

Lecture 11 - the WKB method

Any wave function in coordinate space (1-dim) can be written as

$$\psi(x) = A(x)e^{iS(x)/\hbar}.$$

When plugged into Schrödinger equation, we found the two following relations

$$\dot{A} = -\frac{1}{m} \frac{\partial A}{\partial x} \frac{\partial S}{\partial x} - \frac{1}{2m} A \frac{\partial^2 S}{\partial x^2} \quad (1)$$

$$\dot{S} = \frac{1}{A} \frac{\hbar^2}{2m} \frac{\partial^2 A}{\partial x^2} - \frac{1}{2m} \left(\frac{\partial S}{\partial x} \right)^2 - V \quad (2)$$

Let's go one step forward. Can we use this way of writing the wavefunction to find stationary solutions ψ_E ?

$$\psi_E(x, t) = A(x)e^{iS(x)/\hbar} e^{-iEt/\hbar}$$

In general, the amplitude depends on time: $A(x, t)$, but for stationary states: $A(x)$. In solving eq. (2), assume

$$\frac{1}{A} \frac{\hbar^2}{2m} \frac{\partial^2 A}{\partial x^2} \ll E, \quad (3)$$

then eq.(2) gives just

$$E = \frac{p^2}{2m} + V \quad \Rightarrow \quad p(x) = \sqrt{2m(E - V(x))}$$

When taking the approximation above, when is the inequality true?

$$\frac{1}{A} \frac{\partial^2 A}{\partial x^2} \ll \left(\frac{p}{\hbar} \right)^2 = \left(\frac{2\pi}{\lambda} \right)^2,$$

this means that the amplitude of the wavefunction should not change much over a wavelength. The phase is given by

$$S(x) = \int_{x_0}^x p(x') dx'.$$

From eq. (1),

$$2 \frac{\partial A}{\partial x} p = -A \frac{\partial p}{\partial x}$$

$$\Rightarrow \frac{\partial A}{A} = -\frac{1}{2} \frac{\partial p}{p}$$

$$\Rightarrow \ln\left(\frac{A}{A_0}\right) = -\frac{1}{2} \ln\left(\frac{p}{p_0}\right),$$

and finally, taking the exponential in both sides and absorbing all constants into C ,

$$A(x) = \frac{C}{\sqrt{p(x)}},$$

recall also that eq. (1) reproduces the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0.$$

For stationary states, the first term vanishes and thus $\nabla \cdot \vec{J} = 0$. Recall also that we wrote

$$\vec{J} = \frac{p}{m} \cdot \rho = \frac{p}{m} A^2,$$

which should be a constant, since it can not depend on x . The density $\rho = A^2$ is largest where the momentum is small,

$$A^2 \sim \frac{1}{p}.$$

A pretty good approximation to a stationary solution is then

$$\psi_E(x) = \frac{C}{\sqrt{p(x)}} e^{i \int_{x_0}^x p(x') dx' / \hbar},$$

unless the approximation (3) doesn't hold. Note also that there are actually two solutions ψ_E^+ and ψ_E^- , with normalization constant C_+ , $-C_-$.

Particle in a box

For a 1-dim box located at the interval $[0..a]$, we must have $C_+ = -C_-$ and the stationary solution is

$$\psi(x) = \frac{B}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_{x_0}^x p(x') dx'\right),$$

but it is also required that $\psi(x = a) = 0$, thus it is required

$$\int_{x_0}^x p(x') dx' = n\pi\hbar,$$

which is equivalent to Bohr-Sommerfeld quantization condition:

$$\frac{1}{\hbar} \oint_{\text{orbit}} p(x) dx = 2\pi n.$$

Note that the factor 2 comes about because for a "closed path" as required in the Bohr-Sommerfeld condition we have to go from 0 to a and back to 0.

Constant potential V

If a particle follows a closed path where $V(\vec{r})$ is constant, then the closed loop integral around a path of length L simply becomes $p \cdot L = 2n\pi\hbar$. This condition can help us understand why only certain orbits are allowed. For a classical path around the Hydrogen atom, circular orbit of radius R :

$$\begin{aligned} \frac{1}{\hbar} \oint_{\text{orbit}} p(x) dx &= \frac{1}{\hbar} \int p dx \\ &= 2n\pi \\ &= 2\pi R p \\ \Rightarrow R p &= n\hbar. \end{aligned}$$

For a Hydrogen atom, the binding energy E

$$T_{kin} = |E| = \frac{|V(R)|}{2} = \frac{e^2}{2R}.$$

In addition, $p = \sqrt{2mT_{kin}}$, then

$$\sqrt{2mE} \cdot \frac{e^2}{2E} = n\hbar$$

and finally

$$E = -\frac{me^4}{2\hbar^2 n^2},$$

which corresponds to what we already know. However, for non-circular orbits, this procedure can get really messy.

Potential barrier $V > E$

If $V(x) > E$, $p(x)$ is imaginary and the solution is then

$$e^{\pm(i^2/\hbar) \int_{x_0}^x |p(x')| dx'} = e^{\pm(i^2/\hbar) \int_{x_0}^x |\sqrt{2m(V-E)}| dx'}.$$

The wavefunction must be exponentially falling, otherwise is not normalizable.

Consider a short range nucleus potential. Classically, the particle cannot escape. The probability of finding it at $x \gg a$ is

$$P(x \gg a) \sim P(x < a) \cdot e^{-2 \int_a^x \sqrt{2m(V-E)}}.$$

the exponent factor in the exponential is known as the barrier (to get through). For example, an α -particle (He^4) inside a big fat Uranium (U) atom: it will bounce between the potential like a pinball, and eventually (\sim billion years), the α particle will get through the potential barrier, i.e. the U atom emits an

α -particle.

Smooth Potential

If the potential has a smooth but non-trivial dependence on x where for some x_e it becomes equal to E , we can always restrict the solution to the Schrödinger equation to a short interval around x_e , where a linear approximation for the potential is helpful

$$V(x) = V(x_0) + V'(x_0)(x - x_0),$$

then it is possible to solve the Schrödinger equation in this region with the approximated potential

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V'(x - x_0)\psi = 0.$$

and use the WKB method elsewhere (with the usual imaginary exponent where $V < E$ and the negative, real exponent where $V > E$) to smoothly connect on both sides.

Typically, this leads to a modification of the quantization condition,

$$\int_0^a p(x') dx' = n\pi\hbar + \frac{1}{2}n\hbar.$$