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A simple model of a decaying quantum mechanical state

August Ludviksson

Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Postfach 6980, D-7500 Karlsruhe 1, West Germany

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Abstract. A model featuring a one-dimensional particle in a tilted potential which may be trapped in a δ type potential well is considered. The time dependence of a state where the particle is trapped and where it decays via the quantum mechanical tunnel effect is calculated explicitly. Since the background potential decreases without limit (in one direction), the decay is purely exponential for long times and the decay rate is equal to the imaginary part of the eigenenergy in a Schrödinger equation that is solved for a quasi-stationary state.

The decay of a metastable state by quantum mechanical tunnelling is a problem which has received much attention recently in connection with questions concerning the validity of quantum mechanics on a macroscopic scale (see Leggett 1978, 1980). Usually the calculation of the wavefunction or decay rate of such a state relies, even in the one-dimensional case, on a mathematical approximation scheme of quasiclassical type (Schmid 1986, Coleman 1985). Therefore, the simple model to be discussed here may be of some interest, since it allows explicit discussion of many general features occurring in the theory of quantum decay.

The model I wish to consider is that of a particle in a tilted potential which may be trapped in a δ type potential well at the origin. Thus

$$\begin{aligned} H &= H_0 - \Omega\delta(x) \\ H_0 &= p^2/2m - Fx. \end{aligned} \tag{1}$$

If the dimensionless quantities

$$\xi = x/x_0 \qquad z = E/E_0 \qquad \tau = tE_0/\hbar \qquad \omega = \Omega/x_0E_0 \tag{2a}$$

are introduced where

$$x_0 = \left(\frac{\hbar^2}{2mF}\right)^{1/3} \qquad E_0 = Fx_0 \tag{2b}$$

the Hamiltonian is given by

$$h(\xi) = -\partial_\xi^2 - \xi - \omega\delta(\xi). \tag{3}$$

I will calculate the resolvent $\mathscr{R}(\xi, \xi'; z)$ which is defined as the solution of

$$(z - h(\xi))\mathscr{R}(\xi, \xi'; z) = \delta(\xi - \xi') \tag{4}$$

subject to the boundary conditions that $\mathscr{R}(\xi, \xi'; z)$ remains bounded as $\xi \to \pm\infty$. Regarding the δ well as a perturbing potential, $v(\xi) = -\omega\delta(\xi)$, the integral equation

$$\mathscr{R}(\xi, \xi'; z) = \mathscr{R}_0(\xi, \xi'; z) + \int d\xi''\mathscr{R}_0(\xi, \xi''; z)v(\xi'')\mathscr{R}(\xi'', \xi'; z) \tag{5}$$

where $\mathcal{R}_0$ is the resolvent of the particle in the tilted potential, can be easily solved to yield

$$\mathcal{R}(\xi, \xi'; z) = \mathcal{R}_0(\xi, \xi'; z) - \frac{\mathcal{R}_0(\xi, 0; z)\mathcal{R}_0(0, \xi'; z)}{1/\omega + \mathcal{R}_0(0, 0; z)}. \tag{6}$$

Note that $\mathcal{R}$ automatically obeys the same boundary conditions as $\mathcal{R}_0$.

The solutions of the differential equation for $\mathcal{R}_0(\xi, \xi'; z)$

$$(\partial_\xi^2 + \xi + z)\mathcal{R}_0(\xi, \xi'; z) = \delta(\xi - \xi')$$

are linear combinations of the Airy functions $\mathrm{Ai}(-\xi - z)$ and $\mathrm{Bi}(-\xi - z)$. At $\xi = \xi'$, $\mathcal{R}_0$ is continuous but its derivative has a jump

$$\partial_\xi \mathcal{R}_0(\xi, \xi'; z)|_{\xi=\xi'+0} - \partial_\xi \mathcal{R}_0(\xi, \xi'; z)|_{\xi=\xi'-0} = 1. \tag{7}$$

The solution satisfying the boundary conditions is

$$\mathcal{R}_0(\xi, \xi'; z) = \begin{cases} \mathcal{G}_0^{\mathrm{R}}(\xi, \xi'; z) & \mathrm{Im}\, z > 0 \\ \mathcal{G}_0^{\mathrm{A}}(\xi, \xi'; z) & \mathrm{Im}\, z < 0 \end{cases} \tag{8}$$

where $\mathcal{G}_0^{\mathrm{R/A}}$ are given by

$$\mathcal{G}_0^{\mathrm{R/A}}(\xi, \xi'; z) = -\pi \begin{cases} \mathrm{Ci}^{+/-}(-\xi' - z)\,\mathrm{Ai}(-\xi - z) & \xi \leqslant \xi' \\ \mathrm{Ci}^{+/-}(-\xi - z)\,\mathrm{Ai}(-\xi' - z) & \xi \geqslant \xi' \end{cases} \tag{9}$$

corresponding to the retarded and advanced Green functions respectively. We have introduced the notation $\mathrm{Ci}^{\pm} = \mathrm{Bi} \pm \mathrm{iAi}$ for brevity.

As is well known the spectrum of the Hamiltonian can be derived from the properties of the resolvent on the real z axis (Economou 1983). Bound states correspond to poles of the resolvent whereas a continuum of states gives rise to a discontinuity on the real axis. In the present case $\mathcal{R}_0(\xi, \xi'; z)$ is discontinuous everywhere on the real axis and it follows that H_0, and therefore H, possesses a continuum of eigenstates without any bound state, the spectrum stretching over the whole real axis.

The Airy functions are entire, i.e. they possess no singularities in any finite region of the complex plane. Correspondingly, the function $\mathcal{G}_0^{\mathrm{R}}(\xi, \xi'; z)$ can be continued analytically in the entire z plane. We remark, however, that the continuation of $\mathcal{G}_0^{\mathrm{R}}(\xi, \xi'; z)$ into the lower half-plane does not satisfy the boundary conditions.

The analytic continuation of $\mathcal{G}^{\mathrm{R}}(\xi, \xi'; z)$ into the lower half-plane

$$\mathcal{G}^{\mathrm{R}}(\xi, \xi'; z) = \mathcal{G}_0^{\mathrm{R}}(\xi, \xi'; z) - \frac{\mathcal{G}_0^{\mathrm{R}}(\xi, 0; z)\mathcal{G}_0^{\mathrm{R}}(0, \xi'; z)}{1/\omega + \mathcal{G}_0^{\mathrm{R}}(0, 0; z)} \tag{10}$$

has poles whenever the denominator of the second term vanishes. Considering the alternative expression

$$\mathcal{G}_0^{\mathrm{R}}(0, 0; z) = -2\pi \exp(\mathrm{i}\pi/6)\,\mathrm{Ai}[-z \exp(2\mathrm{i}\pi/3)]\,\mathrm{Ai}(-z)$$

one finds that $\mathcal{G}_0^{\mathrm{R}}(0, 0; z)$ has zeros on the positive real axis and on the ray $\arg z = -2\pi/3$ (Abramowitz and Stegun 1968). Therefore one expects that, in the limiting case $\omega \gg 1$, the function $\mathcal{G}^{\mathrm{R}}(\xi, \xi'; z)$ has poles in the vicinity of these zeros. To the lowest non-vanishing order in $1/\omega$ the poles close the the real axis are located at

$$\mathrm{Re}\, z_n = \left(-\frac{3\pi}{8} + n\frac{3\pi}{2}\right)^{2/3} \tag{11}$$

$$\mathrm{Im}\, z_n = -\frac{1}{\omega^2}\left(-\frac{3\pi}{8} + n\frac{3\pi}{2}\right) \qquad n = 1, 2, \ldots \tag{12}$$

whereas the poles close to the ray $\arg z = -2\pi/3$ are given by

$$\hat{z}_n = \operatorname{Re} z_n \exp(-2i\pi/3). \tag{13}$$

Most important, however, is an isolated pole z_0, since it is very close to the negative real axis. If $\omega \gg 1$, we may use the asymptotic expansion of the Airy functions and we find that this pole is given by

$$\operatorname{Re} z_0 = -\tfrac{1}{4}\omega^2 \tag{14}$$

$$\operatorname{Im} z_0 = -\tfrac{1}{4}\omega^2 \exp(-\tfrac{1}{6}\omega^3). \tag{15}$$

In this limit, $\operatorname{Re} z_0$ coincides with the energy of a particle bound in a δ type potential well without any background potential ($F = 0$). Perhaps surprisingly, it is possible to establish a connection between some of the above results and the WKB approximation. Thus one arrives at condition (11) if one demands that the WKB wavefunction has a node at the location of the δ function. Furthermore, the exponent in the expression for $\operatorname{Im} z_0$ is the classical action of a particle of energy $\frac{1}{4}\omega^2$ performing a complete periodic motion ('bounce') in the inverted potential, in which case the δ function acts as a reflecting wall.

The residue of $\mathscr{G}^{\mathrm{R}}(\xi, \xi'; z)$ at any pole $z = \bar{z}$ is of the form of a product of wavefunctions† $\psi_{\bar{z}}(\xi)\psi_{\bar{z}}(\xi')$ where $\psi_{\bar{z}}(\xi)$ is proportional to $\mathscr{G}_0^{\mathrm{R}}(\xi, 0; z)$. Explicitly, we have

$$\psi_{\bar{z}}(\xi) = \pi \left(-\frac{\partial}{\partial \bar{z}} \mathscr{G}_0^{\mathrm{R}}(0, 0; \bar{z}) \bigg|_{z=\bar{z}} \right)^{-1/2} \begin{cases} \operatorname{Ai}(-\bar{z}) \operatorname{Ci}^+(-\xi - \bar{z}) & \xi > 0 \\ \operatorname{Ci}^+(-\bar{z}) \operatorname{Ai}(-\xi - \bar{z}) & \xi < 0. \end{cases} \tag{16}$$

Note that $\psi_{\bar{z}}(\xi)$ may be called a quasi-stationary wavefunction since it satisfies the (quasi-stationary) Schrödinger equation

$$h(\xi)\psi_{\bar{z}}(\xi) = \bar{z}\psi_{\bar{z}}(\xi)$$

as $1/\omega + \mathscr{G}_0^{\mathrm{R}}(0, 0; \bar{z}) = 0$ by construction. The asymptotic expressions for the Airy functions reveal that far to the left the wavefunction falls off exponentially, whereas far to the right it represents an outgoing wave. It should be noted, however, that because of the negative imaginary part of $\bar{z}$ the wavefunction will not be bounded at infinity.

Given an initial state $\psi_i(\xi)$ its evolution in time is governed by

$$\psi(\xi, \tau) = \int \mathrm{d}\xi' \, \mathscr{K}(\xi, \xi'; \tau)\psi_i(\xi')$$

where $\mathscr{K}(\xi, \xi'; \tau)$ is the Fourier transform of the retarded Green function. Thus

$$\psi(\xi, \tau) = \mathrm{i} \int \mathrm{d}\xi' \int \frac{\mathrm{d}u}{2\pi} \exp(-\mathrm{i}u\tau)\mathscr{R}(\xi, \xi'; z = u + \mathrm{i}0)\psi_i(\xi'). \tag{17}$$

As demonstrated in the appendix, for $\tau > 0$ it is possible to close the contour of integration with respect to u in the lower half-plane if one regards the propagator $\mathscr{K}(\xi, \xi'; \tau)$ as an operator acting upon integrable initial wavefunctions. By the theorem of residues we obtain

$$\psi(\xi, \tau) = \int \mathrm{d}\xi' \, \psi_i(\xi') \sum_n \exp(-\mathrm{i}z_n\tau)\psi_{z_n}(\xi)\psi_{z_n}(\xi') \tag{18}$$

† Observe that there is no complex conjugation.

where the z_n denote the poles of $\mathscr{G}^R(\xi, \xi'; z)$ in the lower half-plane and the wavefunctions ψ_{z_n} are defined as in (16). Let us introduce $z_n = z'_n - iz''_n$. Then, far to the right, the quasi-stationary wavefunction $\psi_{z_n}(\xi)$ is asymptotically given by $\psi_{z_n}(\xi) = \psi^0_{z_n}(\xi)\exp(z''_n\xi^{1/2})$, where

$$\psi^0_{z_n}(\xi) \approx \frac{1}{\sqrt{\pi}} \frac{\exp(i\pi/4)}{(\xi + z_n)^{1/4}} \exp[i(\tfrac{2}{3}\xi^{3/2} + z'_n\xi^{1/2})] \tag{19}$$

i.e. it grows exponentially with $\xi^{1/2}$ due to the negative imaginary part of z_n. We may now express the temporal behaviour of the wavefunction in the form

$$\psi(\xi, \tau) = \sum_n \{\psi_{z_n} | \psi_i\} \psi^0_{z_n} \exp(-iz'_n\tau) \exp[-z''_n(\tau - \xi^{1/2})] \tag{20}$$

where we have introduced the shorthand notation† $\{\psi_{z_n} | \psi_i\} = \int d\xi' \, \psi_{z_n}(\xi')\psi_i(\xi')$. The behaviour of $\psi(\xi, \tau)$ will be dominated by the real exponential factor. For ξ fixed and $\tau \gg \xi^{1/2}$ only the term containing z''_0 needs to be retained because in the limit $\omega \gg 1$ the ratio z''_0/z''_n becomes arbitrarily small as can be seen by comparing equations (12) and (13) with (16). We thus obtain

$$\psi(\xi, \tau) \simeq \{\psi_{z_0} | \psi_i\} \psi^0_{z_0} \exp(-iz'_0\tau) \exp[-z''_0(\tau - \xi^{1/2})]. \tag{21}$$

Another quantity of interest is the probability amplitude for still finding the system in the initial state after time τ, which, provided that $\psi_i(\xi)$ is integrable, is given by

$$P(\tau) = \langle \psi_i | \psi(\tau) \rangle = \sum_n \exp(-iz_n\tau) \langle \psi_i | \psi_{z_n} \rangle \{\psi_{z_n} | \psi_i\}. \tag{22}$$

Again, due to its small imaginary part, only the term containing z_0 survives if τ is sufficiently large.

These results allow the following interpretation. The projections of the initial wavefunction on quasi-stationary states with a large imaginary part of the energy leave the well quickly and then move in a classical fashion, accelerating uniformly to the right. Classically, in a time τ, the particle falls a distance $\xi = \tau^2$. At a fixed position ξ, for times which are much larger than the classical passage time from the origin to ξ, only the projection on the quasi-bound state ψ_{z_0} is seen and this decays exponentially with the rate z''_0.

If the potential tilt flattens out to reach a constant value, the exponential decay law breaks down for long times (Höhler 1958), in contrast to the present case, where the exponential decay prevails forever. This can be ascribed to the fact that, in the former case, the decay products move away from the decaying state so slowly that interference between the decaying state and the decayed amplitude will occur.

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Appendix

We wish to show that it is possible to close the contour of integration with respect to z in (16) by a half-circle of infinite radius in the lower half-plane. For this purpose

† Observe that there is no complex conjugation.

we consider the asymptotic behaviour of $\mathscr{G}^{\mathrm{R}}(\xi, \xi'; z)$. The asymptotic expansions of the function $\mathrm{Ai}(-z)$ and $\mathrm{Ci}^{+}(-z)$ are as follows.

Sector 1: $-2\pi/3 \leqslant \arg z \leqslant 0$

$$\mathrm{Ai}(-z) \sim \frac{1}{2\sqrt{\pi}} \exp(-\mathrm{i}\pi/4) z^{-1/4} [\exp(\mathrm{i}\tfrac{2}{3} z^{3/2}) - \mathrm{i} \exp(-\mathrm{i}\tfrac{2}{3} z^{3/2})]$$

$$\mathrm{Ci}^{+}(-z) \sim \frac{1}{\sqrt{\pi}} \exp(\mathrm{i}\pi/4) z^{-1/4} \exp(\mathrm{i}\tfrac{2}{3} z^{3/2})$$

Sector 2: $-\pi \leqslant \arg z \leqslant -2\pi/3$

$$\mathrm{Ai}(-z) \approx \frac{1}{2\sqrt{\pi}} \exp(-\mathrm{i}\pi/4) z^{-1/4} \exp(\mathrm{i}\tfrac{2}{3} z^{3/2})$$

$$\mathrm{Ci}^{+}(-z) \sim \frac{1}{\sqrt{\pi}} \exp(-\mathrm{i}\pi/4) z^{-1/4} [\exp(-\mathrm{i}\tfrac{2}{3} z^{3/4}) + \tfrac{1}{2}\mathrm{i} \exp(\mathrm{i}\tfrac{2}{3} z^{3/2})].$$

Let us now write $\mathscr{G}^{\mathrm{R}}(\xi, \xi'; z)$ as

$$\mathscr{G}^{\mathrm{R}}(\xi, \xi' z) = \mathscr{G}_1^{\mathrm{R}}(\xi, \xi'; z) - \mathscr{G}_2^{\mathrm{R}}(\xi, \xi'; z)$$

where

$$\mathscr{G}_1^{\mathrm{R}}(\xi, \xi'; z) = \frac{1}{\omega} \cdot \frac{\mathscr{G}_0^{\mathrm{R}}(\xi, \xi'; z)}{1/\omega + \mathscr{G}_0^{\mathrm{R}}(0, 0; z)}$$

$$\mathscr{G}_2^{\mathrm{R}}(\xi, \xi'; z) = \frac{\mathscr{G}_0^{\mathrm{R}}(\xi, \xi'; z) \mathscr{G}_0^{\mathrm{R}}(0, 0; z) - \mathscr{G}_0^{\mathrm{R}}(\xi, 0; z) \mathscr{G}_0^{\mathrm{R}}(0, \xi'; z)}{1/\omega + \mathscr{G}_0^{\mathrm{R}}(0, 0; z)}.$$

In sector 1 we find that $\mathscr{G}_0^{\mathrm{R}}(0, 0; z)$ becomes dominant and the denominator can be replaced by $-\frac{1}{2} z^{-1/2} \exp(\mathrm{i}\frac{4}{3} z^{3/2})$. In sector 2, on the other hand, $\mathscr{G}_0^{\mathrm{R}}(0, 0; z)$ becomes arbitrarily small with the modulus of z so that in this region the denominator must be replaced by $1/\omega$. In the following we treat only the case $\xi > 0$ and we always assume $|z| \gg |\xi|, |\xi'|$. Let us first consider $\mathscr{G}_1^{\mathrm{R}}(\xi, \xi'; z)$. In sector 1, where $\mathscr{G}_0^{\mathrm{R}}(0, 0; z)$ is dominant, the asymptotic behaviour is simply

$$\mathscr{G}_1^{\mathrm{R}}(\xi, \xi'; z) \sim z^{1/2} (\xi + z)^{-1/4} (\xi' + z)^{-1/4} \exp[\mathrm{i}\sqrt{z}(\xi + \xi')]. \tag{A1}$$

In sector 2 one obtains

$$\mathscr{G}_1^{\mathrm{R}}(\xi, \xi'; z) \sim -\tfrac{1}{2}(\xi + z)^{-1/4} (\xi' + z)^{-1/4} \{\tfrac{1}{2} \exp[\mathrm{i}\tfrac{4}{3} z^{3/2} + \mathrm{i}\sqrt{z}(\xi + \xi')] - \mathrm{i} \exp(-\mathrm{i}\sqrt{z}|\xi - \xi'|)\}. \tag{A2}$$

In this case both exponential terms are subdominant.

The asymptotic behaviour of $\mathscr{G}_2^{\mathrm{R}}(\xi, \xi'; z)$ is as follows.

Sector 1:

$$\mathscr{G}_2^{\mathrm{R}}(\xi, \xi'; z) \sim -\tfrac{1}{2}\mathrm{i}(\xi + z)^{-1/4} (\xi' + z)^{-1/4} \{\exp(\mathrm{i}\sqrt{z}|\xi - \xi'|) - \exp[\mathrm{i}\sqrt{z}(\xi + \xi')]\} \tag{A3}$$

Sector 2:

$$\begin{aligned}\mathscr{G}_2^{\mathrm{R}}(\xi, \xi'; z) \sim -\tfrac{1}{4}\mathrm{i} z^{-1/2} (\xi + z)^{-1/4} (\xi' + z)^{-1/4} [\![\tfrac{1}{2} \exp(\mathrm{i}\tfrac{4}{3} z^{3/2}) \{\exp[\mathrm{i}\sqrt{z}(\xi + \xi')] \\ - \exp[\mathrm{i}\sqrt{z}|\xi - \xi'|]\} - \mathrm{i} \exp(-\mathrm{i}\sqrt{z}|\xi + \xi'|) + \mathrm{i} \exp[-\mathrm{i}\sqrt{z}(\xi + \xi')]]\!].\end{aligned} \tag{A4}$$

In this case also the expression in shadow brackets is subdominant.

In sector 2 we obtain by the lemma of Jordan that a path at infinity contributes nothing to the integral

$$\int \mathrm{d}z \exp(-\mathrm{i}z\tau)\mathscr{G}^{\mathrm{R}}(\xi, \xi'; z)$$

because expressions (A2) and (A4) both vanish at infinity.

In sector 1 the term (A3) also brings no contribution. To see this let us evaluate

$$I = \int \mathrm{d}z \exp(-\mathrm{i}z\tau)\frac{\exp(\mathrm{i}\sqrt{z}\alpha)}{\sqrt{z}} \qquad \alpha, \tau > 0$$

and by putting $z = r\,\mathrm{e}^{-\mathrm{i}\varphi}(0 < \varphi < \frac{2}{3}\pi)$ one derives

$$|I| \leqslant \sqrt{r} \int_0^{2\pi/3} \mathrm{d}\varphi \exp(r\tau \sin\varphi + \sqrt{r}\alpha \sin\varphi/2).$$

If r is large enough one can always find a number c $(0 < c < \tau)$ such that $\exp(-r\tau\sin\varphi + \sqrt{r}\alpha\sin\varphi/2) \leqslant \exp(-rc\sin\varphi)$. Thus

$$|I| \leqslant \sqrt{r} \int_0^{2\pi/3} \mathrm{d}\varphi \exp(-rc\sin\varphi) \propto 1/\sqrt{r}.$$

The expression (A1) itself brings a non-vanishing contribution to the z integration. However, if we first perform the integration over ξ' with an absolutely integrable initial wavefunction ψ_i in (16) we obtain a function which goes to zero as z goes to infinity that, by an argument similar to the one above, would bring no contribution to the z integration. We conclude that, in the restricted context that ψ_i is an integrable function, the contour of integration with respect to z can be closed by a half-circle of infinite radius in the lower half-plane. The restriction on ψ_i means that the sum (18) only has a meaning in this restricted sense as well.

References

Abramowitz M and Stegun I A 1968 *Handbook of Mathematical Functions* (Washington, DC: Govt Printing Office)

Coleman S 1985 *Aspects of Symmetry* (Cambridge: Cambridge University Press) ch 7

Economou E N 1983 *Green's Functions in Quantum Physics* (Berlin: Springer)

Höhler G 1958 *Z. Phys.* **152** 546

Leggett A J 1978 *J. Physique* C **6** 1264

—— 1980 *Prog. Theor. Suppl.* **69** 80

Schmid A 1986 *Ann. Phys., NY* **170** 333