2008 - 12 - 05

Free particle $\psi = \exp\left(\pm \frac{i}{\hbar}S\right)$ where S is a classical action, $S = \int^x dx' p(x')$. For a particle bound in a potential, what is the wave function? What is the quantisation condition? (Bohr, Pauli!) Einstein noticed that Bohr's method would fail for most systems. Periodic orbits are in general not stable.

Stationary phase approximation

$$I = \int_{x_1}^{x_2} \mathrm{d}x \, g(x) \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}f(x)}$$

 $\hbar \to 0$: the integrand oscillates rapidly. The main contribution to I is from the vicinity of x_j^* where $f'(x_j^*) = 0$. Assume that x_j^* is sufficiently far from the boundary $(x_1 \text{ and } x_2)$. Also assume that the x_j^* are sufficiently far from each other.

$$f(x) = f(x_j^*) + \frac{1}{2} f''(x_j^*) (x - x_j^*)^2 + \cdots$$

Change of variables: $x \rightarrow t$, so that

$$\frac{1}{2}f_j'' \cdot (x - x_j^*)^2 = s_j t^2 \quad \text{where } s_j = \text{sgn}(f_j''); \quad \frac{\mathrm{d}x}{\mathrm{d}t} = \sqrt{\frac{2}{|f_j''|}}$$
$$I = \sum_j g(x_j^*) e^{\frac{\mathrm{i}}{\hbar}f(x_j^*)} \int_{-\infty}^{\infty} \mathrm{d}t \, \frac{\mathrm{d}x}{\mathrm{d}t} \, \exp\left(\frac{\mathrm{i}}{\hbar}s_j t^2\right)$$

This is a Fresnel integral.

$$\int_{-\infty}^{\infty} dt \, e^{\pm it^2} = \int_{-\infty}^{\infty} dt \left[\cos t^2 \pm i \sin t^2 \right] = \sqrt{\pi} \, \frac{(1\pm i)}{\sqrt{2}} = \sqrt{\pi} \, e^{\pm i\pi/4}$$
$$I = \sum_j \, g(x_j^*) \, e^{\frac{i}{\hbar} f(x_j^*)} \frac{\sqrt{2}}{\sqrt{|f_j''|}} \cdot \sqrt{\pi} \, \exp\!\left(\frac{i\pi}{4} \operatorname{sgn} f_j''\right)$$
$$I = \int_{x_1}^{x_2} \, dx \, g(x) \, e^{\frac{i}{\hbar} f(x)} \approx \sum_j \, g(x_j^*) \, \sqrt{\frac{2\pi}{|f''(x_j^*)|}} \, \exp\!\left(\frac{i}{\hbar} \, f(x_j^*) + \frac{i\pi}{4} \operatorname{sgn} f''(x_j^*)\right)$$

where x_j^* is such that $f'(x_j^*) = 0$.

WKB wave function with $p(x) = \pm \sqrt{2 m (E - V(x))}$.



Figure 1. The blue curve is the exact solution to the Schrödinger equation with the linearised potential. The red and green parts are the WKB approximations.

In the allowed region, the red part of figure 1:

$$\frac{A_+}{\sqrt{p(x)}} \exp\left(\frac{\mathrm{i}}{\hbar} \int_{x_0}^x \mathrm{d}x' \, p(x)\right) + \frac{A_-}{\sqrt{p(x)}} \exp\left(-\frac{\mathrm{i}}{\hbar} \int_{x_0}^x \mathrm{d}x' \, p(x')\right)$$

The green part:

$$\frac{B}{\sqrt{|p(x)|}} \exp\left(-\frac{\mathrm{i}}{\hbar} \int_{x_0}^x \mathrm{d}x' \, p(x')\right)$$

The linear approximation to the actual potential:

$$V(x) \approx E - F \cdot (x - a)$$

 $\Rightarrow p(x) = \pm \sqrt{2 m F \cdot (x - a)}$

The exact wave function for the linear potential, the blue part of figure 1:

$$\psi(x) = C \int_{-\infty}^{\infty} \mathrm{d}p \, \exp\left(-\frac{\mathrm{i}}{\hbar} \left(\frac{p^3}{6\,m\,F} - p(x-a)\right)\right)$$

This is a situation where we can use the stationary phase approximation:

$$-f(p) = \frac{p^3}{6 \, m \, F} - p(x-a)$$

The $\psi(x)$ above is actually closely related to the Airy function:

$$\operatorname{Ai}(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}u}{2\pi} \exp\left(\mathrm{i}\left(u^3 + x\,u\right)\right).$$

There is one combination that occurs frequently in the final result:

$$\int_{a}^{x} dx' \, p(x') = \frac{2}{3} \sqrt{2 \, m \, F} \left(x - a\right)^{3/2}$$

E > V(x):

$$\psi(x) = \frac{A}{\sqrt{p(x)}} \left[\exp\left(\frac{\mathrm{i}}{\hbar} \int_a^x \mathrm{d}x' \, p(x') - \frac{\mathrm{i}\pi}{4}\right) + \exp\left(-\frac{\mathrm{i}}{\hbar} \int_a^x \mathrm{d}x \, p(x') + \frac{\mathrm{i}\pi}{4}\right) \right]$$

E < V(x):

$$\psi(x) = \frac{B}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar} \int_x^a dx' |p(x')|\right)$$

Studying E > V(x) we find that we should choose $|A_-| = |A_+|$, but give A_- and A_+ different phases.



Figure 2. Next, we have to match the wave functions in the middle.

$$\begin{split} \psi_{\text{left}}(x) &= \frac{C}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_{a}^{x} dx' \, p(x') + \frac{\pi}{4}\right) \\ \psi_{\text{right}}(x) &= \frac{C'}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_{a}^{b} dx' \, p(x') + \frac{\pi}{4}\right) \\ \psi_{\text{right}}(x) &= \frac{C'}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_{a}^{b} dx' \, p(x') - \frac{1}{\hbar} \int_{a}^{x} dx' \, p(x') + \frac{\pi}{4}\right) = \\ &= \frac{-C'}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_{a}^{x} dx' \, p(x') - \frac{\pi}{4} - \frac{1}{\hbar} \int_{a}^{b} dx' \, p(x')\right) \stackrel{!}{=} \frac{C}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_{a}^{x} dx' \, p(x') + \frac{\pi}{4}\right) \\ &\quad -\frac{1}{\hbar} \int_{a}^{b} dx' \, p(x') - \frac{\pi}{4} + \pi + n \cdot \pi = \frac{\pi}{4}, \quad n \in \mathbb{Z} \end{split}$$

Maupertuis action.

$$p(x) = \sqrt{2\pi(E - V(x))}$$
$$\frac{1}{\hbar} \int_{a}^{b} dx' \, p(x') = \left(n + \frac{1}{2}\right)\pi$$
$$\frac{C'}{C} = (-1)^{n}$$
$$2 \int_{a}^{b} dx' \, p(x') = \left(n + \frac{1}{2}\right) 2\pi\hbar$$



Figure 3. $2\int_{a}^{b}=\oint$

$$\oint \,\mathrm{d}x'\,p(x') = \left(n + \frac{1}{2}\right) 2\pi\hbar$$



Figure 4. A plot in phase space.

 $i\pi\nu$. $\nu = \frac{1}{2}$. Maslov index. The fraction of π you pick up when passing a turning point is the Maslov index.

Turning points. Caustics.



Figure 5. Particle trajectories. x versus t.



Figure 6. v(x) folds over.