Lecture 1

Approaches to barrier penetration in one and several dimensions

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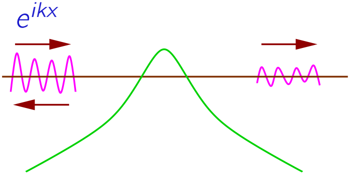
Barrier penetration in one dimension



Barrier penetration in one dimension is characterised using **transmission** and **reflection** coefficients which can be approximated uniformly by

$$t \approx \frac{\mathrm{e}^{-\theta-\mathrm{i}\delta}}{\sqrt{1+\mathrm{e}^{-2\theta}}} \qquad \text{and} \qquad r \approx \frac{-\mathrm{i}\mathrm{e}^{-\mathrm{i}\delta}}{\sqrt{1+\mathrm{e}^{-2\theta}}}$$

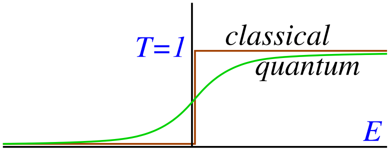
where

$$2\mathrm{i}\theta = \frac{1}{\hbar}\oint p\,\mathrm{d}q$$

is a complex action integral around turning points and the phase δ is described later.

The transmission and reflection **probabilities** are simpler

$$R \equiv |r|^2 \approx \frac{1}{1+\mathrm{e}^{-2\theta}} \qquad \text{and} \qquad T \equiv |t|^2 \approx \frac{\mathrm{e}^{-2\theta}}{1+\mathrm{e}^{-2\theta}}$$



and note also the **primitive** approximations

$$r \approx -\mathrm{i} \qquad \text{and} \qquad t \approx \mathrm{e}^{-\theta}$$

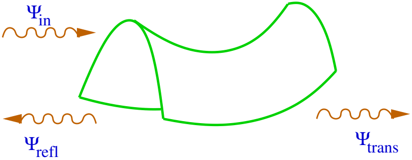
and

$$R \approx 1 \qquad \text{and} \qquad T \approx \mathrm{e}^{-2\theta}$$

valid when $E < E_{\text{barrier}}$ and $\mathrm{e}^{-\theta} \ll 1$.

Allowing also for waves incident on either side of the barrier, these coefficients can be arranged in a scattering matrix

$$S = \begin{pmatrix} r & t \\ t & r \end{pmatrix}$$



which will have multidimensional generalisations later. Notice that the approximations given satisfy the flux conservation condition

$$|r|^2 + |t|^2 = 1$$

and the scattering matrix is **unitary**

$$S^\dagger S = I.$$

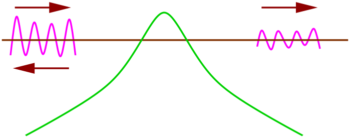
Method I: extension to the complex plane

The standard WKB ansatz

$$\psi_\pm(x) = A(x)\mathrm{e}^{\mathrm{i}S_\pm(x,x_0)/\hbar}, \quad S_\pm(x,x_0) = \pm\int_{x_0}^{x} p(x)\mathrm{d}x, \quad A(x) \propto \frac{1}{\sqrt{p(x)}}$$

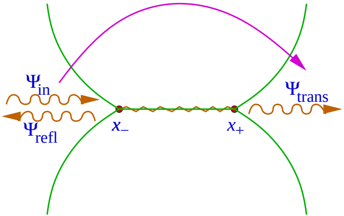
breaks down at turning points $p(x) = 0$, where $A(x) \to \infty$.

$A\mathrm{e}^{\mathrm{i}S_+(x,x_-)} + rA\mathrm{e}^{\mathrm{i}S_-(x,x_-)}$



$tA\mathrm{e}^{\mathrm{i}S_+(x,x_+)}$

We can skirt around this by promoting x to be a complex variable.



Stokes' phenomenon eliminates one of ψ_{in}, ψ_{refl} but the surviving term is simply continued.

Notice that

$$S(x, x_-) = S(x, x_+) + S(x_+, x_-) = S(x, x_+) + \mathrm{i}\hbar\theta$$

so

$$\psi_{\text{in}}(x) = A(x)\mathrm{e}^{\mathrm{i}S(x,x_-)/\hbar} \to \psi_{\text{trans}}(x) = tA(x)\mathrm{e}^{\mathrm{i}S(x,x_+)/\hbar}$$

where

$$t \approx \mathrm{e}^{-\theta}$$

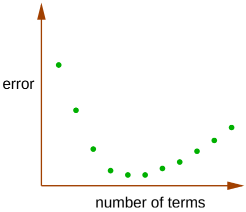
is a **primitive approximation** for the transmission amplitude. A very clear description of the mechanics of this calculation can be found in Berry and Mount Rep. Prog. Phys. **35**, 315 (1972)...

The Stokes phenomenon, briefly

... but it is now possible to give a much clearer explanation of the **Stokes phenomenon** which is a manifestation of the fact that a fully developed WKB approximation

$$\psi_{\pm}(x) = A(x)\mathrm{e}^{\mathrm{i}S_{\pm}(x,x_0)/\hbar} \quad \rightarrow \quad \mathrm{e}^{\mathrm{i}S_{\pm}(x,x_0)/\hbar}\left(a_0(x) + \hbar a_1(x) + \cdots\right)$$

is **divergent**



• Borel resummation [Eg, Balian and Bloch (1974), Ecalle, Voros (1983), Delabære et al (1997).]

• Sum to term with least error [Eg. Stokes, Balian et al (1978), Berry (1989).] (which can also involve Borel resummation)

Borel resummation for dummies

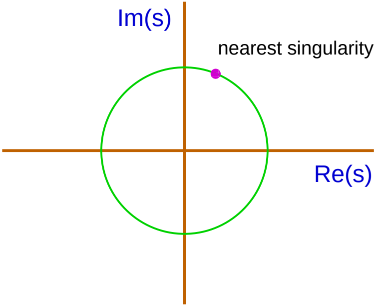
If the formal sum

$$f(\hbar, x) = a_0(x) + \hbar a_1(x) + \cdots + \hbar^n a_n(x) + \cdots$$

is divergent, there is some chance that the alternative sum

$$\hat{f}(s, x) = a_0(x) + s a_1(x) + \cdots + s^n \frac{a_n(x)}{n!} + \cdots$$

converges for s small enough, perhaps defining in a disk in the complex plane, for each x, an analytic function



which might even be **analytically continued** beyond the disk of convergence of the original series.

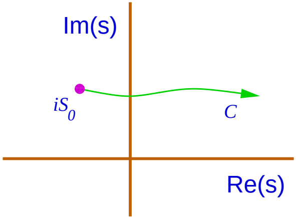
More generally we could make the association

$$\psi(\hbar, x) = \mathrm{e}^{\mathrm{i}S_0/\hbar} \sum_\lambda \hbar^\lambda a_\lambda \quad \sim \quad \hat{\psi}(s, x) = \sum_\lambda \frac{a_\lambda(x)}{\Gamma(\lambda+1)} (s - \mathrm{i}S_0)^\lambda$$

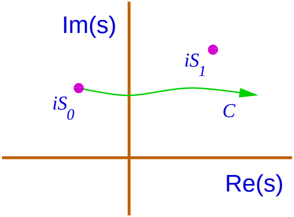
where the connection $\hat{\psi}(s, x) \to \psi(\hbar, x)$ is made using a variation of the Laplace transform

$$\psi(\hbar, x) = \frac{1}{\hbar} \int_C \mathrm{e}^{-s/\hbar} \hat{\psi}(s, x) \mathrm{d}s$$

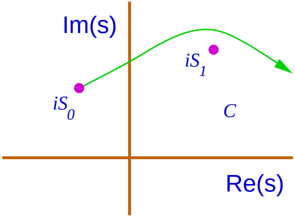
with an appropriately chosen contour C in the complex plane.



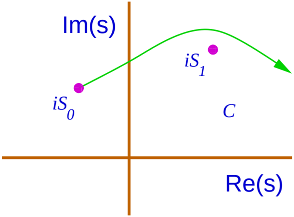
The path taken by the contour is a matter of **convention**, which is important when there are other singularities about!



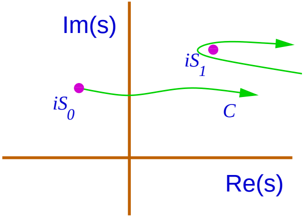
$$\neq$$



The difference is an integral of the same type



$$=$$

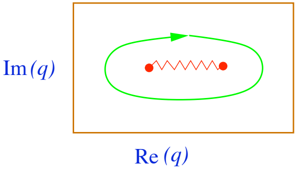


but exponentially smaller!

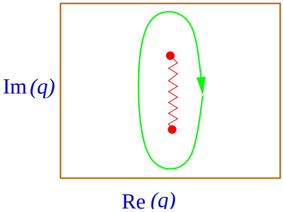
Complex dynamics

The action integral $S(x_+, x_-) = i\hbar\theta$ can be interpreted as a contour integral

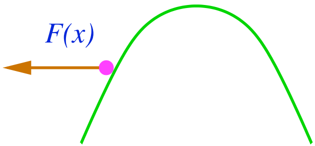
$$2i\theta = \frac{1}{\hbar}\oint p\,dq$$



which can naturally be extended to energies above barrier:



Barrier-crossing action integrals are associated with **complex dynamics**.



In dynamical equations let

$$t = -\mathrm{i}\tau, \qquad p = \mathrm{i}u, \qquad q = x$$

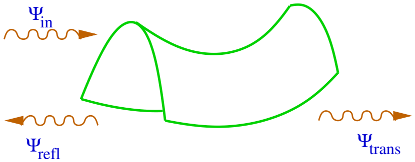
then

$$\frac{\mathrm{d}x}{\mathrm{d}t} = p \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = F(x) \qquad H = \frac{p^2}{2m} + V(x)$$

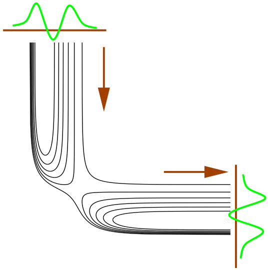
maps to

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = u \qquad \frac{\mathrm{d}u}{\mathrm{d}\tau} = -F(x) \qquad H = -\frac{u^2}{2m} + V(x)$$

The same basic approach can be used to treat transmission across multidimensional barriers

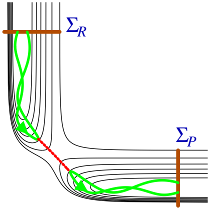


with the difference that in this case transmission depends on what is going on in transverse degrees of freedom also

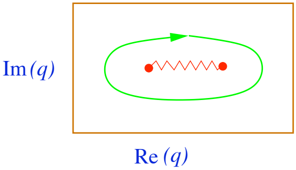


such as in a **scattering matrix** or a **Green function**.

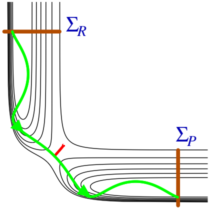
Here the **instanton orbit**



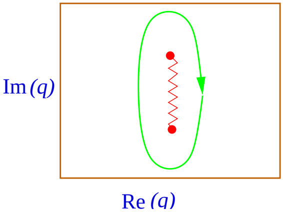
generalising



is a periodic orbit in the upside-down potential which can be extended to other Hamiltonian types and to above-barrier energies



generalising



but which provides only part of the story.