Z. Phys. B – Condensed Matter 68, 181–191 (1987)

Condensed Matter
Zeitschrift für Physik B

Dissipative Tunneling

P. Hänggi
Lehrstuhl für Theoretische Physik, Universität Augsburg,
Federal Republic of Germany

Received April 27, 1987

Dedicated to Professor Harry Thomas on the occasion of his 60th birthday

The rate of escape of a metastable state is studied in a temperature regime where quantum tunneling acts as the rate limiting process. The particle is coupled to a heat bath so that it can dissipate energy in tunneling across an obstructing barrier. This objective then gives the generalization of the classical Kramers treatment of escape from a metastable state for the quantum regime, thereby providing a description for dissipative escape at all temperatures. For a (memory)-damped particle moving in a metastable potential the dissipative quantum decay rate is evaluated by use of a thermodynamic scheme (imaginary free energy method). This free energy method (bounce technique) is contrasted with the semiclassical approximation to finite temperature quantum decay in full phase-space of system plus environment. This comparison sheds new insight into the type of approximations that are inherent in the semiclassical bounce technique for the dissipative quantum system. The validity of the results is discussed as function of the barrier height, the temperature and the dissipation strength. In particular, we point out that dynamical nonequilibrium effects due to weak damping have with decreasing temperature an exponentially smaller effect for the thermodynamic rate expression (i.e. the Boltzmann average in full phase space over energy-dependent reactive tunneling probabilities). The regime of validity of the thermodynamic rate is depicted in a three-dimensional rate phase diagram, named the "Thomas-diagram".

1. Introduction

Kinetic processes hindered by one or a series of intervening potential barriers are of fundamental importance in a variety of systems, including chemical reactions, biological transport, diffusion in solids, nuclear reactions, and possibly even the birth of the universe. At high enough temperatures, the rate of such processes obeys the ubiquitous law by Svante Arrhenius, according to which the rate, Γ, of escape from a metastable state is proportional to the Boltzmann factor for thermal activation up to the barrier top. This process of thermal activation across barriers has been studied extensively in recent years, accounting for various physical complexities. In particular, the study of the prefactor for the rate, A, becomes a highly nontrivial task if one attempts to describe its dependence on friction strength, noise correlation time, external periodic driving forces, dimension of the reaction coordinate, influence of nonadiabatic transport, etc. For more details on the many facets of the problem of classical escape from a metastable state in various situations we refer to a recent review [1], and to the historical overview by Landauer [2].

As one continuously lowers the temperature, the classical rate

$$\Gamma = A \exp(-E_b/kT)$$

predicts an exponential fast decrease with no action taking place at absolute zero temperature. It is in this very low temperature regime where the effect of quantum tunneling becomes increasingly important.

As is well known, quantum mechanics allows a tunnel effect whereby the particle penetrates the classically forbidden regime under the barrier (Fig. 1). Naturally, the role of quantum effects in reactive processes has been recognized long ago, during the hey-

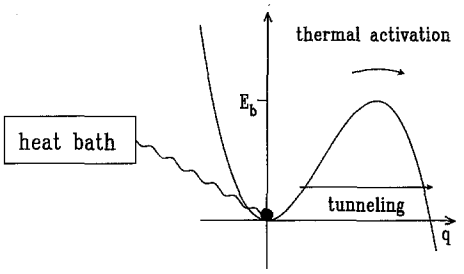

Fig. 1. Escape of a particle from a metastable state. The particle can leave the potential well either via thermal activation over the barrier, or via tunneling through the classically forbidden region. The interaction between the particle and the heat bath is modelled by frictional forces

days of quantum mechanics. In 1927, F. Hund [3] demonstrated that quantum tunneling occurs for intramolecular rearrangements as manifested by tunnel-splittings of spectra in pyramidal molecules such as ammonia. The tunneling phenomenon became a well known effect shortly after 1928, when G. Gamow [4], as well as R.W. Gurney and E.U. Condon [5] convincingly explained the decay of nuclei such as α-decay, and R. Fowler and L. Nordheim [6] applied tunneling to the phenomenon of electron emission in intense electric fields. As early as in 1929, D. Bourgin [7] hinted the possible role of the tunnel effect in chemical kinetics. Around the same time, the work of A.H. Wilson, L. Nordheim and C. Zener opened the important chapter of tunneling phenomena in solid state sciences. Since then, the tunneling mechanism has been invoked, and developed further in a multitude of fields, encompassing biology, electronics, crystalline and amorphous solids, or tunneling microscopy [8].

Our focus, here will be on the problem of *dissipative quantum tunneling*. This area has been evolving recently rather rapidly after Leggett [9] has initiated studies on the problem of low temperature tunneling and quantum coherence of macroscopic quantum variables (known as macroscopic quantum tunneling, MQT) such as the decay of the zero-voltage state in a biased Josephson junction, or the fluxoid quantum transitions in a single junction superconducting quantum interference device (SQUID) ring. In the following I shall restrict myself to a discussion of *incoherent tunneling* decay processes only, as they occur in Josephson junctions, quantum chemical and biological reactions, quantum diffusion in solids and at surfaces, etc. For a discussion of related dissipative quantum phenomena such as dissipative quantum coherence [10], response to microwaves and macroscopic energy quantization [11], or Bloch oscillations in Josephson junctions [12], we refer the readers to the literature.

2. Formulation of the Problem

The quantum description of metastable and unstable states has been a subject of many investigations since the early days of quantum mechanics. As is well known, the description of such states gives rise to several conceptual problems that arise from the difficulty of finding a satisfactory characterization of these states. There are several methods available in the literature that characterize the decay of a metastable state at zero temperature. Some of the more familiar ones are:

(a) The axiomatic S-matrix theory, wherein one associates decay rates in a one-to-one correspondence with poles of the S-matrix close to the real axis on the unphysical sheet of the energy Riemann surface, provided that the S-matrix can be analytically continued there.

(b) A time-dependent wave function approach, whereby one considers the outgoing scattered wave near a resonance energy. In this case, there occurs a typical delay, $t_D = 2/\Gamma$, in the arrival of the scattered wave of the order of the inverse of the decay rate, Γ, with respect to the case in which no resonance occurs.

(c) A dynamical semigroup approach for the evolution of the density operator [13].

The approaches in *(a)* and *(b)* are not readily extended to finite temperatures and to situations where the interactions with the environment become important. For the following, we should also remind ourselves that a pure exponential decay at all times can only occur if a rescattering from the decay products (backscattering) were to be absent*. However, the rescattering phenomenon cannot be forbidden unless one chooses a Hamiltonian that is not bounded from below. Khalfin [14] has pointed out, by use of a fundamental theorem due to Paley and Wiener, that the quantum nondecay probability, $P(t)$, cannot be purely exponential for very large times if the minimum of the energy spectrum of the Hamiltonian is bounded from below at $E_{\min} \neq -\infty$. Moreover, the quantum nondecay probability then also possesses a vanishing derivative at the origin of time evolution; that is, $P(t)$ is also not of exponential form for very short times. Throughout the rest of the paper, therefore, we will focus our attention only on the decay at intermediate times for which the decay law has approximately exponential form. In practice, this intermediate time regime is very large, it usually extends over a time scale at which 99% of the reduction in $P(t)$ has occurred already.

* For a recent study of the role of such backscattering effects in quantum decay at weak bias see [37]

Over the last two decades, probably the most developed theory to describe dissipative quantum mechanics at finite temperatures has been the semigroup approach. This type of method has been very popular in describing damping phenomena in nonlinear optics and in spin relaxation theory. However, these dissipative semigroup methods treat the coupling to the environment perturbatively (weak coupling regime). This restricts the treatment only to the weak damping regime, where the largest damping coefficient, γ, typically obeys

$$\gamma \ll \omega_0, \quad \hbar\gamma \ll kT. \tag{2.1}$$

Here, ω_0 is the smallest frequency typical for reversible motion. In a tunneling system, ω_0 may differ from zero just by the tunnel splitting. Thus, the first inequality is violated already for very weak damping. Furthermore, macroscopic tunneling phenomena occur at extreme low temperatures; that is, the second inequality is then also violated for an appreciable amount of dissipation. Hence, for tunneling systems, a more complete and more accurate description of dissipation is needed.

Our emphasis will be on the study of quantum decay of a damped particle moving in a metastable potential $V(q)$ (see Fig. 1) whose classical equation of motion (or its Ehrenfest equation) for the coordinate q has the form

$$M\ddot{q} + M\int_0^t \gamma(t-s)\,\dot{q}(s)\,\mathrm{d}s + \frac{\partial V(q)}{\partial q} = 0. \tag{2.2}$$

As is well known, tunneling problems are advantageously investigated in terms of complex-time path integrals [15–29].

3. Path Integral Approach

In this subsection I shall present, for reasons of completeness, a brief outline of the main ingredients of the method. Let me start with the partition function Z

$$Z = \mathrm{Tr}\{\exp(-\beta H)\}, \quad \beta = \frac{1}{kT}. \tag{3.1}$$

With the usual replacement by a pure imaginary time, $t \to -i\hbar\beta$, following Feynman, this quantity is recast in the form of a (Euclidean) functional path integral

$$Z = \int \mathscr{D}q(\tau)\exp\{-(S_E[q(\tau)]/\hbar\}, \tag{3.2}$$

where $\tau = it$ is a real variable (Wick rotation). The integral in (3.2) runs over all paths that are periodic with period $\theta = \hbar\beta$. Each path is weighted by the Euclidean action S_E. In order to account for dissipation we start out from the functional integral expression in full phase space of particle plus environment. Moreover, we assume that the environment couples bilinearly to the tunneling coordinate q. The surroundings is represented by a set of harmonic bath oscillator modes such that upon a contraction onto the coordinate q one arrives at an Ehrenfest equation equivalent with (2.2). This procedure yields an effective action S_E [1, 9, 15, 16, 26, 27] that reads

$$S_E[q] = \int_{-\theta/2}^{\theta/2} \mathrm{d}\tau\,[\tfrac{1}{2}M\dot{q}^2 + V(q)] + \tfrac{1}{2}\int_{-\theta/2}^{\theta/2}\mathrm{d}\tau \int_{-\theta/2}^{\theta/2}\mathrm{d}\tau' k(\tau-\tau')\,q(\tau)\,q(\tau'). \tag{3.3}$$

The first term describes the reversible motion, while the second, nonlocal part describes the influence of dissipation. The influence kernel is periodic with period θ, and may be represented in terms of a Fourier series as

$$k(\tau) = \frac{M}{\theta}\sum_{n=-\infty}^{\infty} |\nu_n|\,\hat{\gamma}(|\nu_n|)\exp(i\nu_n\tau); \qquad \int_{-\theta/2}^{\theta/2} k(\tau)\,\mathrm{d}\tau = 0, \tag{3.4a}$$

where we used

$$\nu_n = n2\pi/\theta, \quad \hat{\gamma}(z) = \int_0^\infty \gamma(t)\,\exp(-zt)\,\mathrm{d}t. \tag{3.4b}$$

This result implies a relationship between the quantum mechanical dissipative influence kernel $k(\tau)$ and the *real time* memory damping $\gamma(t)$ in (2.2) [16], i.e.

$$k(\tau) = \frac{M}{\theta}\int_0^\infty \mathrm{d}s\,\gamma(s)\frac{\partial}{\partial s}\left(\frac{\sinh(\nu s)}{\cos(\nu\tau)-\cosh(\nu s)}\right) + M\gamma(0)\,[\delta(\tau)] \tag{3.5}$$

where $\nu = \nu_1 = 2\pi/\theta$ and $[\delta]$ is the δ-fct periodically repeated at $\tau = n\theta$. Because of this connection there is no need to refer further to the specific microscopic model. Also note that $k(\tau)$ remains nonlocal for memory-free damping (i.e. pure Ohmic dissipation $\gamma(t) = 2\gamma\delta(t)$); the nonlocal character is clearly due to the dissipative (non-reversible) part of the motion.

4. The Tunneling Rate: Imaginary Free Energy Method

4.A. The Bounce Solution

Now we are prepared enough to discuss the dissipative quantum decay rate from a metastable state (see Fig. 1). Initially, the particle is located near the origin

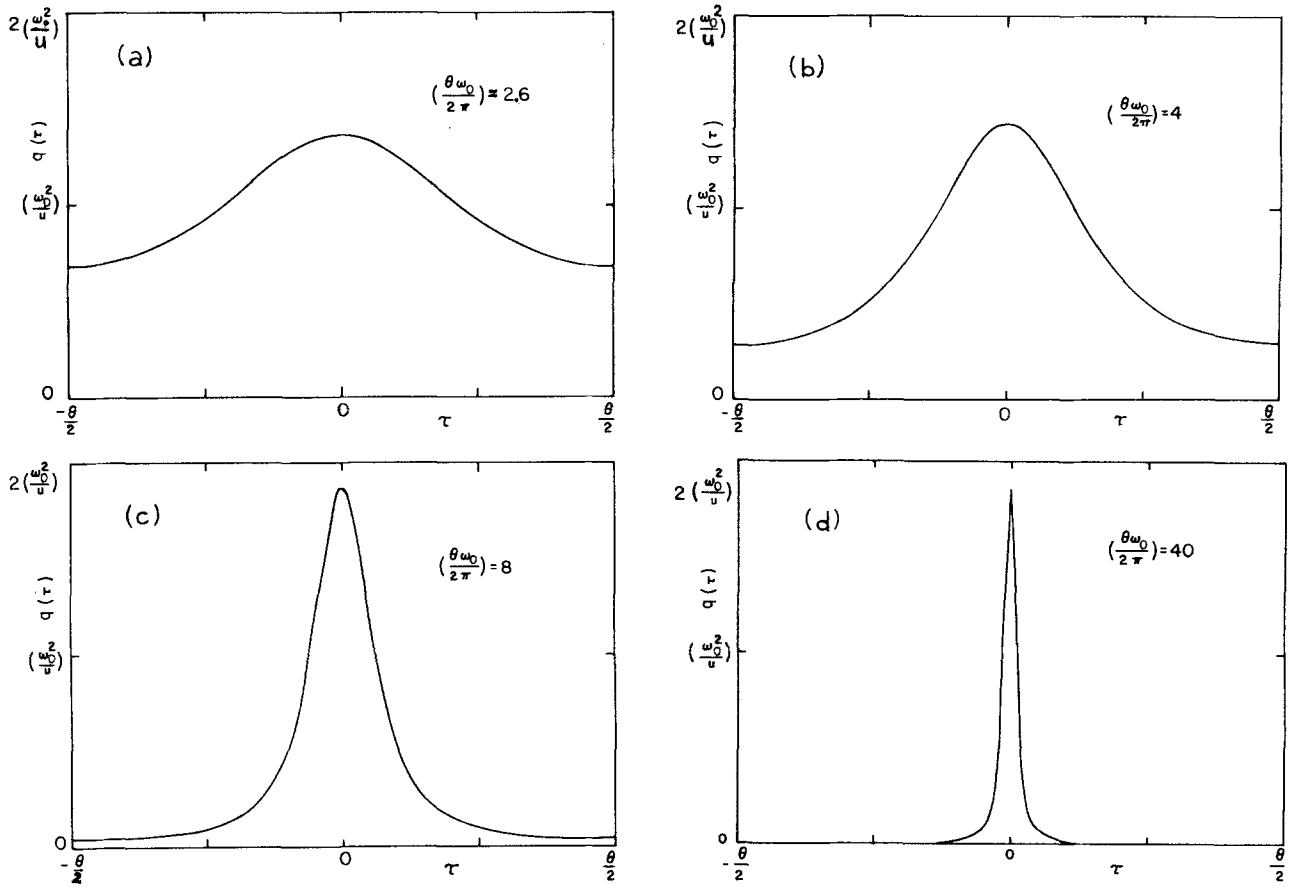

Fig. 2. The bounce trajectories $q_B(\tau)$ in a cubic metastable potential as a function of four decreasing temperatures ($\theta=\hbar\beta$). Note the approach of the bounce trajectory towards the constant saddle point solution $q_b=\omega_0^2/u$ with increasing temperature. At the crossover temperature ($\theta_0\,\omega_0/2\pi)=\sqrt{6}$, $q_B(\tau)$ coincides with the trivial bounce solution $q_B(\tau)=q_b$ (taken from [21])

$q=0$. The free energy, F, of the particle is from (3.1) given by

$$F=-kT\ln Z=-kT\ln\{\int\mathscr{D}q\,\exp(-S_E[q]/\hbar)\}, \quad (4.1)$$

where S_E is given in (3.3). The state $q=0$ is metastable if its lifetime $\tau_0\equiv\Gamma^{-1}$, is long compared to all other characteristic time scales that describe relaxation towards the locally stable state at $q=0$. Keeping this physical situation in mind, it now turns out that the functional integral in (4.1) acquires an exponentially small imaginary part that is proportional to the decay rate. The origin of this behavior is as follows: We shall assume that the barrier height E_b (see Fig. 1) is large compared with the other relevant energy scales, i.e.

$$kT\ll E_b, \quad \hbar\omega_0\ll E_b, \quad (4.2)$$

where $\omega_0^2=M^{-1}V''(q=0)$. The main contributions to the functional integral then stem from paths that make the Euclidean action S_E stationary, or almost stationary. It follows from (3.3), that S_E is stationary for those paths that are solutions of the classical equation of motion in the inverted potential, $V(q)\to -V(q)$; that is

$$M\ddot{q}_B=\frac{\partial V}{\partial q_B}+\int_{-\theta/2}^{\theta/2}\mathrm{d}\tau' k(\tau-\tau')\,q_B(\tau'), \quad (4.3)$$

with $q_B(\tau)$ obeying the periodic boundary condition $q_B(\tau=-\theta/2)=q_B(\tau=\theta/2)$.

Because of the second property in (3.4a), we note that (4.3) has two trivial solutions: $q_1(\tau)=0$, where the particle just sits on top of the inverted potential, $-V(q)$ (i.e. at the minimum of $V(q)$), and the saddle point solution $q_2(\tau)=q_b$, where the particle is located at the minimum of $-V(q)$ (i.e. at the barrier top of $V(q)$). Solutions of (4.3) at different temperatures ($\theta=\hbar\beta$) in a cubic potential $V(q)=M(\omega_0^2\,q^2/2-uq^3/3)$ are depicted in Fig. 2. Note the broadening of the bounce solution with increasing temperature towards the constant $q_2=q_b=\omega_0^2/u$.

A nontrivial solution $q_B(\tau)$ of (4.3) exists below the crossover temperature $T=T_0$ to quantum dominated escape (see below). We call this solution the "bounce" solution $q_B(\tau)$. The bounce $q_B(\tau)$ is a θ-periodic orbit that rocks back and forth through the classically forbidden region of the potential $V(q)$ [19]. This bounce trajectory is not a minimum of the action S_E; but a saddle point solution with an *unstable* direction. For temperatures $T>T_0$, the role of $q_B(\tau)$ is taken over by the constant saddle-point solution $q_2(\tau)=q_b$. Thus, there exists at all temperatures a fluctuation mode in function space with respect to which the bounce is a maximum of the action. Therefore, this characteristic fluctuation mode ($q(\tau)=q_b$, for $T>T_0$; $q(\tau)=q_B(\tau)$, for $T<T_0$) has a *negative* eigenvalue. Below $T=T_0$, the action $S_E[q(\tau)=q_b]$ exceeds the value obtained by the nontrivial bounce $q_B(\tau)$; hence with $S_E[q_B(\tau)]<S_E[q(\tau)=q_b]=\theta E_b$, the trivial solution can be disregarded for $T<T_0$ (except within the crossover region $T\sim T_0$).

This feature obviously plagues the evaluation of the free energy (partition function). What is needed is an analytical continuation [17, 20], where the integral of the unstable (negative eigenvalue) mode is distorted in the complex plane so that it passes through the saddle point, and then into the complex plane. This omnipresent negative eigenvalue is thus the origin for the exponentially small imaginary part of the free energy F in (4.1).

4.B. Energy Loss During Tunneling

In Fig. 3 we depict the "exit" and "entrance" points of the bounce solution $q_B(\tau)$, as a function of increasing temperature $T\uparrow T_0$. Note that at finite temperatures the particle may loose or gain energy in tunneling across the potential barrier [21]. The difference in energy between the two reference points at "exit" and "entrance" may then be identified with the energy loss (or gain) in quantum tunneling [21, 22]. At zero temperature, there is always an energy loss ΔE, which in terms of the bounce solution is expressed as [22]

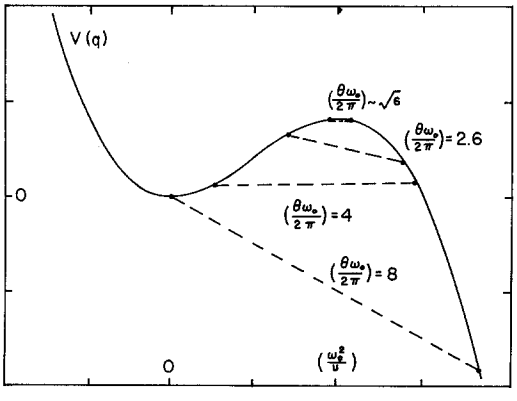

Fig. 3. The "entrance" and "exit" points of bounce solutions $q_B(\tau)$ depicted in Fig. 2. The "entrance" point corresponds to the minimal value at $\tau=\pm 1/2\theta$, the "exit" point is the maximum of the bounce at $\theta=0$ (taken from [21])

$$\Delta E=\int_0^\infty d\tau \int_0^\infty d\tau' \dot{q}_B(\tau)\,\tilde{k}(\tau+\tau')\,\dot{q}_B(\tau'), \tag{4.4a}$$

where

$$\tilde{k}(\tau)=\int_{-\infty}^{\tau} k(s)\,ds. \tag{4.4b}$$

4.C. The Tunneling Rate Formula

Just as in the usual quantum mechanical theory for decay widths (or decay rates) of metastable quantum states, where the rate Γ is related to the imaginary part of the resonance energy, i.e. $\Gamma_n=-(2/\hbar)\,\mathrm{Im}\,E_n$, we define by analogy the temperature averaged decay rate Γ by [15, 16, 21, 23–29]

$$\Gamma=-\frac{2}{\hbar}\,\mathrm{Im}\,F, \qquad T<T_0. \tag{4.5}$$

For temperatures $T>T_0$, however, Affleck [23] has shown that the rate Γ and the imaginary free energy part are connected by

$$\Gamma=-\frac{2}{\hbar}\left(\frac{T_0}{T}\right)\mathrm{Im}\,F, \qquad T>T_0. \tag{4.6}$$

At $T\cong T_0$, (4.6) matches smoothly onto the expression in (4.5). The additional factor (T_0/T) is a remnant of the transition near T_0 where both $q_B(\tau)$ and $q(\tau)=q_b$ induce two zero modes [21, 24, 25]. In previous works [1, 15, 16, 21, 24, 26, 27] we used the above formulas by evaluating the imaginary part of the free energy F, (4.1), with the Euclidean action given by (3.3), after we integrated (exactly) over the environmental modes. Schmid [28] has shown that at $T=0$ this procedure yields the same result as the direct evaluation of the quantum decay rate within the quasi-classical approximation in N-dimensional phase space of system plus environment.

Alternatively, at finite temperatures, a direct Boltzmann average in N-dimensions (system plus bath) gives for the quantum rate Γ the expression

$$\Gamma=Z_0^{-1}\frac{1}{2\pi\hbar}\int_0^\infty dE(\exp-\beta E)\,\Gamma(E), \tag{4.7}$$

being valid for all temperatures. Z_0 is the partition function of the degrees of freedom in the N-dimensional metastable well. The semiclassical approximation for the reactive probability $\Gamma(E)$ is given [19]

$$\Gamma(E)=\sum_{k=1}^{\infty}(-1)^{k-1}\exp(-k\phi(E)/\hbar)\cdot\prod_{i=1}^{N-1}[2\sinh(\tfrac{1}{2}kT(E)\,\omega_k(E))]^{-1}, \tag{4.8a}$$

with

$$\phi(E)=\oint_0^{T(E)}\mathrm{d}\tau\,\mathbf{p}(\tau)\cdot\dot{\mathbf{q}}(\tau),\qquad p_i=M_i\dot{q}_i \tag{4.8b}$$

being the "small" action integral along the periodic orbit of period $T(E)$ that rocks forth and back through the saddle-point region on the upside-down potential energy surface in N-dimensions. This motion is described by a coordinate q_1, along-side this orbit; the remaining $(N-1)$ degrees of freedom are the orthogonal displacements away from this (energy-dependent) periodic orbit in the classically forbidden regime. The parameters $\{\omega_k(E)\}$ denote stability frequencies (dynamical normal mode analysis; for details see Miller [19]) characterizing the unstable periodic orbit $q_1(\tau)$ with period $T(E)=-\phi'(E)$.

At low temperatures, $T<T_0$, only the first term with $k=1$ will contribute significantly to the sum in (4.8a). Then we can evaluate the integral in (4.7) by the method of steepest descent, yielding the condition

$$0=\beta+\phi'(E)/\hbar$$

i.e. the period becomes $T(E)=\hbar\beta=\theta$, which is precisely the period of the (dissipative) bounce in (4.3). Completing the steepest descent approximation in (4.7) then yields with $E=E_\theta$, such that $T(E_\theta)=\theta$ holds, the main result

$$\Gamma=Z_0^{-1}\left|\left(2\pi\hbar\frac{\partial T}{\partial E}\bigg|_{E=E_\theta}\right)\right|^{-\frac{1}{2}}\exp(-\bar{\phi}(\theta)/\hbar)\cdot\prod_{i=1}^{N-1}[2\sinh(\tfrac{1}{2}T(E_\theta)\,\omega_i(E_\theta))]^{-1} \tag{4.9}$$

where the "total" extremal action is given by*

$$\bar{\phi}(\theta)=\theta E_\theta+\phi(E_\theta)=\oint_0^{\theta}\mathrm{d}\tau[V(\mathbf{q}(\tau))+\tfrac{1}{2}\dot{\mathbf{q}}(\tau)\cdot\mathbf{p}(\tau)]. \tag{4.10}$$

This total action $\bar{\phi}(\theta)$ equals (again we assume a bilinear coupling to a heat bath of harmonic oscillators) the bounce action $S_E[q_B(\tau)]$ in (3.3) of the reduced system, i.e.

$$\bar{\phi}(\theta)=S_E[q_B]\equiv S_B=\int_{-\theta/2}^{\theta/2}\mathrm{d}\tau\left[V(q_B)-\frac{1}{2}q_B\frac{\partial V}{\partial q_B}\right]. \tag{4.11}$$

Hereby, we made use of the equation of motion of $q_B(\tau)$ in (4.3). The explicit evaluation of the prefactor in (4.9) is cumbersome and nontrivial. In previous works [21, 27] we have evaluated this prefactor within Gaussian approximation, i.e. we consider up to second order the fluctuations around the nonlinear bounce trajectory in (4.3); and likewise, for the quantity Z_0, we take into account the Gaussian fluctuations around the stable solution $q(\tau)=0$. This procedure induces another *technical* difficulty: Note that the bounce trajectory is not uniquely defined in the sense that a translation $q_B(\tau)\to q_B(\tau+b)$ also generates a solution that leaves the Euclidian action (3.3) invariant. The invariance of the action under translation $q_B(\tau)\to q_B(\tau+b)$ induces an eigenmode $y_1(\tau)\propto\dot{q}_B(\tau)$ with zero eigenvalue $\lambda_1=0$. This problem can be remedied if we perform a change of coordinates and integrate directly over the translation variable b [15, 17], rather than over the zero mode $y_1(\tau)$. This process then induces a zero mode normalization factor W

$$W=\left\{\frac{M}{2\pi\hbar}\int_{-\theta/2}^{\theta/2}\dot{q}_B^2\,\mathrm{d}\tau\right\}^{\frac{1}{2}}. \tag{4.12}$$

Collecting everything, the final result for the low temperature rates is then given explicitly by [1, 9, 15, 16, 21, 25, 27–29]

$$\Gamma=W\left\{\frac{\mathrm{Det}(\delta^2S_E/\delta q^2)_{q(\tau)=0}}{|\mathrm{Det}'(\delta^2S_E/\delta q^2)_{q(\tau)=q_B(\tau)}|}\right\}^{\frac{1}{2}}\exp(-S_B/\hbar),\qquad T<T_0. \tag{4.13}$$

Here Det′ indicates that the eigenvalue zero must be omitted. An *analytical* evaluation of the formula (4.13) is possible only for a cubic potential at a few specific ohmic damping values [21]. Approximative calculations are based either on a variation ansatz for the bounce [30], or on semiclassical methods as they apply for parabolic-like shaped wells and barriers [31, 32]. For a numerical study of the quantum decay rate in a cubic metastable potential we refer the readers to the article by Grabert, Olschowski and Weiss [29] in this very issue.

5. Crossover Temperature T_0

On inspecting the bounce solutions $q_B(\tau;\theta)$ in Fig. 2 we note that $q_B(\tau;\theta)$ approaches the trivial solution

* Here, $V(\mathbf{q})$ denotes the potential in full phase space of system plus environment (N-dimensions)

$q_2(\tau)=q_b$ with increasing temperature. Thus, any linear combination of the two solutions is an almost stationary solution of the Euclidian action S_E. Each one of these two quasi-stationary solutions separately induces a quasi zero mode (an exact zero mode and a quasi-zero mode) [16, 21]. For the solution $q_2(\tau)=q_b$, the Gaussian fluctuation modes are seen to possess the eigenvalue spectra ($\nu=2\pi/\theta$)

$$\lambda_n^{(b)}=n^2\nu^2-\omega_b^2+|n|\nu\hat{\gamma}(|n|\nu), \qquad n=0,\pm1,\pm2,\ldots \quad (5.1)$$

where

$$\omega_b^2=-\left(\frac{1}{M}\right)\frac{\partial^2 V}{\partial q_b^2}>0,$$

is the angular frequency at the barrier top. Note the negative eigenvalue $\lambda_0=-\omega_b^2$ (being independent of temperature) characteristic for the saddle point solution $q_2(\tau)=q_b$. More importantly, the eigenvalues $\lambda_{-1}=\lambda_1$ become mutually zero (zero modes) at

$$\nu^2-\omega_b^2+\nu\hat{\gamma}(\nu)=0, \qquad \nu=\frac{2\pi}{\hbar\beta}. \quad (5.2)$$

The largest temperature satisfying (5.2) thus determines the crossover temperature T_0 as [26, 33]

$$T_0=\frac{\hbar}{2\pi k}\mu \quad (5.3)$$

with μ being the *largest positive solution* of (5.2). With $\hat{\gamma}=0$, this yields the undamped crossover temperature; i.e. $\mu=\omega_b$. Interestingly enough, the quantity μ just coincides with the memory-friction renormalized diffusive (angular) barrier frequency which enters the prefactor of the classical diffusion-controlled rate Γ_{cl} across the barrier, i.e. [1]

$$\Gamma_{cl}=\left(\frac{\mu}{\omega_b}\right)\frac{\omega_0}{2\pi}\exp(-E_b/kT) \quad (5.4)$$

with μ being determined from (5.2). Alternatively, the quantity μ can be recast as

$$\mu=\left(\frac{\hat{\gamma}^2(\mu)}{4}+\omega_b^2\right)^{\frac{1}{2}}-\frac{\hat{\gamma}(\mu)}{2}, \quad (5.5)$$

which makes explicit the connection with the memory-friction $\hat{\gamma}(\omega)$.

The temperature T_0 is the threshold temperature below which quantum tunneling (as manifested by the existence of an oscillating periodic orbit in the classically forbidden regime) dominates over thermal activated hopping processes. Below $T=T_0$ the Arrhenius factor no longer describes the exponential leading part of the rate; this role is now taken over by the bounce action S_B (see 4.11). At $T=T_0$ itself, the bounce action S_B smoothly matches onto the Arrhenius factor (E_b/kT).

This crossover temperature T_0 can with

$$T_0=(1.216\cdot10^{-12}\ \mathrm{s\ K})\mu \quad (5.6)$$

be quite large, depending on the value of the dissipation and memory-renormalized angular barrier frequency μ. Typical atomic/molecular barrier frequencies are of the order of 10^{13}–10^{14} Hz; thus, crossover temperatures of the order of 10–100 K are quite common [33]. For MQT-experiments in Josephson junctions and SQUIDS, however, μ is typically around 10^{11} Hz; i.e. T_0 is around 100 m K. Thus, MQT experiments do require all the necessary expertise for a low temperature experiment. (Notice, however, that all of this might change with the recent discovery of high T_c-superconductors.)

As it follows from (5.5), T_0 is reduced with increasing dissipation strength. On the other hand, the crossover temperature increases monotonically towards its undamped value (given by $\mu=\omega_b$) with increasing memory-friction relaxation time and the zero-frequency dissipation, $\hat{\gamma}(\omega=0)=\gamma_0$ kept constant [33]. For an exponential memory friction

$$\gamma(t)=\frac{\gamma_0}{\tau_c}\exp(-t/\tau_c) \quad (5.7)$$

we depict in Fig. 4 the corresponding crossover temperature $T_0(\gamma_0;\tau_c)$.

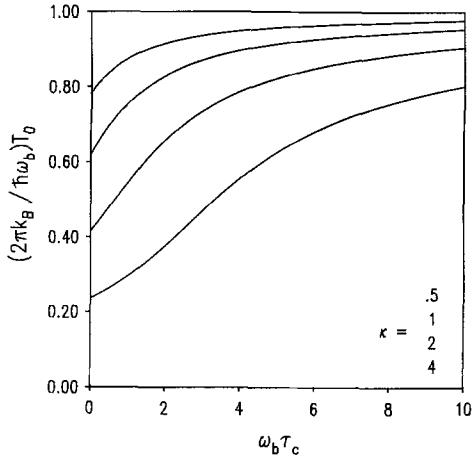

Fig. 4. The dimensionless crossover temperature $(2\pi k/\hbar\omega_b)T_0=\mu/\omega_b$ for the exponential memory damping (5.7) as a function of the dimensionless memory relaxation time $\omega_b\tau_c$, for various values of the noise strength $\kappa=\gamma_0/\omega_b$ (taken from [33])

6. Results for the Tunneling Rate

In this subsection we briefly summarize general analytic results for the dissipative tunneling rate, Γ (see 4.7).

6.A. Above T_0: Quantum Corrections to Thermal Activation

Based on the (high-temperature) rate expression in (4.6) one finds [15, 16, 24, 25, 32, 33] a quantum rate enhancement factor Q; i.e. with (5.4) we obtain

$$\Gamma = \Gamma_{cl} Q. \tag{6.1a}$$

The quantum enhancement factor Q reads explicitly [33]

$$Q = \prod_{n=1}^{\infty} \frac{n^2\nu^2 + \omega_0^2 + n\nu\hat{\gamma}(n\nu)}{n^2\nu^2 - \omega_b^2 + n\nu\hat{\gamma}(n\nu)}. \tag{6.1b}$$

For $T \gg T_0$, Q approaches unity. For weak-to-moderate damping strength there exists an accurate and very simple approximation to (6.1b) [33] which in leading order is independent of the dissipation $\hat{\gamma}$, i.e.

$$Q \simeq \exp\left\{\frac{\hbar^2}{24}\frac{(\omega_0^2+\omega_b^2)}{(kT)^2}\right\}. \tag{6.2}$$

Thus, above $T > T_0$, the Arrhenius factor becomes renormalized towards smaller values:

$$E_b \to E_b - \frac{\hbar^2}{24}\left(\frac{\omega_0^2+\omega_b^2}{kT}\right). \tag{6.3}$$

6.B. Near T_0: The Crossover Region [16, 21, 24, 25]

As mentioned previously, near $T \sim T_0$ the rate evaluation is more complicated due to the presence of two quasi zero modes. This problem has been dealt with by treating the two dangerous modes in the effective action, S_E, up to cubic and quartic order [21, 24, 25]. Moreover, Grabert and Weiss [24] have shown that in this crossover region there exists a frequency scale and a temperature scale (which both depend on the particular system under consideration) such that the rate exhibits a universal scaling behavior (for further details see [16 and 24]).

6.C. Below T_0: Tunneling Behavior

At sufficiently low temperatures we can use the steepest decent expression in (4.13). In this regime both, the exponential leading part as well as the prefactor, are strongly influenced by dissipation. The temperature dependence of the exponential part drastically differs from the Arrhenius law. Grabert, Weiss and Hänggi [26] have shown that the quantum decay rate exhibits a universal temperature enhancement (i.e. it holds independent of potential shape and damping strength) which takes on the form of a power law, $\ln \Gamma \propto T^n$. For Ohmic-like dissipation ($\hat{\gamma}(\omega=0) > 0$) we obtain a universal T^2-enhancement of the form

$$\ln\{\Gamma(T)/\Gamma(T=0)\} = aT^2, \tag{6.4}$$

with

$$a = \frac{\pi}{6}\hat{\gamma}(\omega=0)\, M\left\{\frac{k^2}{\hbar^3}\left(\int_{-\infty}^{\infty} q_B(\tau; T=0; \hat{\gamma})\, d\tau\right)^2\right\}. \tag{6.5}$$

This characteristic law has recently been observed in decisive experiments on MQT in current biased Josephson junctions [34] and SQUID rings [35].

7. Discussion: Rate-Phase-Diagram

The general rate expression in (4.7) is clearly based on a thermodynamic method which does not involve a fully dynamical description of the rare rate events. In the evaluation of the rate formula, via the imaginary free energy method, we made use of the semiclassical approximation (see also (4.2)), i.e.

$$kT \ll E_b, \quad \hbar\omega_0 \ll E_b,$$

and utilized ($T < T_0$) the steepest descent approximation in function space (bounce technique). At $T > T_0$, we thoroughly made use of the Gaussian approximation around the stationary points $q_1 = 0$, and $q_2 = q_b$. Thus, this theory does not account for nonequilibrium effects which result in a deviation from the thermal Boltzmann equilibrium distribution for the energy-distribution inside the metastable well. For very weak dissipation, such effects are known to be important in the classical (high-temperature) regime (see e.g. [1, 2]); at lower temperatures $T < T_0$, however, the role of weak damping plays an increasingly less important role [15, 36].

First let us recall [1] the validity of the classical rate expression in (5.4). This expression is based on the assumption that thermal equilibrium inside the well holds at all times, i.e. it is valid for barrier heights $E_b > kT$, and for moderate-to-strong friction strengths

$$\hat{\gamma}(\mu) \gtrsim \omega_b, \tag{7.1}$$

for which the equilibrization process inside the well away from the barrier occurs on a sufficient fast time

scale. For high barriers, $\beta E_b \gg 1$, the regime of friction values extends to even lower friction, – approaching the result of simple transition state theory [1] –, i.e. we have for the condition of validity of the classical rate Γ_{cl} in (5.4)

$$\hat{\gamma}(\mu) \gtrsim kT\omega_b/E_b, \quad T > T_0. \tag{7.2}$$

Put differently, a very high energy barrier implies an extreme long time scale for escape so that there remains sufficient time for thermalization inside the initial well, even for weak friction obeying (7.2). The crossover value $\hat{\gamma}(\mu) = kT\omega_b/E_b$ is obtained as follows: At very weak friction, energy-diffusion becomes the rate limiting mechanism. In order for it to be the dominant mechanism, the dissipative energy-loss δ for a round trip inside the initial well must be small compared to kT. The classical energy loss in the metastable well is given by

$$\delta = \hat{\gamma}(\mu) \oint p \, dx = \hat{\gamma}(\mu) S_0, \tag{7.3}$$

where S_0 is the classical action for a particle with energy at the barrier energy $E = E_b$ (in absence of friction). Because $S_0 \sim E_b/\omega_b$ we thus obtain from $kT = \delta$ the threshold value $\hat{\gamma}(\mu) = kT\omega_b/E_b$.

Upon a lowering of temperature we reach the crossover temperature $T_0(\hat{\gamma})$, see (5.3, 5.5). In view of quantum tunneling the following three dimensionless parameters determine the behavior of the rate

$$x_1 = \frac{kT}{E_b}, \quad x_2 = \frac{\hat{\gamma}(\mu)}{\omega_b}, \quad x_3 = \frac{\hbar\omega_b}{2\pi kT}. \tag{7.4}$$

The cylinder $1 \geqq x_1 \geqq 0$, cutting the positive (x_2, x_3)-plane at

$$\frac{\hbar\omega_b}{2\pi kT} = \frac{\hbar\omega_b}{2\pi kT_0(\hat{\gamma})} = \frac{\omega_b}{\mu} \xrightarrow[\hat{\gamma}(\mu) \gg \omega_b]{} \frac{\hat{\gamma}(\mu)}{\omega_b}, \tag{7.5}$$

describes the crossover between thermal activation controlled, and quantum tunneling controlled escape from a metastable state.

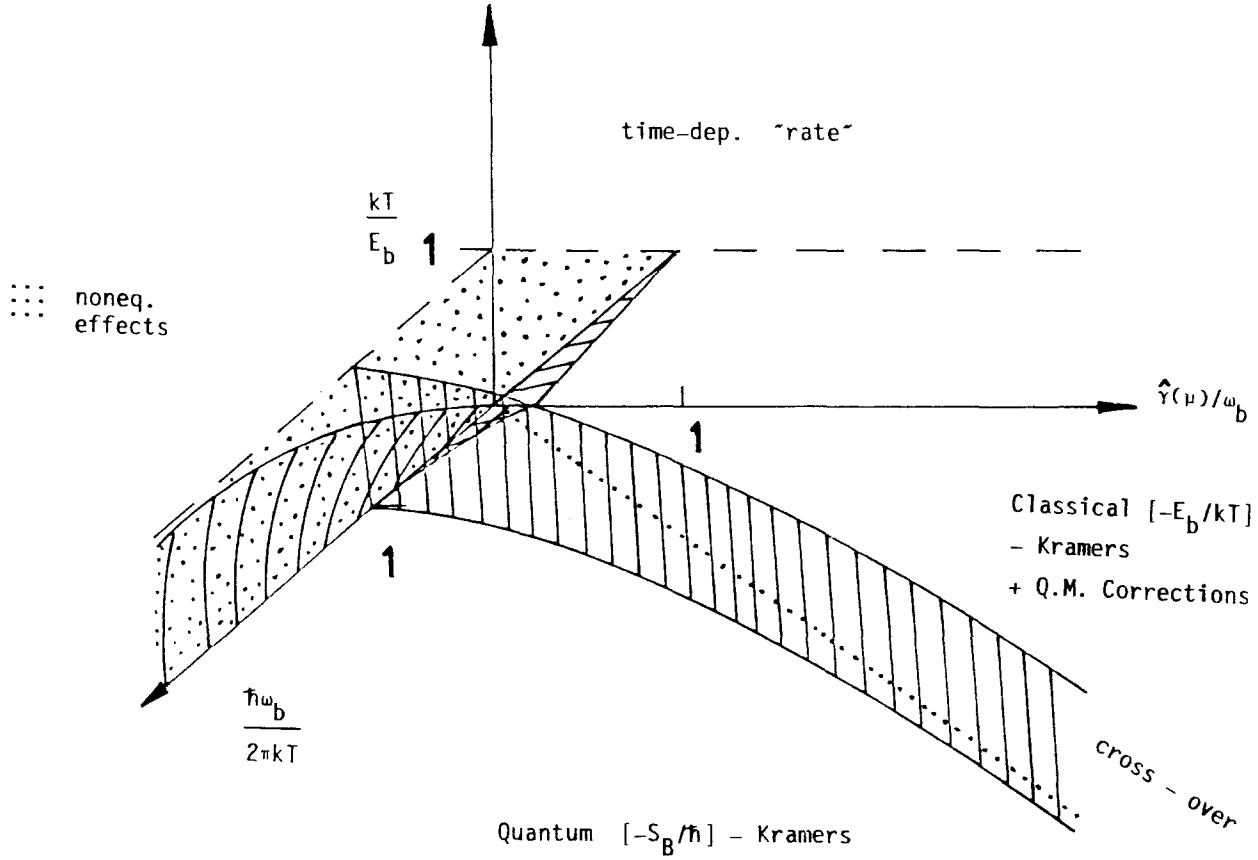

Fig. 5. The "Thomas-diagram". The crossover cylinder [hatched vertically] separates the classical thermal activation regime (including quantum corrections) from the tunneling dominated regime in which the role of the Arrhenius factor is taken over by the dissipative bounce action $S_B(\gamma; T)$, (4.11). The volume [dotted] at the left-side corner indicates the regime as a function of damping, barrier height and temperature in which weak damping induces nonequilibrium effects that are not accounted for by the thermodynamic rate formula (4.7) (imaginary free energy method). For $kT/E_b > 1$, the rate becomes generally a time-dependent function, i.e. $\Gamma \to \Gamma(t)$; $\dot{x}(t) = -\Gamma(t)\, x(t)$

For temperatures below crossover, $T<T_0$, the quantum rate is sufficiently small so that for almost all practical purposes weak friction does not have any impact on deviations from the thermal Boltzmann distribution of population inside the well; i.e. the validity of the rate expression (4.7, 4.8), or the validity of the imaginary free energy method, respectively, holds practically for the whole damping regime. A simple Fermi's Golden Rule calculation for a metastable well containing two quantum levels indicates that the rate at which thermal equilibrization occurs is governed by $\hat{\gamma}(\mu)$. The rate for the decay from one quantum level to a lower one, emitting the excess energy into the normal modes of the heat bath is thus directly proportional to $\hat{\gamma}(\mu)$. Using as an upper limit the zero-temperature decay rate at zero dissipation we can expect possible deviations from the low temperature rate formula (4.13) only for exponentially small friction; that is, for [15, 36]

$$\frac{\hat{\gamma}(\mu)}{\omega_0} \ll \frac{\Gamma(T=0, \hat{\gamma}=0)}{\omega_0} = \frac{12}{\sqrt{2\pi}} \left(\frac{3E_b}{\hbar\omega_0}\right)^{\frac{1}{2}} \exp\left(-\frac{36E_b}{5\hbar\omega_0}\right). \tag{7.6}$$

Typically we have $E_b \gtrsim 2\hbar\omega_0$, in order for the semiclassical approximation to be valid. Then the condition (7.6) becomes

$$\frac{\hat{\gamma}(\mu)}{\omega_0} \lesssim 10^{-6}. \tag{7.7}$$

Clearly, for rate processes in stationary nonequilibrium situations, e.g. for decay rates in presence of external microwaves, etc., or decay rates in systems prepared far from thermal equilibrium, one is required to use a dynamical (real-time) rate approach (e.g. by use of the Feynman-Vernon technique).

The physics of (7.1)–(7.7) can be summarized in a rate-phase-diagram given in Fig. 5. The author would like to dedicate this diagram to Professor Harry Thomas ("Thomas-diagram"): Because of repeated clarifying and helpful discussions with him and his persistent encouragement, my motivation finally crossed the threshold to draw up the three-dimensional rate-phase-diagram in Fig. 5.

The author would like to thank H. Grabert, G.L. Ingold, P. Olschowski, P. Schramm and U. Weiss (University of Stuttgart) and E. Freidkin and P.S. Riseborough (Polytechnic University) for the many helpful discussions and the enjoyable collaboration in tunneling problems.

References

1. Hänggi, P.: J. Stat. Phys. **42**, 105 (1986); **42**, 1003 (1986) (Addendum)
2. Landauer, R: In: Nonlinearity in condensed matter. Bishop, A.R., Campbell, D.K., Kumar, P., Trullinger, S.E. (eds.). Berlin, Heidelberg, New York: Springer 1986
3. Hund, F.: Z. Phys. **43**, 805 (1927)
4. Gamow, G.: Z. Phys. **51**, 204 (1928)
5. Gurney, R.W., Condon, E.U.: Nature **122**, 439 (1928); Phys. Rev. **33**, 127 (1929)
6. Fowler, R.H., Nordheim, L.: Proc. R. Soc. (London) Ser. A **119**, 173 (1928)
7. Bourgin, D.G.: Proc. Natl. Acad. Sci. USA **15**, 357 (1929)
8. For a recent survey see in: Tunneling. Jortner, J., Pullmann, B. (eds.). Boston: Reidel 1986
9. Leggett, A.J.: Progr. Theor. Phys. Suppl. **69**, 80 (1980); **80**, 10 (1984); Quantum Mechanics at the Macroscopic Level: In: Directions in Condensed Matter Physics, Advanced Series in Condensed Matter Physics. Vol. 1, pp. 187–248. Grinstein, G., Mazenko, G. (eds.). Philadelphia: World Scientific Publ. Co. 1986
10. For a recent review see: Leggett, A.J., Chakravarty, S., Dorsey, A.T., Fisher, M.P.A., Garg, A., Zwerger,W.: Rev. Mod. Phys. **59**, 1 (1987)
11. Devoret, M.H., Martinis, J.M., Esteve, D., Clarke, J.: Phys. Rev. Lett. **53**, 1260 (1984)
    Martinis, J.M., Devoret, M.H., Clarke, J.: Phys. Rev. Lett. **55**, 1543 (1985)
12. Ben-Jacob, E., Gefen, Y.: Phys. Lett. **108** A, 289 (1985)
    Likharev, K.K., Zorin, A.B.: J. Low Temp. Phys. **59**, 347 (1985)
    Guinea, F., Schön, G.: Europhys. Lett. **1**, 585 (1986)
13. Sinha, K.: Helv. Phys. Acta **45**, 619, (1972)
    Alicki, R.: Rep. Math. Phys. **1**, 1 (1977)
    Grabert, H.: Springer Tracts in Modern Physics. Vol. 95, Berlin, Heidelberg, New York: Springer 1982
14. Khalfin, L.A.: Sov. Phys. JETP **6**, 1053 (1957)
15. Hänggi, P.: Ann. NY Acad. Sci. **480**, 51 (1986)
16. Grabert, H.: The role of dissipation in quantum tunneling. In: Tunneling. Jortner, J., Pullman B. (eds.), pp. 165–182. Boston: Reidel 1986
17. Coleman, S.: In: The whys of subnuclear physics. Zichichi, A. (ed.), pp. 805–916. New York: Plenum 1979; Phys. Rev. D **15**, 2929 (1977)
    Callan, C.G., Coleman, S.: Phys. Rev. D **16**, 1762 (1977)
18. Pechukas, P.: Phys. Rev. **181**, 166 (1969); **181**, 174 (1969)
19. Miller, W.H.: J. Chem. Phys. **62**, 1899 (1975); Adv. Chem. Phys. **25**, 69 (1974); **30**, 77 (1975); Science **233**, 171 (1986)
20. Langer, J.S.: Ann. Phys. (NY) **41**, 108 (1967)
21. Riseborough, P.S., Hänggi, P., Freidkin, E.: Phys. Rev. A **32**, 489 (1985)
22. Weiss, U., Riseborough, P.S., Hänggi, P., Grabert, H.: Phys. Lett. **104** A, 10 (1984); **104** A, 492 (1984)
23. Affleck, I.: Phys. Rev. Lett. **46**, 388 (1981)
24. Grabert, H., Weiss, U.: Phys. Rev. Lett. **53**, 1787 (1984)
25. Larkin, A.I., Orchinnikov, Yu.N.: Sov. Phys. JETP **59**, 420 (1984)
26. Grabert, H., Weiss, U., Hänggi, P.: Phys. Rev. Lett. **52**, 2193 (1984)
27. Grabert, H., Weiss, U.: Z. Phys. B – Condensed Matter **56**, 171 (1984)
28. Schmid, A.: Ann. Phys. (NY) **170**, 333 (1986)
29. Grabert, H., Olschowski, P., Weiss, U.: Z. Phys. B – Condensed Matter **68**, 193 (1987)
30. Freidkin, E., Riseborough, P.S., Hänggi, P.: Phys. Rev. B **34**, 1952 (1986); Physica **142** A, 178 (1987)
31. Hontscha, W., Hänggi, P.: Phys. Rev. A (in press)
32. Pollak, E.: Phys. Rev. A **33**, 4244 (1986)

33. Hänggi, P., Grabert, H., Ingold, G.L., Weiss, U.: Phys. Rev. Lett. **55**, 761 (1985)
34. Washburn, S., Webb, R.A., Voss, R.F., Faris, S.M.: Phys. Rev. Lett. **54**, 2712 (1985)
35. Schwartz, D.B., Sen, B., Archie, C.N., Jain, A.K., Lukens, J.E.: Phys. Rev. Lett. **55**, 1547 (1985); see also: Grabert, H., Olschowski, P., Weiss, U.: Phys. Rev. Lett. **57**, 265 (1986) (Comment)
36. Freidkin, E., Riseborough, P.S., Hänggi, P.: Z. Phys. B – Condensed Matter **64**, 237 (1986); **67**, 271 (1987); see Sect. V
37. Hänggi, P., Weiss, U., Riseborough, P.S.: Phys. Rev. A**34**, 4558 (1986)

P. Hänggi
Lehrstuhl für Theoretische Physik
Universität Augsburg
Memminger Strasse 6
D-8900 Augsburg
Federal Republic of Germany