

<span id="page-3-2"></span>
$$
W_{E,E'} = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dt \operatorname{Tr}_R\{\langle E|\tilde{H}_I(t)|E'\rangle\langle E'|\tilde{H}_I|E\rangle \rho_R^{eq}\}, \quad (20)
$$

and reflection probabilities  $R(E)$  from the barrier and transmission probabilities  $T(E) = 1 - R(E)$  through the barrier. In the transition rates the system-reservoir coupling appears in the interaction picture  $\widetilde{H}_I(t) = e^{i(\widetilde{H}_S + \widetilde{H}_R)t/\hbar} \widetilde{H}_I e^{-i(\widetilde{H}_S + \widetilde{H}_R)t/\hbar}$  with  $\rho_R^{eq} = e^{\beta H_R}/Z_R$  being the equilibrium bath density matrix. Note that unitary transformation  $(10)$  $(10)$  $(10)$  does not affect the equilibrium density of the bath since  $[U_R, H_R] = 0$ .

The transition rates  $[Eq. (20)]$  $[Eq. (20)]$  $[Eq. (20)]$  can be evaluated explicitly in case of a bilinear system-bath coupling as in Eq.  $(12)$  $(12)$  $(12)$ , and one arrives at a golden rule type of formula

<span id="page-3-4"></span>
$$
W_{E,E'} = \frac{D_{QQ}(E - E')}{\hbar^2} [Q_{qm}(E',E)|^2 + |P_{qm}(E',E)|^2] + \frac{D_{QP}(E - E')}{\hbar^2} 2i \operatorname{Im}[Q_{qm}(E',E)^* P_{qm}(E',E)],
$$
\n(21)

with  $Q_{qm}(E', E) \equiv \langle E' | Q | E \rangle$ ,  $P_{qm}(E', E) \equiv \langle E' | P | E \rangle / (\omega_d M)$ , and  $Im[\cdot]$  denoting the imaginary part. The bath correlation functions  $D_{xy}$  represent the Fourier transforms of the bath correlations  $K_{xy}$  according to Eqs. ([16](#page-2-5)) and ([17](#page-2-6)), respectively,

$$
D_{xy}(E) = \hbar \int_{-\infty}^{\infty} dt K_{xy}(t) e^{itE/\hbar}.
$$
 (22)

In accordance with an effectively Markovian dynamics, we consider a purely Ohmic environment with a spectral density  $I(\omega) = M\gamma\omega$  in the laboratory frame. The bath correlation functions in the moving frame are then given by  $[18]$  $[18]$  $[18]$ 

<span id="page-3-3"></span>
$$
D_{QQ}(E) = \tilde{\gamma}M\{n_{\beta}(E_F + E)(E_F + E)
$$

$$
+ [n_{\beta}(E_F - E) + 1](E_F - E)\}, \tag{23}
$$

$$
D_{QP}(E) = i \tilde{\gamma} M \{- n_{\beta}(E_F + E)(E_F + E) + [n_{\beta}(E_F - E) + 1](E_F - E) \},
$$
 (24)

<span id="page-3-7"></span>whereas  $E_F = \hbar \omega_d$ ,  $\tilde{\gamma} = \gamma/4$  is the effective friction constant in the rotating frame, and  $n_\beta(E) = 1/(e^{\beta E}-1)$  is the Bose-Einstein distribution. Interestingly, Eq. ([23](#page-3-3)) reveals that physically two channels in the bath are now open and accessible for emission or absorption of quanta, namely, one with energy  $E_F + E$  and one with energy  $E_F - E$  [[18](#page-9-11)].

Following the procedure in  $[11]$  $[11]$  $[11]$  one arrives with  $P(E, t)$  $=f_{-\infty}^{\infty}P(E',t)\delta(E-E')dE'$  at an  $\hbar$  expansion of Eq. ([19](#page-3-1)) in the form

<span id="page-3-6"></span>
$$
\dot{P}(E,t) = \sum_{k=1}^{\infty} \left(\frac{\partial}{\partial E}\right)^k \frac{1}{k!} \int_{-\infty}^{\infty} d\delta W_{\delta}(E) (-\delta)^k
$$

$$
\times \frac{R(E)P(E,t)}{n(E)} - T(E) \frac{\omega(E)}{2\pi} P(E,t), \qquad (25)
$$

with  $W_{\delta}(E) = W_{E,E'}$  for  $E' - E = \delta$ , where  $\delta$  is considered to be of order  $\hbar$ . The leading-order terms in the above sum with  $k=1$  and  $k=2$  are kept to get the energy diffusion equation for finite transmission in the semiclassical limit, i.e.,

<span id="page-3-5"></span>
$$
\dot{P}(E,t) = \left[\frac{\partial}{\partial E} \left( -\langle \delta \rangle + \frac{\partial}{\partial E} \langle \delta^2 \rangle \right) R(E) - T(E) \frac{\omega(E)}{2\pi} \right] P(E,t).
$$
\n(26)

<span id="page-3-8"></span>Here, the moments of the energy fluctuations read as

$$
\langle \delta^k \rangle = \frac{1}{n(E)} \int_{-\infty}^{\infty} d\delta \frac{\delta^k}{k!} W_{\delta}(E). \tag{27}
$$

To derive semiclassical transition rates from this diffusion equation one must evaluate the energy momenta up to corrections of order  $\hbar$  and also include consistently transmission and reflection coefficients. Bath induced quantum corrections appear due to bath correlations  $D_{xy}$  that enter the transition rate  $W_{\delta}(E)$  [see Eq. ([21](#page-3-4))]. Finite tunneling and reflection coefficients appear explicitly in the diffusion equation Eq.  $(26)$  $(26)$  $(26)$ ] but must also be taken into account in the matrix elements  $Q_{qm}$  and  $P_{qm}$ , which determine the system part in the transition rates  $[Eq. (21)]$  $[Eq. (21)]$  $[Eq. (21)]$ . We note that quantum corrections due to tunneling and reflection are substantial in an energy range  $\sim \hbar \omega_b$  around the barrier top, where  $R(E_b) \sim T(E_b)$  $\sim 1/2 \sim O(\hbar^0)$ . They induce leading corrections in the escape rate that are of order  $\hbar$ . Quantum corrections that include combinations of a finite transmission and bath induced fluctuations are at least of order  $\hbar^2$  and can be discarded. The strategy we follow in the sequel is thus this: in a first step we neglect bath induced corrections and concentrate on the impact of tunneling, while in a second step tunneling is neglected and bath fluctuations are accounted for. Eventually, the corresponding individual energy diffusion equations derived from Eq.  $(25)$  $(25)$  $(25)$  are combined to capture both phenomena simultaneously.

### **V. SEMICLASSICAL TRANSITION RATES**

<span id="page-4-0"></span>In the energy range close to the barrier top, where the barrier becomes penetrable in the temperature range considered, the conventional WKB approximation "under" the barrier is not applicable because the classical turning points to the left and to the right are not sufficiently separated. In the domain around the marginal point (barrier top), however, the Hamiltonian  $\tilde{H}_s$  can be approximated by an inverted harmonic oscillator with barrier frequency  $\omega_b$  [see Eq. ([B3](#page-8-5))], and one may exploit the fact that the corresponding Schrödinger equation can be solved exactly. The proper eigenfunctions are then matched asymptotically (sufficiently away from the barrier top in the classically allowed range) onto WKB wave functions to determine phases and amplitudes of the latter ones. This way, one obtains

$$
\langle E|Q\rangle = \frac{1}{2} [\langle E|Q\rangle^- + r(E)\langle E|Q\rangle^+]
$$
 (28)

<span id="page-4-1"></span>with matrix elements

$$
\langle E|Q\rangle^{\pm} = N(E) \sqrt{\frac{2\omega(E)}{\pi \partial_P H_S(Q, E)}} e^{\pm (i/\hbar)S_0(E, Q) \mp (i\pi/4)}, (29)
$$

containing the action  $S_0(E, Q) = \int_{Q_1}^Q P(Q', E) dQ'$  of an orbit starting at the turning point  $Q_1$  and running in time *t* toward  $Q$  with momentum  $P(Q, E)$  at energy *E*. The complex-valued reflection amplitude  $r(E)$  of a parabolic barrier is related to the reflection probability  $R(E) = |r(E)|^2$ . The normalization follows from  $\langle E|E'\rangle = \delta(E-E')$  as

$$
N(E) = \frac{1}{\sqrt{\hbar \omega(E)}} \sqrt{\frac{2}{R(E) + 1}}.
$$
 (30)

In case of vanishing transmission,  $E \ll E_b$  and  $R \rightarrow 1$ , one recovers the standard WKB wave function  $N(E) \rightarrow \sqrt{1/(\hbar \omega)}$ , so that it is possible to use Eq.  $(29)$  $(29)$  $(29)$  for all energies, provided the length scale where a parabolic approximation for the barrier applies is much larger than the quantum-mechanical length scale  $\sqrt{\hbar / M \omega_b}$ .

With Eq.  $(29)$  $(29)$  $(29)$  we calculate in the semiclassical limit the transition matrix elements  $Q_{qm}(E',E)$  for finite transmission through the barrier. According to the restricted interference approximation  $\lceil 22 \rceil$  $\lceil 22 \rceil$  $\lceil 22 \rceil$  we only keep the diagonal contributions of forward or backward waves to obtain

$$
Q_{qm}(E',E) = N(E')N(E)[(Q_{\text{sc}}^{(\delta)})^* + r(E)r(E')^*Q_{\text{sc}}^{(\delta)}],
$$
\n(31)

where  $Q_{\text{sc}1}^{(\delta)}(E) \equiv \frac{1}{4} \int_{Q_1}^{Q_2} dQ \langle E' | Q \rangle^- Q \langle E | Q \rangle^+$  and  $Q_1, Q_2$  denote the left and the right turning points of the periodic orbit with energy  $E$ , respectively. The  $\hbar$  expansion for the matrix elements is thus found to read  $\lceil 11,23 \rceil$  $\lceil 11,23 \rceil$  $\lceil 11,23 \rceil$  $\lceil 11,23 \rceil$ 

$$
Q_{\text{scl}}^{(\delta)} = Q_{\text{cl}}^{(\delta)} + \delta \left[ \frac{1}{2} (Q_{\text{cl}}^{(\delta)})' + K_Q^{(\delta)} \right],\tag{32}
$$

where here and in the sequel the prime  $\prime$  at energy dependent functions denotes the derivative with respect to energy and

$$
Q_{\rm cl}^{(\delta)} = \frac{\hbar \omega(E)}{2\pi i \delta} \int_{Q_1(E)}^{Q_2(E)} dQ e^{-i\delta t(Q,E)/\hbar},\tag{33}
$$

$$
K_Q^{(\delta)} = -\frac{\hbar \omega(E)}{2\pi i \delta} Q(t, E)' e^{-i\delta t/\hbar} \Big|_{Q_1(E)}^{Q_2(E)}.
$$
 (34)

Likewise, we calculate the *P* matrix element

$$
P_{qm}(E',E) = N(E')N(E)[- (P_{\text{sc}}^{(\delta)})^* + r(E)r(E')^*P_{\text{sc}}^{(\delta)}],
$$
\n(35)

with  $P_{\text{sel}}^{(\delta)}(E) \equiv 1/4 \omega_d M \int_{Q_1}^{Q_2} dQ \langle E' | Q \rangle^{-} \hat{P} \langle E | Q \rangle^{+}$  and the expansion

$$
P_{\rm scl}^{(\delta)} = P_{\rm cl}^{(\delta)} + \frac{\delta}{2} (P_{\rm cl}^{(\delta)})',\tag{36}
$$

where

$$
P_{\rm cl}^{(\delta)} = \frac{\hbar \omega(E)}{2\pi \omega_d Mi \delta} \int_{P(Q_1,E)}^{P(Q_2,E)} dP e^{-i\delta t(p,E)/\hbar}.
$$
 (37)

<span id="page-4-2"></span>The combination of matrix elements in the transition probability  $[Eq. (21)]$  $[Eq. (21)]$  $[Eq. (21)]$  can then be rewritten as

$$
|Q_{qm}|^2 + |P_{qm}|^2 \approx N^4 \tilde{A} + \delta \tilde{B},
$$
  

$$
\text{Im}[Q_{qm}(E', E)^* P_{qm}(E', E)] \approx N^4 \tilde{C} + \delta \tilde{D},
$$
 (38)

with coefficients  $\tilde{A}$ ,  $\tilde{B}$ ,  $\tilde{C}$ , and  $\tilde{D}$  specified in Appendix A.

For escape processes near the bifurcation threshold, the energy-level spacings of the eigenstates of Eq. ([6](#page-1-3)) are small compared to  $\hbar \omega_d$ . Hence, the following approximation of the bath correlations  $(23)$  $(23)$  $(23)$  and  $(24)$  $(24)$  $(24)$  applies

$$
D_{QQ}(E) = \tilde{\gamma}M(\kappa - E) + O(\hbar^2),\tag{39}
$$

<span id="page-4-3"></span>where

$$
\kappa = \hbar \omega_d \coth(\hbar \beta \omega_d/2) \tag{40}
$$

<span id="page-4-4"></span>and

$$
D_{QP}(E) = i\tilde{\gamma}M\hbar\omega_d \frac{E}{|E|} + O(\hbar^2). \tag{41}
$$

It is important to note that to lowest order in the  $\hbar$  expansion  $D_{QQ}$  is of order  $\hbar^0$ , while  $D_{QP}$  is of order  $\hbar$ . Consequently, as we shall see later, the  $D_{QP}$  term in Eq. ([21](#page-3-4)) gives no contribution to the *classical* energy diffusion equation [see Eq.  $(46)$  $(46)$  $(46)$ ] but is relevant in the quantum realm.

Now, using Eqs.  $(38)$  $(38)$  $(38)$ ,  $(39)$  $(39)$  $(39)$ , and  $(41)$  $(41)$  $(41)$  the  $\hbar$  expansion of the transition probability  $[Eq. (21)]$  $[Eq. (21)]$  $[Eq. (21)]$  takes the form

<span id="page-4-5"></span>
$$
W_{\delta} = \frac{1}{\hbar^2} M \tilde{\gamma} N^4 \tilde{A} \kappa + \frac{\delta}{\hbar^2} M \tilde{\gamma} \left( -N^4 \tilde{A} + \kappa \tilde{B} - 2 \frac{\hbar \omega_d}{|\delta|} \tilde{C} \right). \tag{42}
$$

Close to the energy minimum of the stable domains, the energy-level spacing  $\delta$  is approximately  $\hbar \omega_m$ , with  $\omega_m$  being the minimum local frequency (see Appendix B). Close to the barrier top the energy-level spacings vanish, so that indeed  $\delta \sim \hbar$  or smaller and Eq. ([42](#page-4-5)) is a systematic semiclassical expansion.

### **VI. SEMICLASSICAL ESCAPE RATES**

Following the discussion at the end of Sec. [IV](#page-3-0) we start in this section to consider the influence of a finite barrier reflection or transmission in presence of a classical reservoir and then proceed to analyze the impact of bath induced quantum fluctuations for classical reflection or transmission. Both mechanisms are eventually combined in Sec. [V.](#page-4-0)

## **A. Finite transmission**

<span id="page-5-5"></span>With the transition probabilities at hand, the semiclassical diffusion equation follows from Eqs.  $(26)$  $(26)$  $(26)$  and  $(27)$  $(27)$  $(27)$  with the semiclassical density of states  $n(E) = \frac{1}{\hbar \omega(E)}$  as

<span id="page-5-2"></span>
$$
\dot{P}(E,t) = \left[\frac{\partial}{\partial E}C(E)\Delta(E)\left(1 + \frac{\kappa}{2}\frac{\partial}{\partial E}\right)R(E)\right] - T(E)\left[\frac{\omega(E)}{2\pi}P(E,t),\right]
$$
\n(43)

where

$$
C(E) = 2\frac{1 + R(E)^2}{[1 + R(E)]^2}
$$
 (44)

<span id="page-5-1"></span>and

$$
\Delta(E) = M \tilde{\gamma} \oint dQ \frac{dQ}{dt} + \frac{\tilde{\gamma}}{M \omega_d^2} \oint dP \frac{dP}{dt}.
$$
 (45)

The second term in the *generalized* action [Eq. ([45](#page-5-1))] stems from the *P*-matrix element  $\langle n|P|m\rangle^2$  in Eq. ([21](#page-3-4)). We emphasize that no terms originating from the mixed matrix elements  $\langle n|P|m\rangle\langle n|Q|m\rangle$  related to  $D_{QP}$  appear in Eq. ([21](#page-3-4)).

<span id="page-5-0"></span>For vanishing transmission  $(R=1, T=0)$  one recovers from Eq.  $(43)$  $(43)$  $(43)$  the classical diffusion operator

$$
\dot{P}(E,t) = \frac{\partial}{\partial E} \Delta(E) \left( 1 + \frac{\kappa}{2} \frac{\partial}{\partial E} \right) \frac{\omega(E)}{2\pi} P(E,t), \quad (46)
$$

which looks like a classical Kramers equation  $[24]$  $[24]$  $[24]$  with an effective temperature  $\kappa$ . Further,  $\Delta(E)$  corresponds to an energy relaxation coefficient that takes into account the position-position and the momentum-momentum interactions [Eq.  $(12)$  $(12)$  $(12)$ ] between system and bath. As shown in [[18](#page-9-11)] the bath correlation functions  $D_{OO}$  and  $D_{OP}$  are associated with two *different* effective temperatures due to the fact that a detailed balance condition is not obeyed in the moving frame. However, since in Eq.  $(46)$  $(46)$  $(46)$  [and in Eq.  $(43)$  $(43)$  $(43)$ ] the bath correlation function  $D_{OP}$  does not play any role, it is possible to define in this regime a unique effective temperature as  $k_B T_{\text{eff}} = \kappa/2$ .

Now, the escape rate is determined by the stationary nonequilibrium distribution  $P_{st}(E)$  to Eq. ([46](#page-5-0)), which is associated with a finite flux across the barrier and obeys the following boundary conditions:  $P_{st} = 0$  for  $E > E_b$  and  $P_{st}(E)$  $\rightarrow$  *P*<sub> $\beta$ </sub>(*E*) with a Boltzmann distribution *P*<sub> $\beta$ </sub> in the well region. Accordingly, one obtains for high barriers  $2V_b / \kappa \ge 1$ the classical Kramers result

$$
\Gamma_{\rm cl} = \frac{\omega_m \gamma \Delta(E_b)}{\kappa \pi} e^{-2V_b/\kappa},\tag{47}
$$

with the well frequency  $\omega_m$  [Eq. ([B2](#page-8-6))].

The escape rate in the quantum regime including tunneling or reflection (but no quantum fluctuations in the reser-voir) can now be evaluated also from Eq. ([43](#page-5-2)). This diffusion equation formally looks like the one already considered in  $\lceil 11 \rceil$  $\lceil 11 \rceil$  $\lceil 11 \rceil$  for undriven systems so that we can use the same methods to solve it. In the relevant energy range close the barrier top approximate Hamiltonian  $(B3)$  $(B3)$  $(B3)$  leads to the parabolic transmission and reflection probabilities,

$$
T = \frac{1}{1 + \exp\left(-\frac{2\pi(E - V_b)}{\hbar \omega_b}\right)},
$$
(48)

$$
R = \frac{1}{1 + \exp\left(\frac{2\pi(E - V_b)}{\hbar \omega_b}\right)}.
$$
(49)

<span id="page-5-3"></span>The quantum partition function in the harmonic well region is given by

$$
Z_0 = \frac{\kappa}{2\omega_m \hbar} \prod_{n=1}^{\infty} \frac{\nu_n^2}{\nu_n^2 + \omega_m^2 + \nu_n \gamma},
$$
(50)

with the Matsubara frequencies  $\nu_n = \pi n \kappa / \hbar$ . For vanishing friction, Eq.  $(50)$  $(50)$  $(50)$  reduces to the known result  $Z_{00}$  $= 1/[2 \sinh(\omega_m \hbar / \kappa)]$ . The escape rate follows again from a quasistationary nonequilibrium state, this time from the quasistationary energy distribution  $P_{st}(E)$  of Eq. ([43](#page-5-2)), given by

$$
\Gamma_{\text{scl}} = \int_0^\infty dE n(E) T(E) P_{\text{st}}(E). \tag{51}
$$

<span id="page-5-4"></span>This way one gains

$$
\Gamma_{\text{scl}} = \frac{\sinh(\omega_m \hbar / \kappa)}{(\omega_m \hbar / \kappa)} |B| \Gamma_{\text{cl}},\tag{52}
$$

<span id="page-5-6"></span>with the coefficients

$$
B = -\frac{1}{4}\frac{{}_2F_1\left[\frac{1}{2} - \frac{\theta}{2} - a, \frac{1}{2} - \frac{\theta}{2} + a, 1 - \theta, -\frac{4}{9}\right]}{{}_2F_1\left[\frac{1}{2} + \frac{\theta}{2} - a, \frac{1}{2} + \frac{\theta}{2} + a, 1 + \theta, -\frac{4}{9}\right]},
$$
(53)

$$
a = \sqrt{\frac{2\tilde{\gamma}\Delta(E_b)(1-\theta)^2/\kappa + 36\theta^2}{8\tilde{\gamma}\Delta(E_b)/\kappa}},
$$
 (54)

and the abbreviation  $\theta = \omega_b \hbar / (\pi \kappa)$ . The first factor in this rate expression captures quantum effects (zero-point fluctuations) in the well distribution, while the second one,  $|B|$ , describes the impact of finite barrier transmission close to the top. The latter one can actually prevail and lead to a reduction of the escape rate compared to the classical situation due to a finite reflection from the barrier also for energies *E*  $\geq E_b$  (see Fig. [3](#page-6-0)). For a fixed  $\tilde{\gamma}$ , the expansion of Eq. ([52](#page-5-4)) for high temperatures is  $[11]$  $[11]$  $[11]$ 

<span id="page-6-0"></span>

FIG. 3. Escape rate [Eq. ([55](#page-6-6))] normalized to the classical rate as a function of the bifurcation parameter  $\alpha$  for  $\hbar \omega_d \beta / (2\pi) = 0.01$ (solid),  $\hbar \omega_d \beta / (2\pi) = 0.05$  (dashed), and  $\hbar \omega_d \beta / (2\pi) = 0.1$  (dotted). For all the lines, we use  $\beta L^2 \omega_d M \delta \omega = 40$ ,  $\delta \omega = 0.1 \omega_0$ , and the dimensionless friction constant  $\beta \tilde{\gamma} M L^2 \delta \omega = 0.1$ .

$$
\Gamma_{\rm scl} = \Gamma_{\rm cl}(1 - b_1 \theta),\tag{55}
$$

<span id="page-6-6"></span>with  $b_1 = 1.04$  originating merely from the expansion of *B*. The well partition function leads to corrections of higher order in  $\hbar$ .

#### **B. Bath induced fluctuations**

<span id="page-6-5"></span>In this section we calculate the impact of the friction terms  $\mathcal{L}_{QP}$  and  $\mathcal{L}_{PQ}$  in Eq. ([14](#page-2-4)) on the energy diffusive decay. According to the above strategy, we assume here to have classical transmission and reflection probabilities and calculate from Eq.  $(25)$  $(25)$  $(25)$  the first-order  $\hbar$  correction to the classical diffusion equation [Eq.  $(46)$  $(46)$  $(46)$ ].

For  $R=1$ ,  $T=0$  the matrix elements  $|Q_{qm}|$  and  $|P_{qm}|$  are symmetric with respect to  $\delta$ , and therefore the terms in the first line of Eq.  $(21)$  $(21)$  $(21)$  do not give contributions of order  $\hbar$  to the diffusion equation  $[25,26]$  $[25,26]$  $[25,26]$  $[25,26]$ . The only relevant contributions of order  $\hbar$  result from the  $\text{Im}[Q_{qm}(E',E)^*P_{qm}(E',E)]$ term. To calculate it, we must take into account also the next order term in the expansion of the respective bath correlation function, namely,

$$
D_{QP}(E) \approx i\,\tilde{\gamma}M \left[\hbar\,\omega_d \frac{E}{|E|} + a\hbar|E|\right] + O(\hbar^3),\tag{56}
$$

with  $a = [\beta \omega_d - \sinh(\hbar \omega_d \beta)/\hbar]/[\cosh(\hbar \omega_d \beta) - 1]$ . We recall that energy-level spacings are considered to be proportional to  $\hbar$ . Accordingly, from Eq. ([25](#page-3-6)) we obtain the energy diffusion equation,

<span id="page-6-2"></span>
$$
\dot{P}(E,t) = \left\{ \frac{\partial}{\partial E} \tilde{\gamma} \left[ \Delta - 2\hbar a \Delta^{(1)} \right] + \left( \Delta \frac{\kappa}{2} + \hbar \omega_d \Delta^{(1)} \right) \frac{\partial}{\partial E} \right] \right\} \frac{\omega}{2\pi} P(E,t), \quad (57)
$$

<span id="page-6-1"></span>where

$$
\Delta^{(1)}(E) = \frac{8M\pi\tilde{\gamma}}{\hbar}N^4 \int_0^\infty d\delta \delta^2 \operatorname{Im}[Q_{\rm cl}^* P_{\rm cl} + Q_{\rm cl}^* P_{\rm cl}^*].
$$
 (58)

For an explicit evaluation of Eq.  $(58)$  $(58)$  $(58)$  it is convenient to return to a discrete representation by replacing the energy difference  $\delta$  with  $\hbar l \omega$  and  $\int d\delta$  with  $\Sigma_l \hbar \omega$  so that

<span id="page-6-4"></span>

FIG. 4. Escape rate  $[Eq. (60)]$  $[Eq. (60)]$  $[Eq. (60)]$  normalized to the classical rate as a function of  $\alpha$  for  $\hbar \omega_d \beta/(2\pi) = 0.01$  (solid),  $\hbar \omega_d \beta/(2\pi) = 0.05$ (dashed), and  $\hbar \omega_d \beta/(2\pi) = 0.1$  (dotted). For all the lines, we use  $\delta \omega = 0.1 \omega_0$  and  $\beta L^2 \omega_d M \delta \omega = 40$ .

$$
\Delta^{(1)}(E) = \tilde{\gamma} 8M \pi \omega \sum_{l=0}^{\infty} l^2 \operatorname{Im} [Q_{\text{cl}}^* P_{\text{cl}} + Q_{\text{cl}}^* P_{\text{cl}}^*]. \tag{59}
$$

This expression is correct for low energies, where the spectrum in the wells is discrete and approximates Eq.  $(58)$  $(58)$  $(58)$  very accurately for energies near the barrier top.

In order to reveal the effects of the  $\mathcal{L}_{OP}$  and  $\mathcal{L}_{PO}$  terms, we calculate the rate of escape from Eq.  $(57)$  $(57)$  $(57)$ . Following the standard procedure  $[24]$  $[24]$  $[24]$  one finds

$$
\Gamma_{\rm scl} = \Gamma_{\rm cl} e^{\theta_F b_2},\tag{60}
$$

<span id="page-6-7"></span><span id="page-6-3"></span>where

$$
b_2 = \frac{4\pi}{\omega_d \kappa} (a\kappa + \omega_d) \int_{E_m}^{E_b} dE \frac{\Delta^{(1)}(E)}{\Delta(E)},
$$
 (61)

with  $\theta_F = \hbar \omega_d / (\kappa \pi)$ .  $E_m$  and  $E_b$  are the energies of points (a) and (b), respectively, in Fig. [1.](#page-1-2) The integral in Eq.  $(61)$  $(61)$  $(61)$  is proportional to the barrier height meaning that Eq.  $(61)$  $(61)$  $(61)$  is on the order of  $\beta V_b$ . It thus gives a significant contribution to the escape rate as depicted in Fig. [4](#page-6-4) for various temperatures.

### **VII. DISCUSSION**

In Secs. [VI A](#page-5-5) and [VI B,](#page-6-5) we have analyzed separately the impact of the two dominant quantum effects on the escape rate including contributions of order  $\hbar$ . Since corrections due to the combination of the two effects in the transition probabilities are at least of order  $\hbar^2$ , a full semiclassical diffusion equation up to order  $\hbar$  is obtained by adding the quantum corrections in the respective diffusion coefficients of Eqs.  $(57)$  $(57)$  $(57)$  and  $(43)$  $(43)$  $(43)$ . Hence, we get

$$
\dot{P}(E,t) = \left[ \frac{\partial}{\partial E} \left( \Delta CR - \hbar 2a \Delta^{(1)} + \Delta C \frac{\kappa}{2} \frac{\partial}{\partial E} R + \hbar \omega_d \Delta^{(1)} \frac{\partial}{\partial E} \right) - T \right] \frac{\omega}{2\pi} P(E,t).
$$
\n(62)

The leading-order quantum corrections to the escape rate are then found as

$$
\Gamma_{\text{scl}} = \Gamma_{\text{cl}} \left[ 1 + \theta_F \left( -b_1 \frac{\omega_b}{\omega_d} + b_2 \right) \right]. \tag{63}
$$

<span id="page-7-2"></span>The first correction is negligible when  $\omega_b \ll \omega_d$ , i.e., when  $\alpha$ approaches the boundaries of the bifurcation range  $(\alpha \rightarrow 0)$ and  $\alpha \rightarrow 4/27$ ). Interestingly, the two types of quantum fluctuations have opposite effects on the escape process: while a finite reflection for energies above the barrier top leads to a suppression of the escape probability (Fig.  $3$ ), bath induced fluctuations produce a substantial increase (Fig. [4](#page-6-4)). The conclusion is thus that in the semiclassical regime finite tunneling through the phase-space barrier does not play an important role, in contrast to quantum fluctuations induced by the reservoir in the moving frame. We recall that the opposite is true for energy diffusive escape processes over static barriers where tunneling leads to a reduction of the rate  $[11]$  $[11]$  $[11]$ .

An interesting issue that has been discussed in the literature recently  $\left[16,27\right]$  $\left[16,27\right]$  $\left[16,27\right]$  $\left[16,27\right]$  is the scaling of the escape rate with respect to the distance in parameter space to the bifurcation point  $\alpha_c$ = 4/27. Accordingly, one writes  $\ln \Gamma | \alpha (\alpha_c - \alpha)$ <sup>§</sup> with a characteristic scaling exponent  $\xi$ . In the classical re-gime it was found [[27](#page-9-20)] that  $\xi = 3/2$  in agreement with experimental observations  $\lceil 5 \rceil$  $\lceil 5 \rceil$  $\lceil 5 \rceil$ . In contrast, the analysis in the quantum domain led to the numerical prediction  $\xi \sim 1$  [[16](#page-9-9)[,28](#page-9-21)]. In view of these findings the above semiclassical rate expression can now be analyzed. Of course, the leading exponential part gives rise to  $\ln(\Gamma_{\text{sel}}) \sim 2V_b / \kappa \sim (\alpha_c - \alpha)^{3/2}$ , so that  $\xi$  $= 3/2$  as expected. However, the quantum contributions display different scaling behaviors: the contribution due to finite tunneling scales with the barrier frequency as  $(\alpha_c - \alpha)^{1/4}$ , while a numerical fit to the environmental contribution Eq. ([61](#page-6-3)) provides  $\xi \sim 1.6$ . The conclusion is thus that the impact of the environment is associated with a scaling exponent  $\xi$  $\approx$  3/2 also in the semiclassical range. The different scaling behaviors of tunneling induced contributions with a substantial smaller exponent may be seen as signature of a changeover when one approaches the full quantum regime. Our analytical results thus support the numerical findings in  $[16]$  $[16]$  $[16]$ .

To end this discussion, it is appropriate to specify the range of validity of the above rate expression. One has to impose that

$$
V_b(\alpha) \ge \kappa \ge \hbar \omega_m(\alpha), \hbar \omega_b(\alpha) \tag{64}
$$

in order to guarantee the existence of a steady-state distribution of a quasicontinuum of thermally smeared states on the one hand and to restrict tunneling to energies close to the barrier top on the other hand. Equivalently, the range of validity is determined by those values of  $\alpha$  which are sufficiently smaller than  $\alpha_c$  (where  $V_b \rightarrow 0$ ) (see Fig. [5](#page-7-0)).

We also have to assume weak dissipation compared to the retardation scale  $\hbar / \kappa$  of the reservoir and to the time scale of the moving frame dynamics  $1/\omega_b$ ,  $1/\omega_m$  for the Born-Markov approximation to be applicable. However, for  $\alpha = 0$ the barrier height stays finite, while  $\omega_b$  tends to zero like  $\alpha^{1/4}$ and the effective mass  $M_b$  [see Eq. ([B3](#page-8-5))] tends to infinity like  $\alpha^{-1/2}$ . The growth of the mass is equivalent to an increase of friction which is most clearly taken into account when one works with a rescaled damping constant  $\gamma_b \equiv \tilde{\gamma} \alpha^{-1/2}$ . Then,

<span id="page-7-0"></span>

FIG. 5. The dimensionless barrier height  $V_b/(L^2 \omega_d M \delta \omega)$  (solid line), the well frequency  $\omega_m/\omega_d$  (dotted line), and the barrier frequency  $\omega_b/\omega_d$  (dashed line) as functions of the bifurcation parameter  $\alpha$  for  $\delta \omega / \omega_d = 0.1$ .

for decreasing  $\alpha$  the effective friction  $\gamma_b/\omega_b$  grows (see Fig. [6](#page-7-1)), meaning that for very small  $\alpha$  the motion near the barrier becomes overdamped.

Higher-order corrections in the friction can be accounted for in the underdamped regime on the one hand through  $\omega_b$  $\rightarrow \lambda_b$  in the prefactor *B* in Eq. ([53](#page-5-6)), where the Grote-Hynes frequency  $\lambda_h$  [[29](#page-9-22)] is given by

$$
\lambda_b = \sqrt{\frac{\tilde{\gamma}^2}{4} + \omega_b^2} - \frac{\tilde{\gamma}}{2}.
$$
 (65)

On the other hand, the friction dependence of the partition function can be included via  $[11]$  $[11]$  $[11]$ 

<span id="page-7-3"></span>
$$
\Gamma_{\text{scl}} = \prod_{n=1}^{\infty} \frac{\nu_n^2 - \omega_b^2}{\nu_n^2 - \omega_b^2 + \nu_n \tilde{\gamma}} \Gamma_{\text{cl}} \left[ 1 + \theta_F \left( -b_1 \frac{\lambda_b}{\omega_d} + b_2 \right) \right],\tag{66}
$$

with the Matsubara frequencies  $\nu_n = 2\pi n/\hbar \beta$ . Note that the motion in the well remains always in the strongly underdamped regime  $\omega_m / \tilde{\gamma} \leq 1$ .

<span id="page-7-1"></span>

FIG. 6. Typical behavior of the effective friction  $\gamma$ <sub>b</sub>. For sufficiently large  $\alpha$ , where  $\gamma_b < \omega_b$ ,  $\kappa/\hbar$ , the rate expressions [Eq. ([63](#page-7-2))] for weak friction, and its extension to somewhat larger friction Eq. ([66](#page-7-3))] apply. In the range  $\omega_b < \gamma_b < \kappa/\hbar$  the dynamics of the escape process in the barrier range follows a classical Smoluchowski equation, which turns into a quantum Smoluchowski equation for  $\gamma_b$  $> \omega_b, \kappa/\hbar$ .

With further decreasing  $\alpha$  the motion near the barrier becomes overdamped,  $\gamma_b > \omega_b$ . A classical description applies as long as  $\hbar \gamma_b < \kappa$  (light gray region in Fig. [6](#page-7-1)) [[30](#page-9-23)[,31](#page-9-24)], leading to a classical Smoluchowski rate  $\lceil 32 \rceil$  $\lceil 32 \rceil$  $\lceil 32 \rceil$ . Eventually, for very small  $\alpha$ , friction becomes so strong that the quantum energy scale for friction even exceeds the thermal scale, i.e.,  $\hbar \gamma_b$   $\geq$   $\kappa$  (dark gray region in Fig. [6](#page-7-1)). Accordingly, the classical Smoluchowski dynamics turns into the quantum Smoluchowski range  $\left[30,31,33\right]$  $\left[30,31,33\right]$  $\left[30,31,33\right]$  $\left[30,31,33\right]$  $\left[30,31,33\right]$ .

### **VIII. CONCLUSIONS**

In this paper we analyzed the impact of quantum fluctuations on the escape process in case of a dynamical barrier and in presence of a dissipative environment. In the energy diffusive domain of weak friction and higher temperatures a semiclassical procedure allows us to derive effective diffusion equations, including leading-order quantum effects. It turns out that there are two dominant mechanisms for quantum fluctuations to appear, namely, finite transmission through and reflection from the barrier and reservoir induced quantum fluctuations in the moving frame. The latter ones dominate by far and lead to a substantial enhancement of the classical escape rate. This enhancement is related to positionmomentum terms in the system-bath interaction that appear in the rotating-frame description and are thus a direct consequence of the external driving on the dissipation. Our analytical results for the escape rate indicate a changeover in the scaling behavior when one tunes the systems from the classical to the quantum domain.

Interestingly, when the bifurcation parameter tends to zero, the strongly underdamped dynamics turns into an overdamped motion around the barrier top with friction strengths that may even exceed the thermal energy scale. This quantum Smoluchowski domain that so far has only been studied for escape over static barriers (see, e.g.,  $[30,31]$  $[30,31]$  $[30,31]$  $[30,31]$ ) will be addressed in a future publication.

### **ACKNOWLEDGMENTS**

The authors thank V. Peano for fruitful discussion. Financial support was provided by the German Israeli Foundation (GIF) and the Landesstiftung BW.

# **APPENDIX A: COEFFICIENTS FOR TRANSITION MATRIX ELEMENTS**

Here we collect the coefficients appearing in the  $\hbar$  expansion of  $|Q_{qm}|^2 + |P_{qm}|^2$  and Im $[Q_{qm}^*P_{qm}^*2]$  in Eq. ([38](#page-4-2)). One has

$$
\tilde{A} = (|Q_{\text{cl}}^{(\delta)}|^2 + |P_{\text{cl}}^{(\delta)}|^2)(R^2 + 1) + R(Q_{\text{cl}}^{(\delta)^2} + Q_{\text{cl}}^{(\delta)^2} - P_{\text{cl}}^{(\delta)^2} - P_{\text{cl}}^{(\delta)^2}),
$$
\n
$$
\tilde{B} = \frac{1}{2}(\tilde{N}^4\tilde{A})' + \tilde{N}^4[-rr^{*'}(Q_{\text{cl}}^{(\delta)^2} - P_{\text{cl}}^{(\delta)^2}) - r^{*}r'(Q_{\text{cl}}^{(\delta)^2} - P_{\text{cl}}^{(\delta)^2}) + (R^2 + 1)(Q_{\text{cl}}^{(\delta)}K_Q^{(\delta)^*} + Q_{\text{cl}}^{(\delta)^*}K_Q^{(\delta)}) + 2R(Q_{\text{cl}}^{(\delta)}K_Q^{(\delta)} + Q_{\text{cl}}^{(\delta)^*}K_Q^{(\delta)^*})],
$$
\n
$$
\tilde{C} = \tilde{N}^4 \operatorname{Im}[(Q_{\text{cl}}^{(\delta)^*}P_{\text{cl}}^{(\delta)} - R^2Q_{\text{cl}}^{(\delta)}P_{\text{cl}}^{(\delta)^*} + R(Q_{\text{cl}}^{(\delta)}P_{\text{cl}}^{(\delta)} - Q_{\text{cl}}^{(\delta)^*}P_{\text{cl}}^{(\delta)^*})],
$$
\n(A1)

$$
\widetilde{D} = \frac{1}{2} (\widetilde{N}^4 \widetilde{C})' + \widetilde{N}^4 \left[ r r^{*} Q_{\text{cl}}^{(\delta)^*} P_{\text{cl}}^{(\delta)^*} - r^* r' Q_{\text{cl}}^{(\delta)} P_{\text{cl}}^{(\delta)} - R^2 P_{\text{cl}}^{(\delta)^*} K^{(\delta)} \right. \\
\left. + P_{\text{cl}}^{(\delta)} K^{(\delta)^*} + R (P_{\text{cl}}^{(\delta)} K^{(\delta)} + P_{\text{cl}}^{(\delta)^*} K^{(\delta)^*}) \right].
$$
\n(A2)

#### **APPENDIX B: POTENTIAL**

Close to its minimum  $[Q = Q_m(\alpha), P = 0]$ , Hamiltonian ([1](#page-1-4)) can be approximated by

$$
H_{\text{eff}}^{(m)} = \frac{P^2}{2M_m} + V_{\text{eff}}^{(m)}(Q),\tag{B1}
$$

where the effective mass is determined by

$$
M_m^{-1} = \left. \frac{\partial^2 \widetilde{H}_S}{\partial P^2} \right|_m = \frac{\delta \omega}{M \omega_d} \left( 1 - \frac{Q_m^2}{L^2} \right),
$$

<span id="page-8-6"></span>and the effective potential is  $V_{\text{eff}}^{(m)}(Q) = \frac{1}{2} M_m \omega_m^2 Q^2$  with the frequency

$$
\omega_m = \delta \omega \sqrt{\frac{1 - 3Q_m^2}{1 - Q_m^2}}.
$$
 (B2)

<span id="page-8-5"></span>In the same way it is possible to approximate the system Hamiltonian close to the saddle point  $[Q = Q_b(\alpha), P = 0]$  by

$$
H_{\text{eff}}^{(b)} = \frac{P^2}{2M_b} + \frac{1}{2}M_b \omega_b^2 Q^2, \tag{B3}
$$

with  $M_b^{-1} = \delta \omega / (M \omega_d) (1 - (Q_b/L)^2)$  and

$$
\omega_b = \delta \omega \sqrt{\frac{1 - 3(Q_b/L)^2}{1 - (Q_b/L)^2}}.
$$
 (B4)

- <span id="page-8-0"></span>1 T. Monz, K. Kim, A. S. Villar, P. Schindler, M. Chwalla, M. Riebe, C. F. Roos, H. Häffner, W. Hänsel, M. Hennrich, and R. Blatt, *[Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.103.200503)* **103**, 200503 (2009).
- <span id="page-8-1"></span>2 D. Vion, A. Assime, A. Cottet, P. Joyez, H. Pothier, C. Urbina, D. Esteve, and M. H. Devoret, [Science](http://dx.doi.org/10.1126/science.1069372) 296, 886 (2002).
- [3] J. Claudon, F. Balestro, F. W. J. Hekking, and O. Buisson, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.93.187003) 93, 187003 (2004).
- <span id="page-8-2"></span>4 J. Koch, T. M. Yu, J. Gambetta, A. A. Houck, D. I. Schuster, J. Majer, A. Blais, M. H. Devoret, S. M. Girvin, and R. J. Schoelkopf, *[Phys. Rev. A](http://dx.doi.org/10.1103/PhysRevA.76.042319)* **76**, 042319 (2007).
- <span id="page-8-3"></span>5 I. Siddiqi, R. Vijay, F. Pierre, C. M. Wilson, M. Metcalfe, C. Rigetti, L. Frunzio, and M. H. Devoret, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.93.207002) **93**, [207002](http://dx.doi.org/10.1103/PhysRevLett.93.207002) (2004).
- <span id="page-8-4"></span>6 I. Siddiqi, R. Vijay, F. Pierre, C. M. Wilson, L. Frunzio, M.

Metcalfe, C. Rigetti, R. J. Schoelkopf, M. H. Devoret, D. Vion, and D. Esteve, *[Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.94.027005)* **94**, 027005 (2005).

- <span id="page-9-0"></span>7 V. Manucharyan, E. Boaknin, M. B. Metcalfe, R. Vijay, I. Siddiqi, and M. H. Devoret, *[Phys. Rev. B](http://dx.doi.org/10.1103/PhysRevB.76.014524)* **76**, 014524 (2007).
- <span id="page-9-1"></span>8 M. I. Dykman and M. A. Krivoglaz, Zh. Eksp. Teor. Fiz. **77**, 60 (1979) [Sov. Phys. JETP **50**, 30 (1979)].
- <span id="page-9-2"></span>9 M. I. Dykman and M. A. Krivoglaz, [Physica A](http://dx.doi.org/10.1016/0378-4371(80)90010-2) **104**, 480  $(1980).$  $(1980).$  $(1980).$
- <span id="page-9-3"></span>10 P. Hänggi, P. Talkner, and M. Borkovec, [Rev. Mod. Phys.](http://dx.doi.org/10.1103/RevModPhys.62.251) **62**, 251 ([1990](http://dx.doi.org/10.1103/RevModPhys.62.251)).
- <span id="page-9-4"></span>[11] A. Verso and J. Ankerhold, *[Phys. Rev. A](http://dx.doi.org/10.1103/PhysRevA.79.022115)* **79**, 022115 (2009).
- <span id="page-9-5"></span>[12] M. I. Dykman, C. M. Maloney, V. N. Smelyanskiy, and M. Silverstein, *[Phys. Rev. E](http://dx.doi.org/10.1103/PhysRevE.57.5202)* 57, 5202 (1998).
- <span id="page-9-6"></span>13 M. I. Dykman and V. N. Smelyanski, Zh. Eksp. Teor. Fiz. **94**, 61 (1988) [Sov. Phys. JETP **67**, 1769 (1988)].
- <span id="page-9-7"></span>14 M. Marthaler and M. I. Dykman, [Phys. Rev. A](http://dx.doi.org/10.1103/PhysRevA.73.042108) **73**, 042108  $(2006).$  $(2006).$  $(2006).$
- <span id="page-9-8"></span>15 I. Serban and F. K. Wilhelm, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.99.137001) **99**, 137001  $(2007).$  $(2007).$  $(2007).$
- <span id="page-9-9"></span>[16] L. Guo, Z. Zheng, and X. Li, **EPL 90**[, 10011](http://dx.doi.org/10.1209/0295-5075/90/10011) (2010).
- <span id="page-9-10"></span>[17] V. Peano and M. Thorwart, [Chem. Phys.](http://dx.doi.org/10.1016/j.chemphys.2005.06.047) **322**, 135 (2006).
- <span id="page-9-11"></span>[18] A. Verso and J. Ankerhold, *[Phys. Rev. A](http://dx.doi.org/10.1103/PhysRevA.81.022110)* **81**, 022110 (2010).
- <span id="page-9-12"></span>19 U. Weiss, *Quantum Dissipative Systems* World Scientific, Singapore, 2007).
- <span id="page-9-13"></span>[20] A. O. Caldeira and A. J. Leggett, *[Physica A](http://dx.doi.org/10.1016/0378-4371(83)90013-4)* **121**, 587 (1983).
- <span id="page-9-14"></span>21 H. P. Breuer and F. Petruccione, *The Theory of Open Quantum* Systems (Oxford University Press, Oxford, 2002).
- <span id="page-9-15"></span>[22] R. M. More and K. H. Warren, [Ann. Phys.](http://dx.doi.org/10.1016/0003-4916(91)90060-L) **207**, 282 (1991).
- <span id="page-9-16"></span>[23] R. Karrlein and H. Grabert, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.475906) **108**, 4972 (1998).
- <span id="page-9-17"></span>[24] H. A. Kramers, *Physica ([Amsterdam](http://dx.doi.org/10.1016/S0031-8914(40)90098-2))* 7, 284 (1940).
- <span id="page-9-18"></span>[25] S. Linkwitz and H. Grabert, *[Phys. Rev. B](http://dx.doi.org/10.1103/PhysRevB.44.11888)* 44, 11888 (1991).
- <span id="page-9-19"></span>[26] S. Linkwitz and H. Grabert, *[Phys. Rev. B](http://dx.doi.org/10.1103/PhysRevB.44.11901)* 44, 11901 (1991).
- <span id="page-9-20"></span>[27] M. I. Dykman, *[Phys. Rev. E](http://dx.doi.org/10.1103/PhysRevE.75.011101)* **75**, 011101 (2007).
- <span id="page-9-21"></span>[28] A. P. Dimitriev, M. I. Dyakonov, and F. Ioffe, Zh. Eksp. Teor. Fiz. **90**, 1430 (1986) [Sov. Phys. JETP **63**, 838 (1986)].
- <span id="page-9-22"></span>[29] R. F. Grote and J. T. Hynes, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.440485) **73**, 2715 (1980).
- <span id="page-9-23"></span>30 J. Ankerhold, P. Pechukas, and H. Grabert, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.87.086802) **87**, [086802](http://dx.doi.org/10.1103/PhysRevLett.87.086802) (2001); J. Ankerhold and H. Grabert, *ibid*. **101**(E), [119903](http://dx.doi.org/10.1103/PhysRevLett.101.119903) (2008).
- <span id="page-9-24"></span>[31] S. A. Maier and J. Ankerhold, *[Phys. Rev. E](http://dx.doi.org/10.1103/PhysRevE.81.021107)* **81**, 021107 (2010).
- <span id="page-9-25"></span>[32] H. Risken, *The Fokker Planck Equation* (Springer, Berlin, 1984).
- <span id="page-9-26"></span>33 J. Ankerhold, *Quantum Tunneling in Complex Systems* (Springer, Berlin, 2007).