

Chapter 15

Tunneling in open quantum systems

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Processes involving quantum tunneling can be found in a huge variety of physical and chemical systems, ranging in length from the mesoscopic scale of a few microns to the subatomic scale of a few fermi. It has been realized already three decades ago that thereby the interaction of the tunneling degree of freedom with environmental degrees of freedom plays a crucial role. Namely, any realistic description has to account for the fact that a purely isolated system is always an idealization, an issue which tends to become more and more relevant with the growing complexity of the system and particularly with increasing system size. A quantitative understanding of experimental observations must include the presence of e.g. electromagnetic modes in electrical circuits, vibrational modes in molecular aggregates, or phonon backgrounds in solid state systems. Moreover, as a genuine quantum effect tunneling processes serve as paradigm to analyze the boundary between the microscopic and the macroscopic world or at least to elucidate how the latter one emerges from the former one.

Experimental studies started in the 1980s mainly in the new field of mesoscopic physics with the detection of the switching out of the zero voltage state in Josephson junctions. In these systems the phase difference between the two superconducting reservoirs is a collective degree of freedom the physics of which is equivalent to that of a fictitious particle in a tilted periodic potential. The tunneling of this phase out of one of the metastable wells, then coined macroscopic quantum tunneling, attracted a substantial amount of research and triggered theoretical developments to describe tunneling in open systems. Presently, advanced fabrication techniques have led to the design and tailoring of quantum systems in atomic, molecular, and solid state physics which allow for the observation of quantum effects in general and tunneling in particular with unprecedented accuracy. In fact, tunneling processes have even been exploited as sensitive detection mechanisms close to the quantum limit [1]. Theory is again challenged to provide a deeper understanding of the interaction of these systems with their surrounding.

Here, we give a brief overview of basic ideas and theoretical concepts for tunneling in presence of dissipation, established ones and recent developments, and illustrate them through specific examples. A formally exact description of the dynamics of dissipative quantum systems is given in terms of path integrals. The explicit evaluation of this expression, however, is even numerically possible only in few cases, which serve as benchmark results for approximate approaches. In the context of tunneling rates there are basically two situations where simplifications can be achieved. In one case the coupling to the environment is sufficiently strong so that on the reactant side of the tunneling system a local thermodynamic state is preserved over long periods of time. Then, thermodynamical methodologies apply and heavily rely on semiclassical techniques to treat imaginary time path integrals. Another case is the domain of weak friction and elevated temperatures, where thermodynamic methods fail, but approximate equations of motion can be derived from the path integral expression. Again semiclassical techniques are of importance to provide explicit expressions for decay rates. This type of approach can also be extended to systems driven by time-periodic forces where escape over and tunneling through dynamical barriers occurs.

15.1 Dynamics of dissipative quantum systems

Dissipative quantum systems are described with system+reservoir models [2, 3], where the position q of a system with potential $V(q)$ is bilinearly coupled to positions x_α of environmental degrees of freedom. Typically, the number of these reservoir degrees of freedom is macroscopically large and they are assumed to reside in thermodynamic equilibrium at inverse temperature $\beta = 1/k_B T$. In this situation the relevant system degree of freedom is effectively subject to fluctuating forces which obey Gaussian statistics. It is thus possible to mimic the reservoir by a quasi-continuum of harmonic oscillators, independent of its actual microscopic realization. In turn, all properties of the bath are captured by the first and the second cumulants of the bath-force interacting with the system.

Accordingly, one considers a Hamiltonian of the form $H = H_S + H_R + H_I$ with a system part H_S , a reservoir H_R and an interaction H_I , i.e.,

$$\begin{aligned} H_S &= \frac{p^2}{2m} + V(q) \\ H_R &= \sum_{\alpha} \frac{p_{\alpha}^2}{2m_{\alpha}} + \frac{m_{\alpha}\omega_{\alpha}^2}{2} x_{\alpha}^2 \\ H_I &= -q \sum_{\alpha} c_{\alpha} x_{\alpha} + q^2 \sum_{\alpha} \frac{c_{\alpha}^2}{2m_{\alpha}\omega_{\alpha}^2}, \end{aligned} \tag{15.1}$$

where the translational invariant form of the coupling between system and reservoir avoids coupling-induced potential renormalizations. The dynamics of the relevant system is described by the reduced density operator with the environmental modes traced out

$$\rho(t) = \text{Tr}_R \left\{ e^{-\frac{i}{\hbar} H t} W(0) e^{+\frac{i}{\hbar} H t} \right\} \tag{15.2}$$

and with $W(0)$ being the initial state of the total compound. The only non-perturbative way to deal with the elimination of the bath degrees of freedom is to apply the path integral

approach. The coordinate representation of (15.2) with $\rho(q_f, q'_f, t) \equiv \langle q_f | \rho(t) | q'_f \rangle$ follows as

$$\rho(q_f, q'_f, t) = \int dq_i dq'_i d\vec{x}_f d\vec{x}_i d\vec{x}'_i G(q_f, \vec{x}_f, t, q_i, \vec{x}_i) \langle q_i, \vec{x}_i | W(0) | q'_i, \vec{x}'_i \rangle G(q'_f, \vec{x}_f, t, q'_i, \vec{x}'_i)^* \quad (15.3)$$

where the $*$ means complex conjugation and $\vec{x}$ collects the x_α . The time dependent transition amplitudes (propagators) on the rhs are expressed as

$$G(q_f, \vec{x}_f, t, q_i, \vec{x}_i) = \int \mathcal{D}[q] \mathcal{D}[\vec{x}] e^{iS[q, \vec{x}]/\hbar} \quad (15.4)$$

with the total action $S = S_S + S_R + S_I$ according to the three parts of the Hamiltonian (15.1). The sum goes over all paths running in time t from $q(0) = q_i, \vec{x}(0) = \vec{x}_i$ to $q(t) = q_f, \vec{x}(t) = \vec{x}_f$. To carry out all integrations over the bath degrees of freedom in (15.4) explicitly, the initial state must be specified.

In the ordinary Feynman-Vernon theory [4] this state is assumed to be a factorizing state, $W(0) = \rho_S(0) \exp(-\beta H_R)/Z_R$ (Z_R is the bath partition function), so that each one, system and equilibrated bath, lives in splendid isolation at $t = 0$. While this assumption may be justified in the weak damping/high temperature limit or in certain experimental situations, in general, it fails particularly for condensed phase systems and for moderate to strong friction and/or lower temperatures. A more general approach is to work with correlated initial states [5], i.e. $W(0) = \sum_j O_j \exp(-\beta H) O'_j / Z$ with preparation operators O_j and O'_j acting onto the system degree of freedom only and the total partition function Z . In fact, the corresponding classical model can be shown to reproduce the well-known generalized Langevin equation.

To keep the formulation transparent we focus in the sequel on the case where the preparation operators depend exclusively on coordinate and refer to [3, 5] for generalizations. As an example think about a position measurement with a Gaussian slit, in which case the preparation operators are Gaussian weighted projection operators onto position. Hence, one has

$$\rho(q_i, q'_i, t = 0) = \rho_\beta(q_i, q'_i) \lambda(q_i, q'_i), \quad (15.5)$$

with the preparation function $\lambda(q, q') = \sum_j \langle q | O_j | q \rangle \langle q' | O'_j | q' \rangle$ and the reduced thermal equilibrium density $\rho_\beta = \text{Tr}_R \{ \exp(-\beta H) \} / Z$. Accordingly, in (15.3) the initial state is represented as a path integral in imaginary time (Euclidian path integral), which sums over system and bath paths connecting the respective endpoints in the time interval $\hbar\beta$.

Having fixed the initial state, the integrations over the bath degrees of freedom in (15.3) can now be performed exactly. One finds

$$\rho(q_f, q'_f, t) = \int dq_i dq'_i J(q_f, q'_f, t, q_i, q'_i) \lambda(q_i, q'_i), \quad (15.6)$$

where the propagating function $J(\cdot)$ is a threefold path integral over the system degree of freedom only

$$J(q_f, q'_f, t, q_i, q'_i) = Z^{-1} \int \mathcal{D}[q] \mathcal{D}[q'] \mathcal{D}[\bar{q}] e^{i\Sigma_0[q, q', \bar{q}]/\hbar} \langle e^{i\Sigma_I[q, q', \bar{q}, \vec{x}, \vec{x}', \vec{x}]/\hbar} \rangle_R. \quad (15.7)$$

The two real time paths $q(s)$ and $q'(s)$ connect in time t the initial points q_i and q'_i with

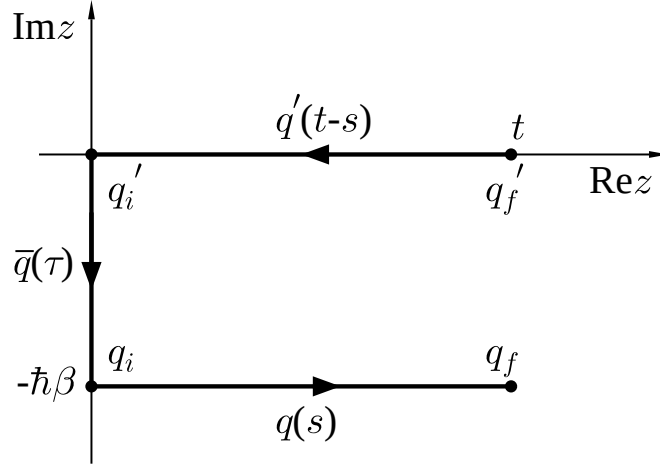


Figure 15.1: Real and imaginary time paths in the complex time plane $Z = s - i\tau$ contributing to the propagating function (15.7).

end points q_f and q_f' , while the imaginary time path $\bar{q}(\sigma)$ runs from q_i to q_i' in the interval $\hbar\beta$ (cf. fig. 15.1). The contribution of each path is weighted with the total bare action $\Sigma_0 = S_S[q] - S_S[q'] + i\bar{S}_S[\bar{q}]$ ($\bar{S}$ denotes the Euclidian action) and with the expectation value $\langle e^{i\Sigma_I/\hbar} \rangle_R$ of the coupling $\Sigma_I = S_I[q, \vec{x}] - S_I[q', \vec{x}'] + i\bar{S}_I[\bar{q}, \vec{x}]$ with respect to the equilibrium distribution of the reservoir. According to (15.1) one has e.g. $S_I[q, \vec{x}] = \int_0^t ds q(s) \xi(s) - \mu \int_0^t ds q(s)^2$ with the bath force $\xi = \sum_\alpha c_\alpha x_\alpha$ and $\mu = \sum_\alpha c_\alpha^2 / (m_\alpha \omega_\alpha^2)$. Hence, $\langle e^{i\Sigma_I/\hbar} \rangle_R$ is the generating functional of the thermal distribution of the bath. For the harmonic model considered here, the first cumulant vanishes $\langle \xi(t) \rangle_R = 0$ and one obtains the so-called influence functional $\langle e^{i\Sigma_I/\hbar} \rangle_R = e^{-\Phi/\hbar}$ with

$$\Phi[\tilde{q}] = \int dz \int_{z > z'} dz' \tilde{q}(z) K(z - z') \tilde{q}(z') + \frac{i}{2} \mu \int dz \tilde{q}(z)^2. \quad (15.8)$$

The ordered time integration is understood along the contour (fig. 15.1): $z = s$ for s from $t \rightarrow 0$, $z = -i\tau$ for τ from $0 \rightarrow \hbar\beta$, $z = -i\hbar\beta + s$ for s from $0 \rightarrow t$ with

$$\tilde{q}(z) = \begin{cases} q'(s) & \text{for } z = s & 0 \leq s \leq t \\ \bar{q}(\tau) & \text{for } z = -i\tau & 0 \leq \tau \leq \hbar\beta \\ q(s) & \text{for } z = -i\hbar\beta + s & 0 \leq s \leq t \end{cases}. \quad (15.9)$$

The effective impact of the bath is completely controlled by the second cumulant $K(z) = \langle \xi(z) \xi(0) \rangle_R / \hbar$, i.e.,

$$K(z) = \int_0^\infty \frac{d\omega}{\pi} I(\omega) \frac{\cosh[\omega(\hbar\beta - iz)]}{\sinh(\omega\hbar\beta/2)}, \quad (15.10)$$

where $I(\omega) = (\pi/2) \sum_\alpha c_\alpha^2 / (m_\alpha \omega_\alpha) \delta(\omega - \omega_\alpha)$ denotes the spectral density of the environment. In particular, for real times the kernel $K(s) = K'(s) + iK''(s)$ is related to the macroscopic damping kernel entering the classical generalized Langevin equation

$$\gamma(s) = \frac{2}{m} \int_0^\infty \frac{d\omega}{\pi} \frac{I(\omega)}{\omega} \cos(\omega s) \quad (15.11)$$

via $K''(s) = (M/2)d\gamma(s)/ds$ and $K'(s) \rightarrow M\gamma(s)/\hbar\beta$ in the classical limit.

The expression (15.6) is a formally exact result for the time dependent reduced dynamics. Its explicit evaluation, however, is very challenging particularly for processes involving quantum tunneling. Namely, due to the non-local time interactions mediated by the reservoir and captured by the influence functional, in general, a time-local evolution equation for the reduced density matrix does not exist. In this situation, progress has been made in basically three directions: (i) application of numerical approaches as e.g. quantum Monte Carlo techniques, which in principle provide numerically exact results but are plagued by the so-called sign problem, (ii) derivation of approximate time evolution equations from the exact path integral expression in certain ranges of parameter space, (iii) development of semiclassical techniques according to the WKB-machinery.

While approach (i) has been used very successfully to describe e.g. the dynamics of tight-binding systems [3], for tunneling in continuous systems it faces two interconnected problems. Namely, one needs to consider the dynamics on sufficiently long time scales *and* with high accuracy to extract exponentially small tunneling rates. To meet these criteria simultaneously, is very demanding and computationally time-consuming. Practically, only very few systems have thus been analyzed. Approach (ii) leads to various types of master equations in the complementary domains of weak [6] and strong friction [7]. In both cases tunneling rates have been derived. Approach (iii) sounds very appealing since path integrals offer a natural starting point for an $\hbar$ -expansion. Unfortunately, a direct semiclassical evaluation of the time-dependent density (15.6) is not feasible. While the minimal action paths can be determined at least numerically, the standard strategies to relate the Gaussian fluctuations around them to the corresponding minimal action or to an equation of motion (Gelfand-Yaglom) do not apply due to the bath induced time retardation and time irreversibility. Moreover, a systematic $\hbar$ -expansion is not straightforward since the minimal action paths do *not* reproduce in the classical limit the classical Langevin equation [3]. If one keeps in mind though that in condensed phase systems tunneling often occurs from a thermal state on the reactant side, a very powerful semiclassical technique has been developed based purely on the imaginary time path integral representation of the partition function. This formalism, known as the imaginary part of the free energy method ("ImF") [3, 8, 9], requires sufficiently high energy barriers and sufficiently strong friction or low temperatures.

In the sequel, we thus proceed as follows: we first consider a case, where the complete tunneling dynamics can be obtained, namely, a situation where tunneling is restricted to the parabolic top of a barrier potential. This result is already non-trivial and confirms corresponding predictions obtained in the 1980s within the ImF technique. The latter approach will be introduced in Sec. 15.3 including its recent generalization to non-Gaussian baths. Section 15.4 deals with semiclassical type of time evolution equations applicable in the regime of low friction and moderate temperatures, where the ImF approach fails. This formulation can be extended to extract rates for dynamical tunneling in driven systems close to a bistability, which have been implemented lately as highly sensitive detectors.

15.2 Barrier dynamics in real-time

We consider a quantum particle in a metastable potential subject to a thermal environment. Initially the system is prepared in a local thermal equilibrium in the well. Then, for a sufficiently high barrier potential $V_b \gg k_B T, \hbar\omega_0$ the dynamics of the reduced density will

approach a steady state within a plateau range of time from which the escape rate can be obtained. For sufficiently high temperatures and sufficiently strong dissipation this steady state distribution coincides in the well region with the local thermodynamic state and deviates from it only in a boundary layer around the barrier top. Accordingly, the tunneling dynamics is obtained from the time evolution in an inverted harmonic potential and from the thermodynamic state in the harmonic well, both situations, for which the three-fold path integral (15.6) can be solved exactly [10].

To be specific, let us consider an archetypical metastable well potential

$$V(q) = \frac{m\omega_0^2}{2}q^2 \left(1 - \frac{2q}{3q_b}\right) \quad (15.12)$$

with a harmonic well around $q = 0$ with frequency ω_0 and a barrier top with energy $V_b = V(q_b)$ located at $q = q_b$ with frequency $-\omega_b^2 \equiv -\omega_0^2$. The initial state is a thermal state restricted to the left of the barrier top

$$\rho(x_i, r_i) = \rho_\beta(x_i, r_i) \theta(q_b - r_i), \quad (15.13)$$

where for convenience we introduced sum and difference coordinates $r = (q + q')/2$ and $x = q - q'$, respectively, and θ denotes the step function. From the imaginary time path integral one first finds the density distribution around the parabolic barrier top as

$$\rho_\beta^{(b)}(x, r) = \frac{1}{Z \sqrt{\omega_0^2 m \beta \Lambda_b}} \sqrt{\frac{m}{2\pi \hbar^2 \beta}} \left(\prod_{n=1}^{\infty} \nu_n^2 u_n^{(b)} \right) \exp \left[-\beta V_b - \frac{(r - q_b)^2}{2\Lambda_b} - \frac{\Omega_b x^2}{2\hbar} \right] \quad (15.14)$$

with the "variances"

$$\Lambda_b = \frac{1}{m\beta} \sum_{n=-\infty}^{\infty} u_n^{(b)}, \quad \Omega_b = \frac{m}{\beta} \sum_{n=-\infty}^{\infty} (|\nu_n| \hat{\gamma}(|\nu_n|) - \omega_b^2) u_n^{(b)} \quad (15.15)$$

which contain the Matsubara frequencies $\nu_n = 2\pi n/\hbar\beta$ and $u_n^{(b)} = 1/[\nu_n^2 - \omega_b^2 + |\nu_n| \hat{\gamma}(|\nu_n|)]$. Friction enters through the Laplace transform $\hat{\gamma}(z)$ of the classical damping kernel $\gamma(t)$ (15.11). As a function of temperature Λ_b displays a non-trivial behavior, which can already be read off from its non-dissipative limit $\Lambda_b^{(0)} = -(\hbar/m) \coth(\omega_b \hbar \beta)$. Apparently, with lowering temperature $\Lambda_b^{(0)}$ vanishes for the first time at a critical temperature $T_c^{(0)} = \hbar\omega_b/(\pi k_B)$ which is *twice* the non-dissipative crossover temperature T_0 introduced below. The effect of friction is to push the critical temperature towards lower temperatures $T_c < T_c^{(0)}$. Physically, at T_c the local harmonic approximation for the equilibrium distribution (15.13) breaks down even in the close vicinity of the barrier top and the global shape of the potential (15.12) must be taken into account.

Now, starting with this initial state the density matrix $\rho(x_f, r_f, t)$ reaches for longer times a quasi-stationary state, the so-called flux state, which can be cast into the form

$$\rho_{\text{fl}}(x_f, r_f) = \rho_\beta(x_f, r_f) g_{\text{fl}}(x_f, r_f), \quad (15.16)$$

where

$$g_{\text{fl}}(x, r) = \frac{1}{2} \operatorname{erfc} \left[(-r + q_b + ix\hbar|\Lambda_b|\omega_R/m)/\sqrt{2|\Lambda_b|} \right] \quad (15.17)$$

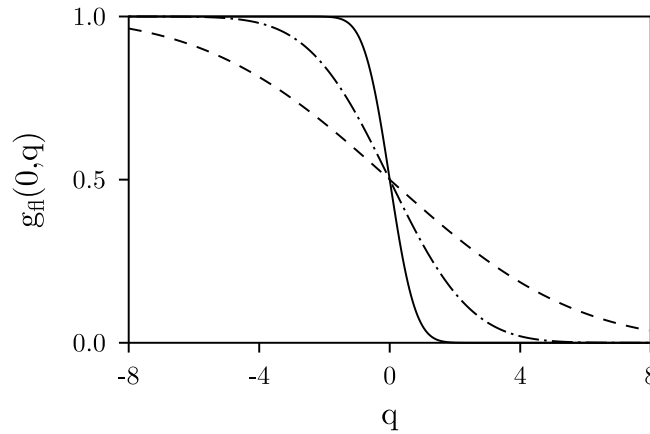


Figure 15.2: Distribution $g(x, r)$ describing deviations from thermal equilibrium in (15.16). Shown is the diagonal part $g_R(0, q)$ for various temperatures $\omega_b \hbar \beta = 0.1$ (dashed), 1 (dotted-dashed), and 2 (solid) for ohmic friction with $\gamma/\omega_b = 1$. Position is scaled with $\sqrt{\hbar/m\omega_b}$.

describes deviations from the equilibrium state around $q = q_b$ on the length scale $l_R = \sqrt{2|\Lambda_b|}$ (see fig. 15.2). This state is approached on time scales large compared to the inverse of the Grote-Hynes frequency ω_R , which is the largest positive root of $\omega_R^2 + \omega_R \hat{\gamma}(\omega_R) - \omega_b^2 = 0$ and captures the local real-time dynamics around the barrier top. Accordingly, the steady state reduces to the thermal state to the left of the barrier top but within the parabolic range of the potential if l_{st} is sufficiently smaller than the anharmonicity length scale q_b . This in turn provides the range of validity of calculations based on local harmonic properties (see the $\text{Im}F$ method discussed in the next Section). Roughly speaking, for a given temperature above the critical temperature T_c friction must be sufficiently strong. Then, deep inside the well around $q = 0$ one reaches the thermal state of a harmonic oscillator $\rho_\beta^{(0)}(x, r)$ obtained from $\rho_\beta^{(b)}(x, r)$ upon replacing $\omega_b \rightarrow i\omega_0$ and putting $q_b = V_b = 0$. To the right of the barrier $g \rightarrow 0$, thus describing an exponentially decreasing population on the product side. The escape rate out of the well is given as the probability flux

$$J_R = \frac{1}{2m} \langle p \delta(q - q_b) + \delta(q - q_b) p \rangle_R \quad (15.18)$$

with respect to the flux state and normalized to the population in the well. The latter one follows from identifying the normalization Z in (15.14) with the harmonic partition function in the well. This way, the escape rate is found to read $\Gamma = \Gamma_{cl} f_q$ with the classical rate $\Gamma_{cl} = (\omega_0 \omega_R / 2\pi \omega_b) \exp(-\beta V_b)$ and the quantum factor

$$f_q = \prod_{n=1}^{\infty} \frac{u_n^{(b)}}{u_n^{(0)}} = \prod_{n=1}^{\infty} \frac{\nu_n^2 + \omega_0^2 + \nu_n \hat{\gamma}(\nu_n)}{\nu_n^2 - \omega_b^2 + \nu_n \hat{\gamma}(\nu_n)} \quad (15.19)$$

describing the impact of quantum fluctuations. For high temperatures one has $f_q \rightarrow 1$ and the barrier escape is purely due to thermal activation over the barrier. For lower temperatures $f_q > 1$ so that barrier escape is enhanced partially due to zero point fluctuations in the well, partially due to tunneling through the top of the barrier. At the so-called crossover temperature T_0 , however, where $\nu_1^2 - \omega_b^2 + \nu_1 \hat{\gamma}(\nu_1) = 0$, the rate expression (15.19) breaks

down. For instance, for ohmic friction $\hat{\gamma}(z) = \gamma$ one derives from the positive solution to $\lambda_0^2 - \omega_b^2 + \lambda_0\gamma = 0$ that $T_0 = \hbar\lambda_0/2\pi k_B$. For vanishing friction this leads to $T_0^{(0)} = \hbar\omega_b/2\pi k_B = T_c^{(0)}/2$. Interestingly, while for temperatures below the critical temperature T_c the steady state distribution is determined by global properties of the potential, the escape process is dominated by tunneling only below the crossover temperature $T_0 < T_c$ [11, 12]. Both temperatures are lowered with increasing friction corresponding to the fact that dissipation tends to drive a quantum system back towards the classical regime even though the reservoir is quantum mechanical in nature as well.

To calculate tunneling rates within a dynamical calculation for temperatures below the crossover temperature is a challenging and yet unsolved problem. The crucial point is that even for non-dissipative systems a semiclassical expression for the time evolution operator (15.4) in the long time limit where deep tunneling occurs, is not known. Some progress has been made by analyzing the phase space dynamics of minimal action paths in the complex plane [7, 11, 12] or by using initial value representations for the quantum propagator [13].

15.3 Thermodynamical approach

Physically, a full dynamical treatment is not always necessary. It seems intuitively clear that this is the case if the state from which tunneling occurs remains close to a local thermal equilibrium. The most prominent of such a thermodynamic approach is the imaginary part of the free energy method ("Im F ") [3, 8, 9], which applies over the whole temperatures range and is based upon a semiclassical treatment of imaginary time path integrals. In the range where it applies, it provides an extremely elegant and powerful formulation.

15.3.1 General formulation and Gaussian heat baths

The underlying idea of the Im F method is this: Inside a metastable well quasi-energy levels $\epsilon_n = E_n - i\hbar\Gamma_n/2$ exist the finite life-time of which are related to imaginary parts Γ_n with $E_n \gg \hbar\Gamma_n$. Equivalently, in a scattering experiment such states appear as resonances with finite widths. Hence, the partition function of the unstable system is (formally) calculated as

$$Z = \sum_{n=0}^{\infty} e^{-\beta\epsilon_n} \approx \sum_{n=0}^{\infty} e^{-\beta E_n} - i\frac{\hbar\beta}{2} \sum_{n=0}^{\infty} \Gamma_n e^{-\beta E_n}.$$

Here, for energies near and above the barrier, the sum is taken as an integral. Obviously, the imaginary part in Z is proportional to the thermally averaged decay rate. In the non-dissipative case a careful WKB treatment proves [8] that

$$\Gamma = -\frac{2}{\hbar}\mu(T)\text{Im}F \quad (15.20)$$

with the free energy $F = -\ln Z/\beta$ and a temperature dependent prefactor $\mu(T)$ with $\mu(T \geq T_0) = T_0/T$ above and $\mu(T < T_0) = 1$ below the crossover temperature $T_0 = \hbar\omega_b/2\pi k_B$. It is not a priori clear that the relation (15.20) also applies to finite dissipation (with T_0 taken as the crossover temperature for finite friction) and, in fact, a rigorous proof has not been

given yet. Qualitatively, one can at least formulate a necessary condition: a thermodynamic approach is supposed to be valid when a thermal state is preserved in the well region over periods of time long compared to intrawell relaxations. For temperatures above T_c the $\text{Im}F$ produces results identical to those derived in the previous Section within the full dynamical calculation. It is thus applicable if friction is sufficiently strong, but certainly fails for weak dissipation where the steady state broadens in position space to cover the entire well domain. For temperatures far below T_0 the population is confined to the ground state in the potential well so that even for weaker dissipation the method applies. All experimental results obtained so far are in complete agreement with its theoretical predictions which indicates that the $\text{Im}F$ approach provides at least an extremely accurate approximation to a full dynamical theory.

The starting point is the representation of the partition function of the composite system in terms of Euclidian path integrals. Upon eliminating the reservoir degrees of freedom along the lines described in Sec. 15.1 one has

$$Z = \oint \mathcal{D}[\bar{q}] e^{-\bar{S}_S[\bar{q}]/\hbar} \langle e^{-S_I[\bar{q}, \bar{x}]/\hbar} \rangle_R, \quad (15.21)$$

where the integral sums over all periodic paths in the interval $\hbar\beta$. As above, the expectation value $\langle e^{-S_I[\bar{q}, \bar{x}]/\hbar} \rangle_R$ can explicitly be evaluated for a Gaussian bath distribution, i.e. for reservoirs consisting of harmonic modes. In this case one obtains the influence functional (15.8) for $z = i\tau$, $\tau \in [0, \hbar\beta]$ and $\langle e^{-S_I[\bar{q}, \bar{x}]/\hbar} \rangle_R = \exp(-\bar{\Phi}[\bar{q}]/\hbar)$. The remaining integral over the system paths with the effective action $\bar{\Sigma} = \bar{S}_S + \bar{\Phi}$ is then evaluated in a semiclassical fashion. In contrast to the conventional recipe, however, exponentially small imaginary parts must be retained against dominating real parts since the imaginary parts determine the escape rate. The fact that the partition function carries an imaginary contribution is a consequence of the instability of the system and follows from a proper steepest descent evaluation of the fluctuation path integral around the minimal action paths. For $T > T_0$ the system supports only the trivial minimal action paths $q_0(\tau) = 0$ with $\bar{\Sigma}[0] = 0$ and $q_b(\tau) = q_b$ with $\bar{\Sigma}[q_b] = \hbar\beta V_b$. Certain fluctuations around the latter path are unstable and must be treated via an analytical continuation procedure [9]. Eventually, this reproduces the result (15.19) that diverges at T_0 . The fact that the full dynamical approach discussed in the previous Section is strongly influenced by anharmonic quantum fluctuations already at the higher temperature T_c , while this temperature does not explicitly appear in the final rate expression (15.19), indicates that the $\text{Im}F$ calculation and the dynamical calculation deviate in the temperature range between T_c and T_0 . These discrepancies are small and vanish for temperatures below T_0 [12], where the path integral (15.21) is dominated by the contribution of a newly emerging periodic orbit in the inverted barrier potential, the so-called bounce $\bar{q}_B(\tau)$ [9]. Its explicit trajectory must be calculated numerically as well as its corresponding minimal action $S_B \equiv \bar{\Sigma}[\bar{q}_B] \ll \hbar\beta V_b$. It can be shown that the bounce is again an unstable orbit giving rise to an imaginary contribution to the partition function. Hence, one arrives at

$$\Gamma = \sqrt{\frac{S_B}{2\pi\hbar}} \sqrt{\frac{\det[L_0]}{\det'[L_B]}} e^{-S_B/\hbar}. \quad (15.22)$$

Here, the first factor accounts for a zero-mode of the bounce orbit related to its invariance against phase shifts $\bar{q}_B(\tau) \rightarrow \bar{q}_B(\tau + \tau_0)$. The operators L_0 and L_B correspond to the second order variational operator of the effective action $\bar{\Sigma}[q]$ around the trivial periodic orbit at the well bottom and the bounce orbit, respectively. The prime indicates that the zero mode has to be omitted. While explicit results can only be obtained numerically, see for instance [9],

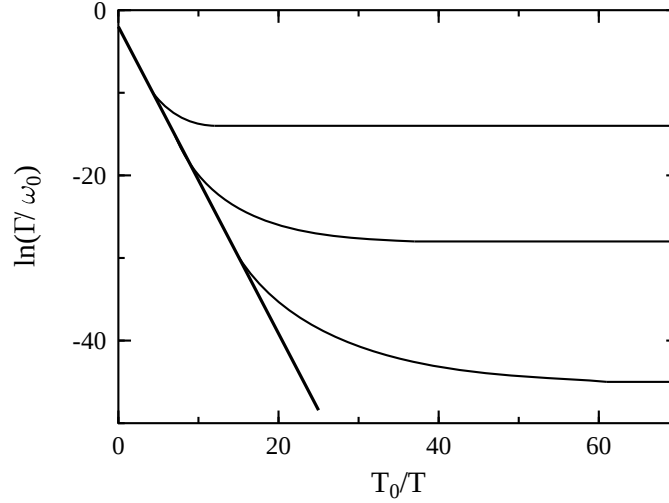


Figure 15.3: Quantum tunneling rate vs. inverse temperature for the potential (15.12) and various ohmic friction strengths $\gamma/\omega_0 = 0$ (top), 1 (middle), 2 (bottom). Barrier height is $V_b/\hbar\omega_0 = 5$ and the thick straight line depicts the classical result.

approximate ones can be given for weak dissipation and for vanishing temperature. In this case one has $\Gamma = \Gamma_0 Y_2$ with the WKB tunneling rate for vanishing dissipation Γ_0 and a dissipative factor stemming from the influence functional evaluated along the zero-friction bounce path $\bar{q}_B^{(0)}$, i.e.,

$$Y_2 = \exp \left[-\frac{1}{2} \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\sigma \bar{q}_B^{(0)}(\tau) k(\tau - \sigma) \bar{q}_B^{(0)}(\sigma) \right]. \quad (15.23)$$

The imaginary time kernel is related to the second cumulant $K(i\tau)$ of the bath distribution (15.10) via $k(\tau) = \mu : \delta(\tau) : -K(i\tau)$ with the static contribution $\mu = 2 \lim_{\hbar\beta \rightarrow 0} K(0)$ and the periodically continued δ function $: \delta(\tau) := \sum_n \delta(\tau - n\hbar\beta)$. This dissipative factor thus adds to the exponential of the bare tunneling rate which contains the bare bounce action $\bar{S}_S[\bar{q}_B^{(0)}]$. It can be shown that the exponential in (15.23) is always positive so that dissipation due to position-position coupling always suppresses tunneling. In case of the metastable potential (15.12) and for ohmic friction the explicit evaluation gives

$$\Gamma_0 \propto e^{-36V_b/(5\hbar\omega)} \quad , \quad Y_2 = e^{-162\zeta(3)V_b\gamma/(\pi^3\omega_0^2)}. \quad (15.24)$$

A typical Arrhenius-plot [$\ln(\Gamma)$ vs. inverse temperature] is shown in fig. 15.3. The changeover from classical thermal escape to quantum tunneling appears for stronger friction at lower temperatures and is also smeared out. At the same time friction suppresses tunneling substantially according to the explicit dependence of the bounce action on dissipation [cf. (15.24)].

These and further predictions have been verified experimentally in Josephson junction (JJ) devices [14]. We also note that alternative formulations, e.g. multi-dimensional transition state theory, are completely equivalent to the $\text{Im}F$ method and provide identical results.

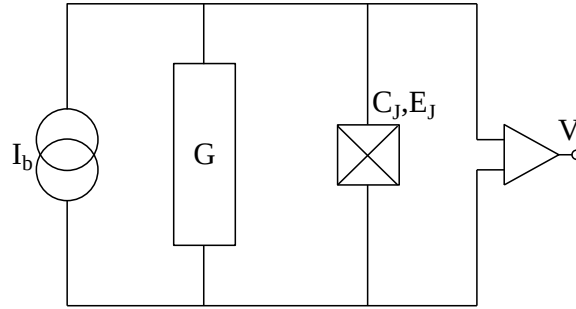


Figure 15.4: Electrical circuit with a mesoscopic conductor G in parallel to a JJ with capacitance C_J and coupling energy E_J biased by an external current I_b .

15.3.2 Extension to reservoirs with non-Gaussian fluctuations

The results discussed so far assume a heat bath environment which obeys Gaussian statistics. As already pointed out, for a large majority of experimentally relevant situations this is indeed an accurate description. In the last years, however, reservoirs with non-Gaussian characteristics have attracted substantial interest in the context of current noise generated by mesoscopic conductors (typically voltage biased) [15] such as tunnel contacts, atomic point contacts, and ballistic wires, to name but a few. In fact, it has been shown that higher than second order current cumulants carry information about the transport process that cannot be gained from usual current-voltage measurements (IV-curves). The granularity of the elementary charge carriers gives rise to non-Gaussian deviations from the mean current, e.g. in the simplest case of a tunnel junction corresponding to Poissonian noise statistics. While this concept of "full counting statistics" is fascinating and has also interesting relations to photon counting in quantum optics, the detection of higher order current cumulants is very challenging due to small signals and strict filtering demands. As we have seen above for Gaussian noise, escape rates depend very sensitively on noise produced by the surrounding, particularly in the quantum regime. Hence, the switching out of the zero-voltage state in JJs has been proposed as detection process. Indeed, very recently the third cumulant produced by a tunnel junction has been retrieved from the asymmetry of the switching rate with the JJ being operated in the classical regime of over-the-barrier-activation. The extension to the tunneling regime, however, is not easy since the second order cumulant of current noise gives rise to additional heating. One proposal to overcome this difficulty has been discussed in [16] (the corresponding circuitry is sketched in fig. 15.4): the noise generating element is placed in parallel to the JJ so that only equilibrium current fluctuations reach the junction. No net current flows through the conductor and due to time reversibility all odd order cumulants vanish so that direct access to higher order even cumulants is obtained.

The tunneling rate at zero temperature is determined by the $\text{Im}F$ -recipe with the representation of the partition function as specified in (15.21). The reservoir distribution is given by the current distribution in equilibrium and the coupling between the detector degree of freedom and the current noise is assumed to be weak. This way, the tunneling rate is formally given by

$$\Gamma = \Gamma_0 \langle e^{-S_I[\theta_B^{(0)}/2, I/e]/\hbar} \rangle_G \quad (15.25)$$

with the non-dissipative bounce orbit $\theta_B^{(0)}$ and the current operator I of the conductor G . Note that the factor $1/2$ appears in S_I since according to the second Josephson relation

$V_J = (\hbar/e)\dot{\theta}/2$ (phase across the JJ is θ), the voltage across the junction equals that across the conductor $V_J = V_G \equiv (\hbar/e)\dot{\varphi}$. (phase across the conductor is φ). The correction to the bare rate is again given by the generating functional of the reservoir, i.e. the conductor. This is a formidable task, but in some cases explicit analytical expressions are available. For instance, in case of a tunnel junction with dimensionless conductance $g_T = \hbar/(2e^2 R_T) = \pi \sum_i T_i$ (tunneling resistance R_T and transmissions T_i) one derives

$$S_T[\varphi] \equiv \Phi[\varphi] = -4g_T \int_{\mathcal{C}} dz \int_{\mathcal{C}} dz' \alpha(z - z') \sin^2 \left[\frac{\varphi(z) - \varphi(z')}{2} \right] \quad (15.26)$$

with the kernel $\alpha(z) = \pi/[2(\hbar\beta)^2 \sinh^2(\pi z/\hbar\beta)]$. $\mathcal{C}$ denotes the integration contour introduced in (15.9) consisting of two segments in real and one segment in imaginary time. For the $\text{Im}F$ calculation only the contribution along this latter branch $z = -i\tau$ is relevant. By expanding the sin-function in a power series of the phase difference, the impact of higher order cumulants on the tunneling process can be studied. Thereby the k -th power corresponds to the k -th cumulant. Approximating a single well-barrier segment of the tilted washboard potential of a JJ by (15.12) and switching from $q \rightarrow \theta$, one finds for the bounce orbit $\theta_B^{(0)}(\tau) = 3\theta_b/[2\cosh^2(\omega_0\tau/2)]$. This way, in lowest order (second order) we have $\Gamma^{(2)} = \Gamma_0 Y_2$ with $Y_2 = \exp[-g_T 54\zeta(3)\theta_b^2/(4\pi^3)]$ so that the known suppression of tunneling due to the second cumulant of the reservoir is regained. In next order (fourth order) one finds $\Gamma^{(4)} = \Gamma^{(2)} Y_4$ with

$$Y_4 = \exp \left[\frac{g_T A_4}{(4\pi)^3} (9\theta_b)^4 \right] \quad (15.27)$$

and a numerical constant $A_4 = 66.3547\dots$. Apparently, the fourth order contribution *enhances* the tunneling rate. Moreover, it displays a characteristic dependence on the tilt (the applied bias current) of the washboard potential different from that of the Gaussian contribution Y_2 . This in turn allows for the experimental detection of the fourth order cumulant of the current noise distribution.

Theoretically, the above scheme extends the standard $\text{Im}F$ approach to reservoirs with non-Gaussian statistics still, however, residing in equilibrium. The calculation of tunneling rates in situations when a finite bias voltage is applied across the conductor so that its current distribution is stationary but out of equilibrium, has not been solved yet. It is related to the open problem of how to obtain deep tunneling rates within a real-time approach.

15.4 Tunneling rates from equations of motion

In the regime of weak friction and for temperatures above the crossover temperature, the $\text{Im}F$ approach is not applicable since then the steady state covers in position space even the well region and does not reduce to a thermal equilibrium. Accordingly, the flux state distribution from which tunneling occurs is not known a priori. In the classical limit this situation refers to the energy-diffusive regime of Kramers' theory [17]. To analyze the impact of quantum fluctuations in this domain, one starts by deriving from the exact path integral expression (15.3) an approximate time evolution equation for the reduced density. Namely, in the domain $\gamma\hbar\beta \ll 1$ the time scale on which relaxation occurs, i.e. $1/\gamma$, by far exceeds the retardation time scale $\hbar\beta$ of the reservoir so that on a coarse grained time scale a time local equation of motion for the density does exist. This leads to master type of

equations corresponding to second order perturbation theory in the system-bath coupling (Born-Markov approximation). Explicit expressions are most conveniently obtained in the eigenstate representation of the bare system Hamiltonian H_S .

15.4.1 Escape over a potential barrier

Let us first illustrate the general concept for a standard situation, namely, a particle initially confined in a metastable potential (15.12). We first assume a high barrier $V_b \gg k_B T, \hbar\omega_0$ so that for weak damping the well supports a ladder of quasi-stationary discrete energy levels which reach the continuum for energies above the barrier top. Second, we consider higher temperatures $k_B T$ which sufficiently exceed $\hbar\omega_0$ so that the energy ladder is smeared out by thermal fluctuations. This is a typical semiclassical situation not only in the sense of barrier tunneling but also with respect to the dynamics inside the well. The crucial question is then: What are the dominating quantum effects that influence the escape rate?

For this purpose, it is convenient to introduce the occupation probability of a well state with energy E via

$$P(E, t) = \sum_{n=0}^N \delta(E - E_n) p_n(t), \quad (15.28)$$

where N is the number of states in the well. Here p_n is the occupation probability of a well eigenstate $|E_n\rangle$ with quasi-energy E_n . It is thus identical to the diagonal part of the reduced density (15.2) matrix in the energy representation $p_n(t) = \langle E_n | \rho(t) | E_n \rangle$. The explicit construction of these eigenstates follows from a type of WKB-recipe as shown below. Starting with a set of master equations for the populations p_n , the corresponding time evolution equation for the occupation probability is found [18] to read

$$\dot{P}(E, t) = \int dE' \left[W_{E,E'} \frac{R(E') P(E', t)}{n(E')} - W_{E',E} \frac{R(E) P(E, t)}{n(E)} \right] - T(E) \frac{\omega(E)}{2\pi} P(E, t) \quad (15.29)$$

with $\omega(E)$ being the frequency of a classical oscillation at energy E . This diffusion equation captures the incoming probability flux to and outgoing probability flux from the state with energy E according to intrawell transition rates [19]

$$W_{E,E'} = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dt \text{Tr}_R \{ \langle E | H_I(t) | E' \rangle \langle E' | H_I | E \rangle \rho_{\beta,R} \}, \quad (15.30)$$

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 $H_I(t) = e^{i(H_S + H_R)t/\hbar} H_I e^{-i(H_S + H_R)t/\hbar}$ with $\rho_{\beta,R} = e^{-\beta H_R} / Z_R$ being the equilibrium bath density matrix. Further, $n(E)$ in (15.29) denotes the density of states.

The transition rate (15.30) can be evaluated explicitly in case of the bilinear system-bath coupling as in (15.1). One arrives at the golden rule type of formula

$$W_{E,E'} = \frac{1}{\hbar^2} |Q_{\text{qm}}(E', E)|^2 D(E - E') \quad (15.31)$$

with $Q_{\text{qm}}(E', E) \equiv \langle E'|q|E \rangle$ and the bath absorption/emission rate captured by

$$D(E) = \hbar \int_{-\infty}^{\infty} dt K(t) e^{itE/\hbar} = \hbar I(E/\hbar) \bar{n}(E) \quad (15.32)$$

with the Bose-Einstein distribution $\bar{n}(E) = 1/[\exp(\beta E) - 1]$. In accordance with an effectively Markovian dynamics we consider a purely ohmic environment with $I(\omega) = m\gamma\omega$. In order to calculate (15.31) semiclassically, we have to construct the energy dependent wave functions inside the well. In the energy range close to the barrier top, however, classical turning points to the left and to the right of the barrier are not sufficiently separated so that the standard WKB approximation is not applicable. In this situation, one exploits (as done already above) that any sufficiently smooth barrier potential can be approximated by a parabolic barrier with barrier frequency ω_b for which the Schrödinger equation can be solved exactly. The proper eigenfunctions are then matched asymptotically (sufficiently away from the barrier top in the well region) onto WKB wave functions to determine phases and amplitudes of the latter ones. This leads us to

$$\langle E|q \rangle = \frac{1}{2} [\langle E|q \rangle^- + r(E) \langle E|q \rangle^+] \quad (15.33)$$

with matrix elements

$$\langle E|q \rangle^{\pm} = \frac{N(E)}{\sqrt{\partial H(q, p)/\partial p}} e^{\pm \frac{i}{\hbar} S_0(E, q) \mp \frac{i\pi}{4}}, \quad (15.34)$$

where $S_0(E, q) = \int_{q_1}^q p(E, q') dq'$ is the action of an orbit starting at a turning point q_1 and running in time t towards q with momentum $p(E, q')$ at energy E . The complex valued reflection amplitudes $r(E)$ of a parabolic barrier [20] are related to the reflection probabilities $R(E) = |r(E)|^2$ and the normalization is determined from $\langle E|E' \rangle = \delta(E - E')$ to read

$$N(E) = 2 \sqrt{\frac{1}{\hbar \pi [R(E) + 1]}}. \quad (15.35)$$

These results match for lower energies onto the standard semiclassical ones. In particular, transmission and reflection coefficients over the full energy range are given by the uniform semiclassical expressions

$$\begin{aligned} T(E) &= |t(E)|^2 = \frac{1}{1 + \exp[-\bar{S}(E)/\hbar]} \\ R(E) &= |r(E)|^2 = \frac{\exp[-\bar{S}(E)/\hbar]}{1 + \exp[-\bar{S}(E)/\hbar]}, \end{aligned} \quad (15.36)$$

where $\bar{S}(E)$ denotes the Euclidian action of a periodic orbit with energy E oscillating in the inverted barrier potential $-V(q)$. With the semiclassical wave function at hand and using the restricted interference approximation [21] one can now calculate the transition matrix elements which enter the transition rates in (15.31).

Upon inserting these transition rates into the time evolution equation (15.29), an expansion in powers of $\hbar$ can be performed, where one has to keep in mind, however, that for energies near the barrier top reflection and transmission probabilities are of order 1, particularly with $T(E = V_b) = R(E = V_b) = 1/2$. This way, we arrive at the semiclassical

expression for the energy diffusion equation (15.29) in the metastable well

$$\dot{P}(E, t) = \left\{ \frac{\partial}{\partial E} C(E) \gamma S_0(E) \left[1 + \frac{1}{\beta} \frac{\partial}{\partial E} \right] R(E) - T(E) \right\} \frac{\omega(E)}{2\pi} P(E, t), \quad (15.37)$$

with

$$C(E) = 2 \frac{1 + R(E)^2}{[1 + R(E)]^2}, \quad (15.38)$$

and $S_0(E)$ the action of a periodic orbit in the well with energy E . Note that for vanishing transmission ($R = 1, T = 0$) one recovers from the above expression the classical Kramers equation [17]. Corrections to the diffusion equation (15.37) are at most of order $\hbar^2$.

The escape rate follows again from a quasi-stationary nonequilibrium state, this time from the quasi-stationary energy distribution $P_{\text{st}}(E)$ corresponding to (15.37), i.e.,

$$\Gamma_{\text{scl}} = \int_0^\infty dE n(E) T(E) P_{\text{st}}(E) \quad (15.39)$$

with the semiclassical density of states $n(E) = 1/[\hbar\omega(E)]$. Taking into account (15.37) one finds

$$\Gamma_{\text{scl}} = \frac{\sinh(\omega_0 \hbar \beta / 2)}{(\omega_0 \hbar \beta / 2)} |B| \Gamma_{\text{cl}}, \quad (15.40)$$

where the classical escape rate is

$$\Gamma_{\text{cl}} = \frac{\omega_0 \gamma S_0(V_b) \beta}{2\pi} e^{-\beta V_b} \quad (15.41)$$

and the coefficients read

$$B = -\frac{1}{4^\theta} \frac{{}_2F_1\left[\frac{1}{2} - \frac{\theta}{2} - a, \frac{1}{2} - \frac{\theta}{2} + a, 1 - \theta, -\frac{4}{9}\right]}{{}_2F_1\left[\frac{1}{2} + \frac{\theta}{2} - a, \frac{1}{2} + \frac{\theta}{2} + a, 1 + \theta, -\frac{4}{9}\right]}, \quad a = \sqrt{\frac{\beta \gamma S_0(V_b)(1 - \theta)^2 + 36\theta^2}{4\beta \gamma S_0(V_b)}} \quad (15.42)$$

with the abbreviation $\theta = \omega_b \hbar \beta$. In (15.40) quantum fluctuations are captured by two factors: the first one describes zero-point fluctuations in the well, while the second one describes the impact of finite barrier transmission close to the top. Interestingly, for weak friction 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 $E \geq V_b$ (fig. 15.5).

15.4.2 Quantum fluctuations in escape processes over dynamical barriers

The situation discussed in the previous Section where escape happens to occur over a static energy barrier is now generalized to a situation, where two stable basins in phase space are separated by a dynamical barrier. Specifically, we consider a system with a weakly anharmonic potential driven by an external time-periodic force (Duffing oscillator), namely,

$$H_S = \frac{p^2}{2m} + \frac{m}{2} \omega_0^2 q^2 - \frac{\Gamma}{4} q^4 + F q \cos(\omega_F t). \quad (15.43)$$

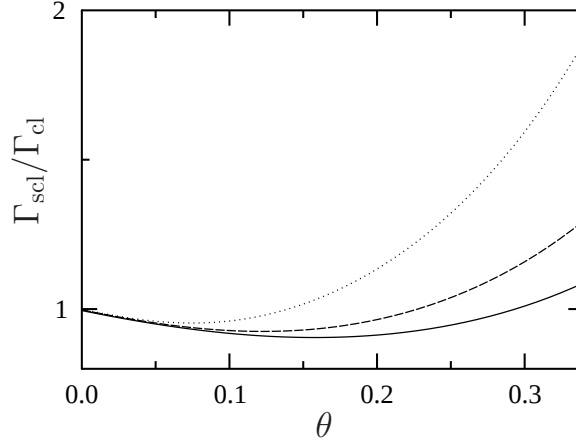


Figure 15.5: Escape rate normalized to the classical rate as a function of the inverse temperature θ for various values of the dimensionless friction strength: $\gamma/\omega_0 = 0.01$ (solid), $\gamma/\omega_0 = 0.005$ (dashed) and $\gamma/\omega_0 = 0.0015$ (dotted) and barrier height $V_b\beta = 10$.

Accordingly, for the anharmonic coefficient we assume $\Gamma/m \ll \omega_0^2/\langle q^2 \rangle$ so that driving is almost resonant for $\delta\omega = \omega_F - \omega_0 \ll \omega_F$. 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, however, can induce switchings between the stable basins leading again to a rate process [22]. In fact, the sensitivity of this rate with respect to e.g. the curvature of the potential surface in (15.43) has recently been exploited as working principle in a very sensitive detection device. In the so-called Josephson Bifurcation Amplifier (JBA) [23, 24] a superconducting tunnel contact (Josephson junction) is placed in parallel to a Cooper-pair box implementing a two level system (qubit) and is driven by microwave fields. In the operational regime of the junction, the device can be described by the Hamiltonian (15.43), where the two qubit states lead to slightly different curvatures ω_0 . Measurements of the switching of the JBA gives thus direct access to the state of the qubit.

Theoretically, the difficulty for a rate description in this kind of system is twofold: first, the Hamiltonian of the isolated system H_S is time-dependent and therefore energy is not conserved, and second, there is no static energy barrier. Due to the coupling to the environment, however, the system approaches, as already discussed for the classical case above, a steady state situation such that the reduced density matrix takes the form $\rho(t) \sim \bar{\rho}(t) \cos(\omega_F t)$ with an only weakly time-dependent density $\bar{\rho}$. Hence, it is convenient to move to a rotating frame described by the unitary operator [25]

$$U(t) \equiv U_S(t)U_B(t) = e^{-i\hat{a}^\dagger \hat{a} \omega_F t - i \sum_n^N \hat{b}_n^\dagger \hat{b}_n \omega_F t}, \quad (15.44)$$

where $\hat{a}$ and $\hat{b}_n$ are annihilation operators for *harmonic* oscillators in the system and in the bath, respectively. In the rotating frame the total Hamiltonian reads

$$\tilde{H} = U^\dagger \left[H - i\hbar \frac{\partial}{\partial t} \right] U = \tilde{H}_S + \tilde{H}_R + \tilde{H}_I \quad (15.45)$$

with H as specified in (15.1) and H_S as in (15.43). The system part follows upon discarding

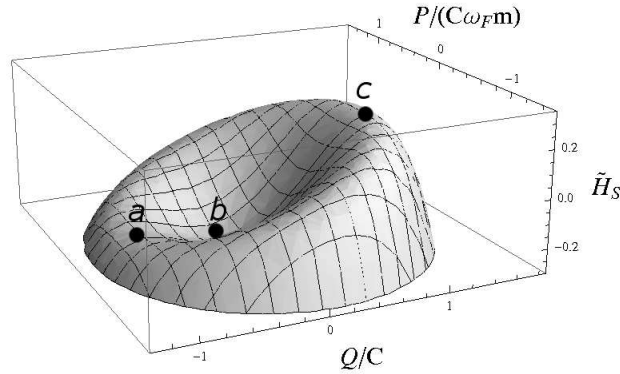


Figure 15.6: The Hamiltonian function (from 15.46) in the rotating frame, for $\alpha = 1/27$. The energy is scaled with $C^2\omega_F m\delta\omega$. The minimum (b) and the maximum (c) in $\tilde{H}_S$ correspond in the laboratory frame to the stable states with low and high amplitude, respectively, separated by a marginal state (a).

fast oscillating terms $\exp(\pm ik\omega_F t)$ with $|k| \geq 1$ as a *time-independent* Hamiltonian [26] of the form

$$\tilde{H}_S = m\omega_F\delta\omega C^2 \left[-\frac{1}{4} \left(\frac{Q^2}{C^2} + \frac{P^2}{(C\omega_F m)^2} - 1 \right)^2 + \frac{\sqrt{\alpha}}{C} Q \right] \quad (15.46)$$

with $C = \sqrt{\frac{8\omega_F\delta\omega m}{3\Gamma}}$ and $\alpha = \frac{3F^2\Gamma}{32(\omega_0\delta\omega m)^3}$. This latter quantity plays the role of a bifurcation parameter: For $0 < \alpha < 4/27$ the Hamiltonian (15.46) has three extrema, where the two stable ones correspond in the laboratory frame to oscillations with low and high amplitude, respectively. They are separated by a phase-space barrier associated with an unstable extremum [see fig. 15.6]. The remaining parts of the composite system (15.45) are written as [27]

$$\begin{aligned} \tilde{H}_R &= \sum_{n=1}^N \left(\frac{p_n^2}{2\tilde{m}_n} + \frac{\tilde{m}_n}{2} \tilde{\omega}_n^2 x_n^2 \right) \\ \tilde{H}_I &= -\sum_{n=1}^N \tilde{c}_n \left(x_n Q + \frac{p_n}{\tilde{\omega}_n \tilde{m}_n} \frac{P}{\omega_F m} \right) + \left[Q^2 + \frac{P^2}{(\omega_F m)^2} \right] \sum_{n=1}^N \frac{c_n^2}{4m_n\omega_n^2}, \end{aligned} \quad (15.47)$$

with new bath parameters

$$\tilde{m}_n = \frac{m_n}{1 - \omega_F/\omega_n}, \quad \tilde{\omega}_n = \omega_n - \omega_F, \quad \tilde{c}_n = \frac{c_n}{2}. \quad (15.48)$$

These parameters determine an effective spectral density and an effective damping kernel (see (15.10)) in the rotating frame [27].

We now calculate the probability for a system prepared initially in one of the stable states, say the low amplitude state, to switch to the other one, say the high amplitude state. Since in the rotating frame the Hamiltonian takes a time-independent form, we can apply the approach presented in the first part of this Section to determine this rate from an equation

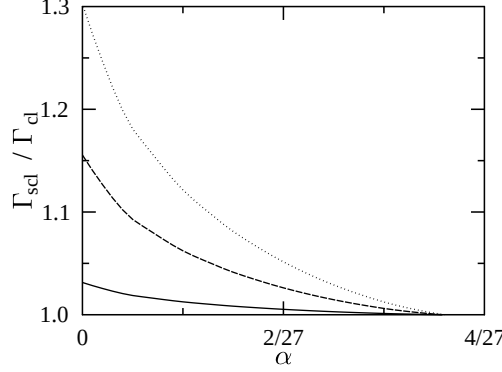


Figure 15.7: Escape rate normalized to the classical rate as a function of the bifurcation parameter α for $\hbar\omega_F\beta/(2\pi) = 0.01$ (solid), $\hbar\omega_F\beta/(2\pi) = 0.05$ (dashed) and $\hbar\omega_F\beta/(2\pi) = 0.1$ (dotted). For all the three lines is $\beta(m\omega_F\delta\omega)^2/\Gamma = 20$, $\delta\omega/\omega_0 = 0.1$ and the dimensionless friction constant $\beta\tilde{\gamma}mD^2\delta\omega = 0.001$.

of motion. The difference here is that the system Hamiltonian is not of standard form and that the system-reservoir coupling carries an additional momentum-momentum interaction. Hence, the transition rates (15.30) appearing in the master equation (15.29) read

$$\begin{aligned}
 W_{E,E'} &= \frac{D_{QQ}(E-E')}{\hbar^2} \left[|Q_{\text{qm}}(E', E)|^2 + \frac{1}{\omega_F^2 m^2} |P_{\text{qm}}(E', E)|^2 \right] \\
 &+ \frac{D_{QP}(E-E')}{\hbar^2 \omega_F m} 2i \operatorname{Im}\{Q_{\text{qm}}(E', E)^* P_{\text{qm}}(E', E)\}, \quad (15.49)
 \end{aligned}$$

with $P_{\text{qm}}(E', E) \equiv \langle E'|P|E \rangle$. Here, the bath functions D_{XY} are defined according to (15.32) with correlations $K_{XY}(t) = \langle \xi_X(t)\xi_Y(0) \rangle / \hbar$ containing those bath forces ξ_X, ξ_Y that couple to system operators X, Y in (15.47). For the escape process near the bifurcation threshold the energy level spacings of the well states in (15.46) are small compared to ω_F and one arrives at [27]

$$\begin{aligned}
 D_{QQ}(E) &= \tilde{\gamma} \{ n_\beta(E_F + E)(E_F + E) + [n_\beta(E_F - E) + 1](E_F - E) \} \\
 D_{QP}(E) &= i\tilde{\gamma} \{ -n_\beta(E_F + E)(E_F + E) + [n_\beta(E_F - E) + 1](E_F - E) \}, \quad (15.50)
 \end{aligned}$$

where $E_F = \hbar\omega_F$ and $\tilde{\gamma} = \gamma/4$ is the effective friction constant in the rotating frame. Notably, the above expressions display that physically two channels of bath modes are accessible for emission or absorption of quanta, namely, one with energy $E_F + E$ and one with energy $E_F - E$ [27].

Now, semiclassical wave functions in the well are constructed as discussed above in (15.34). With their help, transition rates are evaluated and one arrives at the semiclassical energy diffusion equation

$$\dot{P}(E, t) = \left[\frac{\partial}{\partial E} \tilde{\gamma} \left(\bar{\Delta}(E) + \bar{\kappa}(E) \frac{\partial}{\partial E} \right) R(E) - T(E) \right] \frac{\omega(E)}{2\pi} P(E, t) \quad (15.51)$$

with

$$\bar{\Delta}(E) = \Delta(E)C(E) - 2\hbar\nu\Delta^{(1)}(E) \quad (15.52)$$

$$\bar{\kappa}(E) = \Delta(E)C(E)\frac{\kappa}{2} + \hbar\omega_F\Delta^{(1)}(E). \quad (15.53)$$

Here, the coefficient $\kappa = \hbar\omega_F \coth(\hbar\omega_F\beta/2)$ results from the expansion of D_{QQ} in (15.50) and the coefficient $\hbar\nu = [\hbar\beta\omega_F - \sinh(\hbar\omega_F\beta)]/[\cosh(\hbar\omega_F\beta) - 1]$ from D_{QP} in (15.50). The factor $C(E)$ is again due to the finite barrier transmission. Further, Δ can be interpreted as a generalized action and originates from the first term in (15.49), while $\Delta^{(1)}$ is related to the "unconventional" term $\text{Im}\{Q_{\text{qm}}(E', E)^*P_{\text{qm}}(E', E)\}$ in the transition rate (15.49). These two functions are given by

$$\Delta(E) = m \oint dQ \dot{Q} + \frac{1}{m\omega_F^2} \oint dP \dot{P} \quad (15.54)$$

$$\Delta^{(1)}(E) = \frac{\omega}{\pi\omega_F} \lim_{\epsilon \rightarrow 0^+} \int_0^{2\pi/\omega} dt dt' \dot{Q}(t) \dot{P}(t') \frac{\sin[\omega(t-t')]}{1 + e^{-2\epsilon} - 2e^{-\epsilon} \cos[\omega(t-t')]} \quad (15.55)$$

Corrections to (15.51) are of the same order as in (15.37), namely, of order $\hbar^2$ or smaller.

This way, the escape rate gains leading order quantum corrections in the form

$$\Gamma_{\text{scl}} = \Gamma_{\text{cl}} \left[1 + \frac{\hbar\omega_F}{\kappa\pi} \left(-b_1 \frac{\omega_b}{\omega_F} + b_2 \right) \right]. \quad (15.56)$$

The classical rate Γ_{cl} can directly be inferred from (15.41) by replacing

$$S_0 \rightarrow \Delta, \quad \gamma \rightarrow \tilde{\gamma}, \quad \beta \rightarrow 2/\kappa, \quad (15.57)$$

with the barrier height $V_b = E_a - E_b$, where the energies E_a and E_b refer to the unstable point (a) and the stable point (b) in fig. 15.6, respectively, and the well frequency ω_0 determined by (15.46). The quantum factor contains the coefficient $b_1 \simeq 1.04$ originating from a finite barrier transmission/reflection and the bath-induced coefficient

$$b_2 = \frac{4\pi}{\omega_F\kappa} (\nu\kappa + \omega_F) \int_{E_a}^{E_b} dE \frac{\Delta^{(1)}(E)}{\Delta(E)}, \quad (15.58)$$

originating from the position-momentum contribution in the transition rates (15.49). The range of validity of this rate expression is given by those values of α which are sufficiently larger than 0 (where the motion near the barrier top is overdamped) and sufficiently smaller than $\alpha = 4/27$ (where the barrier height tends to zero). Explicit results for the rate (15.56) are depicted in fig. 15.7 for various values of temperature. Interestingly, the two types of quantum fluctuations have opposite effects on the rate expression: while a finite reflection for energies above the barrier top leads to a suppression of the escape probability, bath induced fluctuations produce an increase. In contrast to the situation of a static energy barrier discussed in the previous Section (see fig. 15.5), this latter corrections always prevails in the relevant range of parameters. The corresponding rate enhancement is substantial and grows with decreasing temperature.

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