ENERGY LOSS IN QUANTUM TUNNELLING

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The energy dissipated during the quantum decay of a metastable system which interacts with an environment at zero temperature is considered. It is found that quantum effects reduce the energy loss as compared to simple semiclassical estimates and that the decay is always possible for energetical reasons. Explicit results for the decay rate are obtained from the functional integral of the partition function.

Recently, there has been a great deal of interest in the influence of dissipation on quantum decay of metastable states [1–6] and on quantum coherence in symmetrical [7–9] or slightly asymmetrical [8] two-state systems. One question that is important in this context is that of self-trapping, namely: Can the coupling to a heat bath prevent a particle from tunnelling through a potential barrier, from one potential well to the next. Bray and Moore [7] as well as Chakravarty [8], have addressed this question for the case of a symmetrical double well potential and an ohmic dissipative mechanism. They have come to the conclusion that, if the damping strength exceeds a critical value, there is a spontaneous symmetry breaking at temperature $T = 0$. The large damping situation corresponds to the case of a twofold degenerate ground state, in which there is an unequal average occupation of the two wells and a vanishing of the mean tunnelling rate.

The purpose of this letter is to clarify whether self-trapping can occur at $T = 0$ in an asymmetrical potential. One would expect that a particle is trapped in the higher well when the energy ΔE dissipated during the tunnelling process is greater than v, where v measures the potential drop from the metastable to the lower minimum. From a simple quasiclassical point of view, this should always happen when the coupling to the heat bath is only strong enough.

In the following we calculate the energy loss of a particle escaping from a metastable well along the most probable escape path. We consider two distinct models for the dissipative mechanism and examine the cases of large and small potential drops, $v \approx V_0$ and $v \ll V_0$, where V_0 is the barrier height. In the interesting case of ohmic dissipation and for $v \ll V_0$ we also calculate Im F from the functional integral of the partition function.

Our principal findings are as follows:

(1) The particle is always allowed, from energetical reasons, to escape into the lower well, independent of the precise model for the dissipative mechanism. The associated tunnelling rate, however, is suppressed to extremely small values for very large damping.

(2) At sufficiently high damping the energy loss always saturates at a finite value $\Delta E_c < v$. At very low potential drop $v \ll V_0$ this saturation occurs already at very low damping.

(3) An estimate of the energy loss by quasiclassical

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arguments gives wrong results even for low damping and large potential drop.

Specifically we consider a particle of mass M moving in a potential $V(q)$ with a metastable minimum at $q = 0$, $V(0) = 0$. The system is assumed to be coupled linearly to its environment which at low temperatures can be represented by a bath of harmonic oscillators [2]. Feynman's method [10] of integrating away the environmental modes leaves a one-dimensional problem, the partition function of which is given in terms of an effective euclidean action [2,4]. At temperature $T = 0$ the action can be written

$$S = \int_{-\infty}^{\infty} d\tau [\tfrac{1}{2} M \dot{q}^2 + V(q)]$$

$$+ \frac{1}{2} \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau' k(\tau - \tau') q(\tau) q(\tau'), \qquad (1)$$

from which we identify the three terms

$$S = S_1 + S_2 + S_3 \qquad (2)$$

as being due to the kinetic energy, S_1; the potential, S_2; and the dissipation, S_3. The kernel $k(\tau)$ is related to the spectral density of the environment $J(\omega)$ defined in refs. [2,4,6]:

$$k(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\nu K(\nu) e^{i\nu\tau},$$

$$K(\nu) = \frac{2}{\pi} \int_0^{\infty} d\omega \frac{\nu^2}{\nu^2 + \omega^2} \frac{J(\omega)}{\omega}. \qquad (3)$$

The decay rate of a metastable state in a multidimensional potential is controlled by the most probable escape path [11,12]. After integrating out the environmental coordinates, the most probable escape path becomes an extremal path of the action (1), the so-called bounce trajectory [13,14]. At zero temperature, the bounce starts with zero velocity at time $\tau = -\infty$ from the metastable minimum $q = 0$, traverses the potential well (which is a valley in euclidean time) and bounces off a turning point $\bar{q}$ at time $\tau = 0$ before returning to the metastable minimum at $\tau = \infty$.

An extremal path of the action (1) satisfies the equation of motion

$$-M\ddot{q}(\tau) + \partial V/\partial q + \int_{-\infty}^{\infty} d\tau' g(\tau - \tau') \dot{q}(\tau') = 0, \qquad (4)$$

where

$$g(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\nu e^{i\nu\tau} K(\nu)/i\nu. \qquad (5)$$

For later convenience we have integrated partially the last term in (4) which describes dissipation.

The decay probability of the metastable state is given by [2,3,6]

$$\Gamma = f \exp(-S_b/\hbar), \qquad (6)$$

where S_b is the action (1) evaluated along the bounce trajectory and f is the attempt frequency which can be calculated from the small fluctuations about the bounce trajectory.

When the particle has penetrated the potential well, it emerges from the barrier with zero velocity at the bounce point $\bar{q} = q_b$ ($\tau = 0$), where it continues propagating in real time. In an undamped system one always has $V(\bar{q}) = 0$, whereas in a damped system one finds $V(\bar{q}) < 0$, as will be discussed below. Hence the energy loss in the tunnelling process is simply determined by the relation

$$\Delta E = -V(\bar{q}). \qquad (7)$$

Another exact expression for the energy loss at $T = 0$ is obtained by multiplying (4) by $\dot{q}(\tau)$ and integrating from $\tau = -\infty$ to $\tau = 0$. This yields

$$\Delta E = \int_0^{\infty} d\tau \int_0^{\infty} d\tau' \dot{q}_b(\tau) g(\tau + \tau') \dot{q}_b(\tau'). \qquad (8)$$

Let us first consider a potential with a large drop v between the metastable and the stable well. In a system with linear ohmic dissipation whose classical equation of motion is $M\ddot{q} + \eta\dot{q} + \partial V/\partial q = 0$ the spectral density must have the form $J(\omega) = \eta\omega$ [2]. Then we obtain from (3) and (5) $g(\tau) = g_1(\tau)$, where

$$g_1(\tau) = 2M\omega_0(\alpha/\pi)\tau^{-1}, \qquad (9)$$

and where we have introduced the dimensionless damping constant $\alpha = \eta/2M\omega_0$.

By introducing the scaled time $\sigma = \tau/\alpha$, one finds that the kinetic term in (4) vanishes like $1/\alpha^2$ in the

strong damping limit, while the remaining terms are independent of α. Furthermore, from (1) and (8) it follows that for $\alpha \gg 1$ the bounce action increases linearly with α, while the energy loss saturates at a value ΔE_c which is independent of α. Specifically, for a cubic potential $V(q) = \frac{1}{2}M\omega_0^2 q^2(1 - q/q_0)$, (4) can be solved exactly in the strong damping limit [2]. One obtains

$$q_b(\tau) = \tfrac{4}{3}q_0[1 + (\omega_0\tau/2\alpha)^2]^{-1}, \quad S_b = \tfrac{4}{9}\pi\alpha M\omega_0 q_0^2$$

and

$$\Delta E_c = \tfrac{8}{27}M\omega_0^2 q_0^2 = 4V_0,$$

where V_0 is the barrier height. On the other hand, by insertion of the bounce of the undamped system, $q_b(\tau) = q_0/\cosh(\frac{1}{2}\omega_0\tau)^2$, one finds from (8) the weak damping result $\Delta E = c\alpha M\omega_0^2 q_0^2$, where the constant $c = 0.198$ has been determined numerically. The cross-over from the low-damping to the high-damping situation occurs near $\alpha = 1$.

Recently Büttiker and Landauer [16] have used the concept of the time a particle takes to tunnel through the potential barrier to estimate the energy dissipated during the tunnelling process as

$$\Delta E_{LB} = \eta \int_0^\infty d\tau \dot{q}^2(\tau). \tag{10}$$

This may be evaluated for weak damping by inserting the bounce of the undamped system. We find $\Delta E_{LB} = \frac{8}{15}\alpha M\omega_0^2 q_0^2$ which surmounts the correct numerical value almost by a factor 3. Furthermore, it follows from (8) and (10) that the discrepancy between ΔE and ΔE_{LB} increases when the width of the bounce is increased, i.e., when the potential drop v is decreased.

For tunnelling centers in solids, the spectral density $J(\omega)$ can frequently be described by [6,13] $J(\omega) = \eta\omega^3/(\omega^2 + \omega_D^2)$ where we have chosen a Drude cut-off at high frequencies. We then obtain from (3) and (5) $g(\tau) = g_2(\tau)$, where

$$g_2(\tau) = (4M/\omega_0)(\gamma/\pi)\tau^{-3}, \tag{11}$$

and where $\gamma = \eta\omega_0/2M\omega_D^2$ is a dimensionless dissipation constant. In the strong damping limit $\gamma \to \infty$ the kinetic term in (4) is suppressed by a factor $\gamma^{-2/3}$ as compared to the remaing terms and the bounce action increases with $\gamma^{1/3}$. The energy loss ΔE, however, saturates at a finite value, like in the ohmic case.

In the remainder we consider the case of a small potential drop between the wells at $q = 0$ and $q = 2q_0$, $v \equiv V(0) - V(2q_0) \ll V_0$. Now the "length" of the bounce $2\tau_1$, which corresponds to the sojourn time near $2q_0$, is very large compared to the flip time τ_2. Hence $\dot{q}_b(\tau)$ exhibits two narrow peaks of width τ_2 which are widely separated by $2\tau_1 \gg \tau_2$.

For $v \ll V_0$ the turning point $\bar{q} = q(0)$ is close to $2q_0$. Thus we obtain in a reasonable approximation

$$\Delta E = v - \tfrac{1}{2}M\omega_0^2(2q_0 - \bar{q})^2, \tag{12}$$

where ω_0 is the frequency of small oscillations about the stable well. Next, we determine $\bar{q}$ as a function of τ_1. Observing that the bounce $q_b(\tau)$ is approximately given by a superposition of an instanton with its far separated anti-instanton, i.e., $q_b(\tau) = q_1(\tau_1 + \tau) + q_1(\tau_1 - \tau) - 2q_0$, we obtain

$$\bar{q} = 2q_1(\tau_1) - 2q_0. \tag{13}$$

Here, $q_1(\tau)$ is the instanton solution of (4) in the limit $v = 0$, which interpolates between $q = 0$ at $\tau = -\infty$ and $q = 2q_0$ at $\tau = \infty$ and has its center at $\tau = 0$.

In the undamped case we have for large τ

$$q_1(\tau) = 2q_0 - aq_0 \exp(-\omega_0\tau). \tag{14}$$

The dimensionless constant a is of order unity and depends on the details of the barrier shape [17] [‡1]. In the presence of dissipation we can take advantage of the fact that $\dot{q}_1(\tau)$ is peaked at $\tau = 0$. Thus we immediately obtain from (4) for $v = 0$ and large τ

$$q_1(\tau) = 2[1 - g(\tau)/M\omega_0^2]\, q_0. \tag{15}$$

Putting now the two cases (14) and (15) together we obtain from (13) for the bounce point

$$\bar{q} = 2[1 - a\exp(-\omega_0\tau_1) - 2g(\tau_1)/M\omega_0^2]\, q_0. \tag{16}$$

Here we have kept both the exponential and algebraic behaviour in order to be able to handle the cross-over from an undamped to a damped system.

Next the length of the bounce $2\tau_1$ is determined as a function of v by extremalizing the action with respect to τ_1, $\partial S/\partial\tau_1 = 0$. Again the result can be ex-

[‡1] Note that the parameter A in ref. [17] is related to a by $A = 2\omega_0 q_0 a$.

pressed in terms of the asymptotic properties of the instanton $q_1(\tau)$. In the undamped case one finds for large τ_1 [17]

$$\partial S/\partial \tau_1 = 4M\omega_0^2 q_0^2 a^2 \exp(-2\omega_0\tau_1) - 2v. \qquad (17)$$

In the presence of dissipation the instanton obeys asymptotically a power law, $2q_0 - q_1(\tau) \sim (\omega_0\tau)^{-s-1}$, where s depends on the dissipative mechanism. From (9) and (15) we find $s = 0$ for ohmic dissipation, and from (11) we have $s = 2$. The dissipative part of the action $S_3(\tau_1)$ is most conveniently evaluated in the form

$$S_3 = -\frac{1}{2}\int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau'\, l(\tau-\tau')\,\dot{q}(\tau)\,\dot{q}(\tau'), \qquad (18)$$

where $\partial l/\partial\tau = g(\tau)$. Then we obtain from (1) and (18)

$$\partial S_1/\partial\tau_1 \sim (\omega_0\tau_1)^{-4-2s}, \quad \partial S_2/\partial\tau_1 \sim (\omega_0\tau_1)^{-2-2s},$$

$$\partial S_3/\partial\tau_1 \sim (\omega_0\tau_1)^{-1-s}, \qquad (19)$$

which shows that the leading algebraic behaviour arises from the term S_3. Finally, from $\partial S/\partial\tau_1 = 0$, we obtain by virtue of (17) and (18)

$$v = 2M\omega_0^2 a^2 q_0^2 \exp(-2\omega_0\tau_1) + 4q_0^2 g(2\tau_1). \qquad (20)$$

Eqs. (12), (16) and (20) are general expressions which determine the energy loss ΔE for a small potential drop $v \ll V_0$ for an arbitrary damping mechanism of arbitrary strength.

Let us now specialize to the case of linear ohmic dissipation, where $g(\tau) = g_1(\tau)$ is given in (9). Introducing

$$\lambda = \frac{4}{\pi}\frac{\alpha}{a^2}\frac{\exp(2\omega_0\tau_1)}{2\omega_0\tau_1}, \qquad (21)$$

$$\alpha_0 = \tfrac{1}{16}\pi\,(v/\overline{V})\ln(4a^2\overline{V}/v), \qquad (22)$$

$$\overline{V} = \tfrac{1}{2}M\omega_0^2 q_0^2, \qquad (23)$$

we obtain from (12), (16) and (20)

$$\Delta E = v - \frac{v}{1+\lambda}\left[1 + \lambda\left(\frac{1}{1+\lambda}\frac{v}{\overline{V}}\right)^{1/2}\right], \qquad (24)$$

$$\frac{\alpha}{\alpha_0} = \frac{\lambda}{1+\lambda}\left(1 + \frac{\ln(1+\lambda)}{\ln(4a^2\overline{V}/v)}\right) \qquad (25)$$

From (24) and (25) we see that the low damping region, where ΔE depends linearly on α, is limited to values of λ where $\lambda \ll \overline{V}/v$, which corresponds roughly to the range $\alpha < 0.9\,\alpha_0$ of damping parameters. We then have

$$\Delta E = (\alpha/\alpha_0)\,v. \qquad (26)$$

For $\lambda \gg \overline{V}/v$ the energy loss ΔE has saturated at its maximal value

$$\Delta E_c = v(1 - v/\overline{V}). \qquad (27)$$

This strong damping region corresponds roughly to the range $\alpha > 2.2\alpha_0$. There is a narrow cross-over region $0.9\,\alpha_0 < \alpha < 2.2\,\alpha_0$ in which ΔE changes from (26) to (27). As a result we have found that, from energetical reasons, it is alway possible for the particle to escape.

So far we have concentrated our discussion on the properties of the stationary point of the action (1). But, as is well known, for decreasing potential drop v the "breathing" mode of the bounce becomes increasingly important which may have a dramatic effect on the prefactor in formula (6). In the following we show, however, that our findings can be substantiated from a careful evaluation beyond steepest descent of the functional integral for the partition function Z. For reasons of space we only sketch the calculation of the escape rate and restrict ourselves to the strong damping case $\alpha > 2.2\,\alpha_0$. One starts by writing down an expression for Z as a power series in Δ_0^2, where Δ_0 is the "bare" tunnelling frequency in the symmetrical case $v = 0$ with the flip–flip interactions omitted. Since the time scale of the problem is of the order $\Delta_0^{-1} \gg \omega_0^{-1}$ we may neglect the inter-bounce interactions which can be shown to vanish asymptotically like $(\omega_0\tau)^{-2}$. Proceeding along the lines of Zinn-Justin [18] we then arrive at the following expression

$$Z(\theta = \hbar/k_B T) = \sum_{n=0}^{\infty} Y_{2n}(\theta), \qquad (28)$$

$$Y_{2n} = (\theta/2n)\,\Delta_0^{2n}\int_{-i\infty-\epsilon}^{i\infty-\epsilon} ds\, e^{-s\theta}\,[-s^{-1}I(s)]^n,$$

$$I(s) = \int_{\tau_0}^{\infty} d\tau\, e^{s\tau}\, e^{-U(\tau)}, \qquad (29)$$

where τ_0 is a cut-off parameter and $U(\tau)$ is the intra-bounce interaction, $U(\tau) = -v\tau/\hbar + 2\kappa \ln(\omega_0\tau)$, where $\kappa = 8\alpha\bar{V}/\pi\hbar\omega_0$. Here we have assumed $V''(0) = V''(2q_0) = M\omega_0^2$. (Our parameter κ is identical to the parameter α in ref. [9]). The integral $I(s)$ is only defined by a distortion of the integration contour at the saddle point $\tau_1 = 2\kappa\hbar/(\hbar s + v)$ into the upper half-plane [‡2] along the direction of steepest descent [15,12]. Thus, $I(s)$ acquires an imaginary part which may be expressed in terms of the inverse Γ-function. The sum in (28) can be easily performed,

$$Z(\theta) = -\tfrac{1}{2}(2\pi\mathrm{i})^{-1} \int_{-\mathrm{i}\infty-\epsilon}^{\mathrm{i}\infty-\epsilon} \mathrm{d}s\, \mathrm{e}^{-s\theta}\, \Phi'(s)/\Phi(s), \quad (30)$$

where $\Phi(s) = 1 + \Delta_0^2 I(s)/s$. Furthermore, the integration contour in (30) can be deformed to enclose the poles of $1/\Phi(s)$ in the right-hand-side half plane. Since we have at $T = 0$, $\Gamma_0 = -2\,\mathrm{Im}\,F/\hbar$, we finally obtain for the escape rate (6) the result

$$\Gamma_0 = (2\pi/\omega_0)\,\Delta_0^2 (v/\hbar\omega_0)^{2\kappa-1} [\Gamma(2\kappa)]^{-1}. \quad (31)$$

This result holds in the range $V_0 \gg v \gg \hbar\Gamma_0$ and for damping parameters $\alpha > 2.2\,\alpha_0$ or equivalently

$$\kappa > 1.1\,(v/\hbar\omega_0) \ln(4\bar{V}a^2/v).$$

Eq. (31) exhibits that the escape rate is always non-vanishing, although it is extremely suppressed for very large damping and for $v \ll \hbar\omega_0$.

The same analysis can be carried out in the zero damping limit where $U(\tau) = -v\tau/\hbar - 4\bar{V}a^2 \times \exp(-\omega_0\tau)/h\omega_0$, which gives the escape rate

$$\Gamma_0 = (2\pi/\omega_0)\,\Delta_0^2\,(4\bar{V}a^2/\hbar\omega_0)^{v/\hbar\omega_0} [\Gamma(1 + v/\hbar\omega_0)]^{-1} \quad (32)$$

The crossover from (31) to (32) will be discussed in an extended version of this work, where also different types of the dissipative mechanism are treated.

We would like to thank M. Büttiker and R. Landauer for useful discussions and for stimulating our interest in this problem.

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‡2 The distortion of the integration contour corresponds to a distortion of the potential in such a manner that for $q > 2q_0$ $V(q) < V(\bar{q})$, which is the case in a real decay problem.