

229(3): Background to the WKB Approximation

This is given by E. Merz Sadler, "Quantum Mechanics" (Wiley, 2nd. ed., chapter 7). The WKB approximation is named after Wentzel, Kramers and Brillouin.

Consider the one dimensional Schrodinger equation:

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad - (1)$$

in the limit of the ECE uniform field theory. If:
 $V = \text{constant} \quad - (2)$

then:

$$\psi = \exp(\pm ikx) \quad - (3)$$

If V varies slowly with x , then:

$$\psi(x) = \exp(iu(x)) \quad - (4)$$

with:

$$k(x) = \left(\frac{2m}{\hbar^2} (E - V(x)) \right)^{1/2} \quad \text{if } E > V(x), \quad - (5)$$

and

$$k(x) = -i \left(\frac{2m}{\hbar^2} (V(x) - E) \right)^{1/2} \quad \text{if } E < V(x) \quad - (6)$$

$$= -i \kappa(x)$$

Therefore

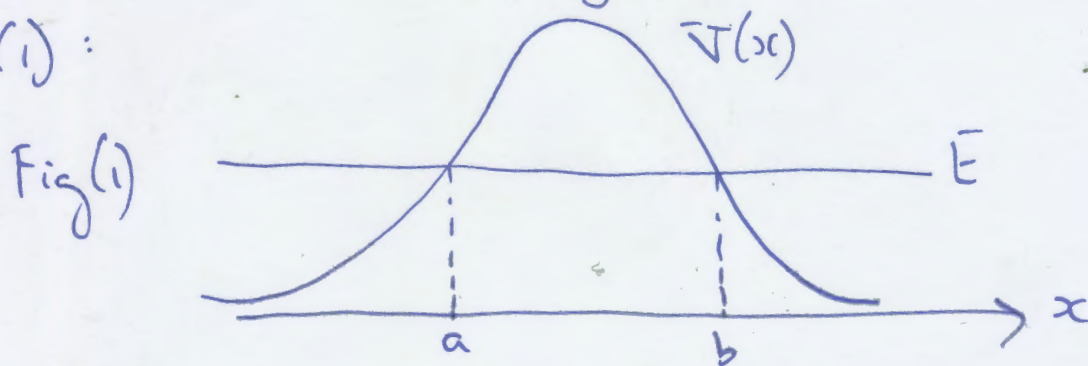
$$\boxed{\kappa(x) = \left(\frac{2m}{\hbar^2} (V(x) - E) \right)^{1/2} \quad \text{if } E < V(x)} \quad - (7)$$

2) and

$$k(x) = \left(\frac{2m}{\hbar^2} (E - V(x)) \right)^{1/2}, \quad - (8)$$

if $E > V(x)$

In low energy nuclear reactions, an atom fuses with another by transmission through a barrier. In molecular dynamics computer simulation the Lennard-Jones potential is used to describe atomic interaction. This is a special case for atom-atom interaction of the general potential of Fig (i):



Using the WKB approximation then:

$$\psi(x) = \frac{A}{(k(x))^{1/2}} \exp \left(i \int_a^x k dx \right) + \frac{B}{(k(x))^{1/2}} \exp \left(-i \int_0^x k dx \right),$$

$x < a;$ - (9)

$$\psi(x) = \frac{C}{(k(x))^{1/2}} \exp \left(- \int_a^x k dx \right) + \frac{D}{(k(x))^{1/2}} \exp \left(\int_a^x k dx \right),$$

$a < x < b;$ - (10)

and

$$\psi(x) = \frac{F}{(k(x))^{1/2}} \exp\left(i \int_b^x k dx\right) + \frac{G}{(k(x))^{1/2}} \exp\left(-i \int_b^x k dx\right), \quad - (11)$$

$b < x.$

If the ratios :

$$\left| \frac{F - iG}{F + iG} \right| \quad \text{and} \quad \left| \frac{B - iA}{B + iA} \right| \quad - (12)$$

are not close to zero, then :

$$\begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 2\theta + \frac{1}{2\theta} & i\left(2\theta - \frac{1}{2\theta}\right) \\ -i\left(2\theta - \frac{1}{2\theta}\right) & 2\theta + \frac{1}{2\theta} \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix} \quad - (13)$$

where

$$\theta = \exp\left(\int_a^b k(x) dx\right) \quad - (14)$$

i.e.

$$\theta = \exp\left(\frac{(2m)^{1/2}}{\hbar} \int_a^b (V(x) - E)^{1/2} dx\right) \quad - (15)$$

The transmission coefficient is :

$$T = \frac{|F|^2}{|A|^2} = \frac{FF^*}{AA^*} \quad - (16)$$

If there is no wave incident from the right then :

4)

$$G = 0 \quad - (17)$$

So:

$$T = \frac{4}{\left(2\theta + \frac{1}{2\theta}\right)^2} \quad - (18)$$

Various potentials $V(x)$ can now be used in eq. (18) to model the interaction of two atoms in a nuclear fusion.

The most obvious feature is that the protons and electrons of one atom interact with those of the other atom with a Coulomb potential developed in note 229(2). There is also nuclear strong force interaction between the nuclei of atom 1 and atom 2. So the next note will consider models of these interactions to determine the conditions for maximum transmission T and maximum quantum tunnelling.
