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The influence of dissipation on the quantal transition state tunnelling rate

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Abstract. We calculate the rate of quantum mechanical tunnelling through a potential barrier. The tunnelling rate is calculated with the WKB approximation. The influence of the dissipation appears both in the leading term of the WKB approximation and in the next leading term. We calculate these corrections exactly and discuss the regions of validity of the results.

1. Introduction

The problem of decay of a metastable state by quantum mechanical tunnelling appears in many different contexts and has been the subject of continuous investigation, since the advent of quantum mechanics. It has long been recognised that the coupling of the system to the degrees of freedom of its environment does have significant influence on these quantum decay rates [1–3]. However, it is only recently that the influence of the environment on quantum dynamics has been formulated in a completely general manner [4–6]. Caldiera and Leggett [4] have evaluated the quantum tunnelling rate in the weak-damping limit, on the assumption that the WKB approximation is valid. In many systems that exhibit tunnelling, the ratio of the barrier height V_0 to the separation of the approximate levels $\hbar\omega_0$ of the metastable well is not very large [7, 8]. Under these circumstances, it is necessary to take into account corrections to the WKB approximation of the next-order by considering the Gaussian fluctuations about the extremal trajectories [9–12].

In this work, we shall examine the effects that a weak dissipative interaction has on these next-order WKB corrections. We shall show that this leads to a multiplicative damping correction to the pre-factor of the tunnelling rate.

2. The general formulation

The system under consideration consists of a particle of mass M, which is moving in the influence of a one-dimensional potential $V(q)$ and is coupled to the environment [4]. The total system, particle and environment system, particle and environment, is described by the Lagrangian

$$L = \frac{M}{2}\dot{q}^2 - V(q) + \sum_{n=1}^{N}\left(\frac{m_n}{2}\dot{\varphi}_n^2 - \frac{m_n}{2}\omega_n^2\varphi_n^2\right) - \sum_{n=1}^{N}\lambda_n\varphi_n q - \sum_{n=1}^{N}\frac{\lambda_n^2}{2m_n}q^2. \tag{2.1}$$

In this, the first two terms represent the motion of the particle in the presence of an effective potential $V(q)$. The second pair of terms corresponds to the normal modes of the thermal reservoir. The last set of terms correspond to a coupling of the particle to the thermal reservoir, and a counter term needed to ensure that the coupling does not change the role of $V(q)$ as the effective potential.

On performing the trace over the normal modes of the thermal reservoir, one finds that the particle motion is governed by the effective action

$$S[q(\tau)] = \int_{-\theta/2}^{\theta/2} \mathrm{d}\tau \left(\frac{M}{2}\dot{q}(\tau)^2 + V(q)\right) + \tfrac{1}{2}\int_{-\theta/2}^{\theta/2}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\tau'\, K(\tau-\tau')[q(\tau)-q(\tau')]^2 \tag{2.2}$$

where $\theta = \hbar/k_B T$ and $q(\tau)$ is a path with period θ. In this expression, we have analytically continued from real to imaginary times. This continuation is appropriate for discussion of motion in the classically forbidden region. The kernel $K(\tau)$ is given by

$$K(\tau) = \int_0^{\infty}\frac{\mathrm{d}\omega}{2\pi}J(\omega)\exp(-\omega|\tau|)$$

where $J(\omega)$ is the spectral density of the coupling to the environment:

$$J(\omega) = \frac{\pi}{2}\sum_{n=1}^{N}\frac{\lambda_n^2}{m_n\omega_n}\delta(\omega-\omega_n). \tag{2.3}$$

The decay rate can be shown to be given by the expression [1]

$$\Gamma = (S_k/2\pi\hbar)^{1/2}(D_0/D_B')^{1/2}\exp[(S_0 - S_B)/\hbar] \tag{2.4}$$

in which S_0 and S_B are, respectively, the minimum and the saddle-point values of the action. The trajectories which extremalise the action are to be calculated from

$$(\delta S/\delta q)|_{q(\tau)} = 0.$$

The factors of D represents the product of the eigenvalues of

$$\delta^2 S/\delta q^2$$

evaluated about the extremal trajectories. The prime in the contribution from the saddle point or bounce trajectory indicates that the zero eigenvalue should be omitted. This zero eigenvalue is replaced by the zero-mode normalisation factor, proportional to S_k. The factor S_k is given by

$$S_k = \int_{-\theta/2}^{\theta/2}\mathrm{d}\tau\, \dot{q}_B(\tau)^2 \tag{2.5}$$

which is evaluated over the saddle-point trajectory.

In the following, we shall specialise to the case of weak damping and zero temperature. However, we shall retain a finite θ in most of our expressions and imply that the limit $\theta \to \infty$ should be taken.

3. The bounce trajectory and the fluctuations

The trajectories that extremalise the action, $\delta S/\delta q = 0$, satisfy the Euler–Lagrange equation

$$-M\ddot{q}(\tau) + \frac{\partial V}{\partial q} + 2\int_{-\infty}^{\infty} \mathrm{d}\tau'\, K(\tau - \tau')[q(\tau) - q(\tau')] = 0 \qquad (3.1)$$

where $q(\tau)$ is subject to periodic boundary conditions $q(\tau + \theta) = q(\tau)$.

We consider the case in which the potential is given by

$$V(q) = (M\omega_0^2/2)q^2 - (Mu/3)q^3$$

and the coupling to the environment is characterised by the spectral density

$$J(\omega) = M\eta\omega.$$

In the limit of zero damping and low temperatures ($\eta = 0$ and $\theta \to \infty$), the non-trivial solution of (3.1) can be found as

$$q_{\mathrm{B}}^{(0)}(\tau) = \tfrac{3}{2}(\omega_0^2/u)\,\mathrm{sech}^2(\omega_0\tau/2). \qquad (3.2)$$

The first-order correction, in η, due to the dissipation [8, 9] is given by $q_{\mathrm{B}}^{(1)}(\tau)$, where

$$q_{\mathrm{B}}^{(1)}(\tau) = \frac{1}{\omega_0}\int_{-\infty}^{\tau} \mathrm{d}\tau'\, \varphi_{\mathrm{C}}(\tau')f(\tau')\varphi_{\mathrm{D}}(\tau) - \frac{1}{\omega_0}\int_{0}^{\tau} \mathrm{d}\tau'\, \varphi_{\mathrm{C}}(\tau)f(\tau')\varphi_{\mathrm{D}}(\tau') \qquad (3.3a)$$

where

$$\varphi_{\mathrm{C}}(\tau) = \mathrm{sech}^2(\omega_0\tau/2)\tanh(\omega_0\tau/2) \qquad (3.3b)$$

and

$$\varphi_{\mathrm{D}}(\tau) = \omega_0\varphi_{\mathrm{C}}(\tau)\int^{\tau} \mathrm{d}\tau'\, \varphi_{\mathrm{C}}(\tau')^{-2} \qquad (3.3c)$$

are two independent solutions of the homogeneous equation, and the inhomogeneous term $f(\tau)$ is given by

$$f(\tau) = 3\frac{\omega_0^2}{u}\left(\frac{\eta}{2\omega_0}\right)\int \frac{\mathrm{d}k}{\pi}\cos\left(k\frac{\omega_0\tau}{2}\right)k\left(\frac{\pi k/2}{\sinh(\pi k/2)}\right). \qquad (3.3d)$$

It can be shown, by successive integration by parts, that the change in the zero-mode normalisation

$$2\int_{-\theta/2}^{\theta/2} \mathrm{d}\tau\, \dot{q}_{\mathrm{B}}^{(0)}(\tau)\dot{q}_{\mathrm{B}}^{(1)}(\tau) = 0$$

is identically zero. This is in agreement with the evaluation of Ovchinnikov and Barone [9]. In our previous work [8], we approximated the integral by a method similar to steepest descents. This approximation is responsible for the non-zero results for the normalisation found in [8], as well as the different results for the bound-state eigenvalues.

The eigenfunctions and eigenvalues of the second functional derivative $(\delta^2 S/\delta q^2)|_{q=0}$ of the action evaluated around the trivial solution are given by the solutions of the equation

$$\left(-\frac{\partial^2}{\partial\tau^2}+\omega_0^2\right)\varphi_n^{(0)}(\tau)+\frac{\eta}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\tau'\,\frac{\partial\varphi_n^{(0)}(\tau')}{\partial\tau'}\left(\frac{1}{\tau-\tau'+\mathrm{i}\delta}+\frac{1}{\tau-\tau'-\mathrm{i}\delta}\right)$$
$$=\frac{\Lambda_n^{(0)}}{M}\varphi_n^{(0)}(\tau) \qquad (3.4)$$

subject to the periodic boundary conditions

$$\varphi_n^{(0)}(\tau+\theta)=\varphi_n^{(0)}(\tau).$$

This equation has solutions for $\eta=0$ which are given by

$$\varphi_n^{(0)}(\tau)=(1/\theta)^{1/2}\exp(\mathrm{i}k_n\,\omega_0\tau/2)$$

where $k_n=4\pi n/\omega_0\theta$ for $n=0,\pm1,\pm2,\pm3,\ldots$ and the corresponding eigenvalues are given by

$$\Lambda_n^{(0)}/M=\omega_0^2(1+k_n^2/4). \qquad (3.5)$$

The dissipative term changes the eigenvalues to the exact expression

$$\Lambda_n^{(0)}/M=\omega_0^2[1+(\eta/2\omega_0)\,|k_n|+k_n^2/4].$$

Thus the change in the eigenvalues due to the dissipation [8–10] is given by

$$\Delta\Lambda_n^{(0)}/M=\omega_0^2(\eta/2\omega_0)\,|k_n|. \qquad (3.6)$$

In addition to these eigenvalues, we require the eigenvalues of the second functional derivative $(\delta S^2/\delta q^2)|_{q_B}$ of the action, evaluated about the bounce trajectory.

In the undamped case, $\eta=0$, these eigenvalues and eigenfunctions satisfy the equation

$$\{-\partial/\partial\tau^2+\omega_0^2[1-3\,\mathrm{sech}^2(\omega_0\tau/2)]\}\varphi_n^{(B)}(\tau)=(\Lambda_n^{(B)}/M)\varphi_n^{(B)}(\tau) \qquad (3.7)$$

and are subjected to periodic boundary conditions. The solutions of this equation consist of three discrete localised solutions and a continuum. The three bound states are given by

$$\varphi_0^{(B)}(\tau)=[(30\omega_0)^{1/2}/8]\,\mathrm{sech}^3(\omega_0\tau/2) \qquad \Lambda_0^{(B)}/M=-\tfrac{5}{4}\omega_0^2$$
$$\varphi_{-1}^{(B)}(\tau)=[(30\omega_0)^{1/2}/4]\,\mathrm{sech}^2(\omega_0\tau/2)\tanh(\omega_0\tau/2) \qquad \Lambda_{-1}^{(B)}/M=0 \qquad (3.8)$$
$$\varphi_1^{(B)}(\tau)=[(6\omega_0)^{1/2}/2]\,\mathrm{sech}(\omega_0\tau/2)\,[1-\tfrac{5}{4}\,\mathrm{sech}^2(\omega_0\tau/2)] \qquad \Lambda_1^{(B)}/M=\tfrac{3}{4}\omega_0^2.$$

The continuum of scattering states $\varphi_{k_m}^{(B)}(\tau)$ are given by

$$\varphi_k^{(B)}(\tau)=\mathcal{N}_k^{-1}\exp(\mathrm{i}k\omega_0\tau/2)\{\mathrm{i}k[k^2-11+15\,\mathrm{sech}^2(\omega_0\tau/2)]$$
$$-[6k^2-6+15\,\mathrm{sech}^2(\omega_0\tau/2)]\tanh(\omega_0\tau/2)\}$$

where $\mathcal{N}_k$ is the normalisation, and k_m are given by the solutions of the equation

$$k_m\theta\omega_0/2=(2m+1)\pi+2\delta(k_m)$$

where $m=0,\pm1,\pm2,\pm3,\ldots$ and $\delta(k)$ is given by

$$\delta(k)=\tan^{-1}(k/3)+\tan^{-1}(k/2)+\tan^{-1}(k/1). \qquad (3.9)$$

The continuum eigenvalues are given by

$$\Lambda^{(B)}/M = \omega_0^2(1 + k_m^2/4).$$

To lowest order in η, the correction to these eigenvalues $\Delta\Lambda_n^{(B)}$, can be calculated from perturbation theory [10]. The leading-order corrections are given by†

$$\frac{\Delta\Lambda_n^{(B)}}{M} = \frac{\eta}{2\pi}\int_{-\theta/2}^{\theta/2} \mathrm{d}\tau \int_{-\infty}^{\infty} \mathrm{d}\tau'\, \varphi_n^{(B)}(\tau)^* \frac{\partial}{\partial\tau}\varphi_n^{(B)}(\tau')\left(\frac{1}{\tau-\tau'+\mathrm{i}\delta}+\frac{1}{\tau-\tau'-\mathrm{i}\delta}\right)$$
$$- 2u\int_{-\theta/2}^{\theta/2} \mathrm{d}\tau\, \varphi_n^{(B)}(\tau)^* q_B^{(1)}(\tau)\varphi_n^{(B)}(\tau). \qquad (3.10)$$

From this expression and the lowest-order eigenfunctions (3.8), we find that the bound-state eigenvalues are given by

$$\Delta\Lambda_0^{(B)}/M = \tfrac{15}{16}\omega_0^2(\eta/2\omega_0)[(1/\pi)\ln 2 - 39\,\xi(3)/\pi^3 + 465\,\xi(5)/\pi^5]$$

and

$$\Delta\Lambda_1^{(B)}/M = \tfrac{9}{16}\omega_0^2(\eta/2\omega_0)\{(3/\pi)\ln 2 - 189\,\xi(3)/\pi^3 + (3875/2)[\xi(5)/\pi^5]\}$$

where the $\xi(n)$ are the Riemann zeta functions.

We note that there is a small discrepancy in the coefficient of $\xi(3)$ in $\Delta\Lambda_0^{(B)}$ between our work and the corresponding work of Ovchinnikov and Barone [9]. Our value of this coefficient is 39, whereas they obtained a value of 37. This difference is insignificant when compared with the discrepancies in the total coefficient expressed in equation (3.17).

The changes in the continuum eigenvalues $\Delta\Lambda_k^{(B)}/M$ are also evaluated from equation (3.10).

We find, after a few integrations by parts, that the last term in (3.10) is evaluated as

$$-\omega_0^2(\eta/2\omega_0)(2\pi/\omega_0\theta)[(216/\pi)/(k^2+1)(k^2+4)(k^2+9)]$$
$$\times\{(k^2+4)[(k^2+4)^2 - 15]\xi(3)/\pi^3 + 125\xi(5)/\pi^5\} \qquad (3.11)$$

where we have neglected terms of order θ^{-2}. The first term in (3.10) can be evaluated by performing the τ' integration by Cauchy's method. There are two contributions to the integration over τ'; one term comes from the poles at $\tau' = \tau \pm \mathrm{i}\delta$, and the other contribution arises from the poles of $\mathrm{sech}^{2n}(\omega_0\tau'/2)$ which are located at

$$\tau' = (\mathrm{i}\pi/\omega_0)(2m + 1)$$

where $m = 0, \pm1, \pm2, \pm3, \ldots$. The contributions from the poles at $\tau' = \tau$ yields a term which is found to have a value that is equal to

$$\omega_0^2(\eta/2\omega_0)\,|k|\{1 + (2\pi/\omega_0\theta)(2/\pi)[\partial\delta(k)/\partial k]\} \qquad (3.12)$$

to order θ^{-2}. In obtaining this expression, it is necessary to retain terms of order θ^0 in $\mathcal{N}_k$. Since Ovchinnikov and Barone do not break down the specific contributions to equation (30), we are unable to locate definitely the origin of the main discrepancy between our calculations. However, as we shall see, it is possible that the origin of the

† Although the eigenfunctions corresponding to the continuum portion of the spectrum are doubly degenerate, since we are only interested in the sum of the eigenvalues, only the diagonal matrix elements enter into the final result.

discrepancy is in the contribution described by (3.12). The remaining contribution is evaluated as

$$+\,\omega_0^2\frac{\eta}{2\omega_0}\frac{2\pi}{\omega_0\theta}\frac{9/\pi}{(k^2+1)(k^2+4)(k^2+9)}\times\left[\sum_{m=1}^{\infty}\frac{\exp(-\pi m|k|)}{\pi m}\left((k^2+4)^2-\frac{60(k^2+4)}{\pi^2m^2}+\frac{3000}{\pi^4m^4}\right)\right]. \qquad (3.13)$$

The terms (3.11) and (3.13) can be identified with identical terms in equation (30) of the work of Ovchinnikov and Barone [9]. However, the terms of odd order in $|k|$ disagree with the corresponding terms in the work of Ovchinnikov and Barone. In our calculation these terms originate solely from equation (3.12). We find that this discrepancy provides the largest difference between this work and that in [9].

To leading order η, the correction to the pre-factor arising from the non-zero eigenvalues is given by a multiplicative factor

$$\exp\left(\tfrac{1}{2}\sum_n\frac{\Delta\Lambda_n^{(0)}}{\Lambda_n^{(0)}}-\tfrac{1}{2}\sum_n\frac{\Delta\Lambda_n^{(B)}}{\Lambda_n^{(B)}}\right). \qquad (3.14)$$

This can be rewritten as

$$\exp\left[\tfrac{1}{2}\frac{\omega_0\theta}{2\pi}\int_0^\infty dk\,\frac{\Delta\Lambda_k^{(0)}}{\Lambda_k^{(0)}}-\tfrac{1}{2}\frac{\Delta\Lambda_0^{(B)}}{\Lambda_0^{(B)}}-\tfrac{1}{2}\frac{\Delta\Lambda_1^{(B)}}{\Lambda_1^{(B)}}-\tfrac{1}{2}\frac{\omega_0\theta}{2\pi}\int_0^\infty dk\left(1-\frac{2\pi}{\omega_0\theta}\frac{2}{\pi}\frac{\partial\delta(k)}{\partial k}\right)\frac{\Delta\Lambda_k^{(B)}}{\Lambda_k^{(B)}}\right]. \qquad (3.15)$$

There are two cancellations that occur within equation (3.15), which involve the $\tau'=\tau\pm i\delta$ pole of the non-local contributions to the eigenvalues. First the plane-wave contributions to $\Delta\Lambda_k^{(0)}$ exactly cancels with the plane term in $\Delta\Lambda_k^{(B)}$. This first cancellation is also apparent in the work of Ovchinnikov and Barone [9]. Secondly, the change in the density of states due to the bounce partly cancels the second term of (3.12). This cancellation eliminates terms of order θ^{-1} in the products in the last term of equation (3.15). This second cancellation is absent in the work of Ovchinnikov and Barone.

On integrating over k, we obtain the final factor

$$\exp[(\eta/2\omega_0)\{\tfrac{3}{8}[-(2/\pi)\ln 2+342\,\xi(3)/\pi^3-1445\,\xi(5)/\pi 5]+6I/\pi^2\}] \qquad (3.16)$$

where $I=-0.182$ is the contribution from the poles of $\mathrm{sech}^{2n}(\omega_0\tau'/2)$. The value of I agrees with the value found by Ovchinnikov and Barone, as are the coefficients of $\xi(5)$. Because of the discrepancy in equation (3.12) discussed above, the coefficient of $\xi(3)$ has an error of less than 1%. The total expression has the numerical form

$$\exp[2.860(\eta/2\omega_0)] \qquad (3.17)$$

which is in close agreement with the value inferred from the numerical calculations of Grabert *et al* [11].

We note that, because of the two cancellations that occur in the non-local contributions of the eigenvalues to (3.15), the change in the pre-factor is completely dominated by the contributions from the local parts of $\Delta\Lambda_n^{(B)}$.

4. Discussion

It has been shown that, at low temperatures and weak damping, the rate of decay of a metastable state by quantum tunnelling is effected by the damping. We have calculated this decay rate using a WKB approximation. We find that, in addition to the leading term of the decay rate, the next-order term in the WKB approximation is also affected by the damping. The tunnelling rate Γ is given by

$$\Gamma = 12\omega_0(3V_0/2\pi\hbar\omega_0)^{1/2} \exp[\![-(36V_0/5\hbar\omega_0)\{1 + [45\xi(3)/\pi^3](\eta/2\omega_0)\}]\!] \times \exp[2.860(\eta/2\omega_0)]$$

where V_0 is the maximum height of the potential (4.2) barrier. This result is expected to be valid when $V_0/\hbar\omega_0 > 1$ and $\eta/2\omega_0 \ll 1$. However, a lower limit of $\eta/2\omega_0$ must also be imposed in order that the quantal transition state theory can be applied.

This limitation stems from the assumption of thermal equilibrium within the metastable potential well. Clearly, if equilibrium is to be maintained throughout the duration of the tunnelling process, the rate of transitions between the approximate metastable levels must be larger than the tunnelling rate. For $V_0 \simeq \frac{3}{2}\hbar\omega_0$, this yields the limit of

$$\eta/2\omega_0 \gtrsim 10^{-4}.$$

This lower limit will decrease for larger values of $V_0/\hbar\omega_0$, and hence this lower limit will usually be exceeded in most practical situations.

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