WKB approximation: α particle decay Masatsugu Sei Suzuki Department of Physics, SUNY at Binghamton (Date: January 13, 2012)

Gregor Wentzel (February 17, 1898, in Düsseldorf, Germany – August 12, 1978, in Ascona, Switzerland) was a German physicist known for development of quantum mechanics. Wentzel, Hendrik Kramers, and Léon Brillouin developed the Wentzel–Kramers–Brillouin approximation in 1926. In his early years, he contributed to X-ray spectroscopy, but then broadened out to make contributions to quantum mechanics, quantum electrodynamics, and meson theory. http://en.wikipedia.org/wiki/Gregor_Wentzel

Hendrik Anthony ''Hans'' Kramers (Rotterdam, February 2, 1894 – Oegstgeest, April 24, 1952) was a Dutch physicist. http://en.wikipedia.org/wiki/Hendrik Anthony Kramers

Léon Nicolas Brillouin (August 7, 1889 – October 4, 1969) was a French physicist. He made contributions to quantum mechanics, radio wave propagation in the atmosphere, solid state physics, and information theory.



http://en.wikipedia.org/wiki/L%C3%A9on_Brillouin

WKB approximation

This method is named after physicists Wentzel, Kramers, and Brillouin, who all developed it in 1926. In 1923, mathematician Harold Jeffreys had developed a general method of approximating solutions to linear, second-order differential equations, which includes the Schrödinger equation. But even though the Schrödinger equation was developed two years later, Wentzel, Kramers, and Brillouin were apparently unaware of this earlier work, so Jeffreys is often neglected credit. Early texts in quantum mechanics contain any number of combinations of their initials, including WBK, BWK, WKBJ,

JWKB and BWKJ. The important contribution of Jeffreys, Wentzel, Kramers and Brillouin to the method was the inclusion of the treatment of turning points, connecting the evanescent and oscillatory solutions at either side of the turning point. For example, this may occur in the Schrödinger equation, due to a potential energy hill. (from http://en.wikipedia.org/wiki/WKB_approximation)

1. Classical limit

Change in the wavelength over the distance δx

$$\delta\lambda = \frac{d\lambda}{dx}dx\,.$$

When $\delta x = \lambda$

$$\delta \lambda = \frac{d\lambda}{dx} \lambda \; .$$

In the classical domain, $\delta \lambda \ll \lambda$

$$\left|\delta\lambda\right| = \left|\frac{d\lambda}{dx}\lambda\right| \ll \lambda \quad \text{or} \quad \left|\frac{d\lambda}{dx}\right| \ll 1,$$

which is the criterion of the classical behavior.

2. WKB approximation

The quantum wavelength does not change appreciably over the distance of one wavelength. We start with the de Broglie wave length given by

$$p = \frac{h}{\lambda}$$
$$\varepsilon = \frac{1}{2m}p^2 + V(x)$$

or

$$p^{2} = \left(\frac{h}{\lambda}\right)^{2} = 2m[\varepsilon - V(x)],$$

or

$$p=\sqrt{2m(\varepsilon-V(x))}.$$

Then we get

$$-2h^2\lambda^{-3}\frac{d\lambda}{dx}=2m\left[-\frac{dV(x)}{dx}\right],$$

or

$$\frac{d\lambda}{dx} = \frac{m}{h^2} \lambda^3 \frac{dV(x)}{dx} = \frac{m}{h^2} \left(\frac{h}{p}\right)^3 \frac{dV(x)}{dx} = \frac{mh}{p^3} \frac{dV(x)}{dx}.$$

When
$$\left|\frac{d\lambda}{dx}\right| << 1$$
, we have
 $\left|\frac{mh}{p^3}\frac{dV(x)}{dx}\right| << 1$ (classical approximation)

If dV/dx is small, the momentum is large, or both, the above inequality is likely to be satisfied

Around the turning point, p(x) = 0. |dV/dx| is very small when V(x) is a slowly changing function of x.

Now we consider the WKB approximation,

$$\varepsilon\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x).$$

When $V \to 0$,

$$\psi(x) = Ae^{ikx} = Ae^{\frac{ipx}{\hbar}}.$$

If the potential *V* is slowly varying function of *x*, we can assume that

$$\psi(x) = A e^{\frac{i}{\hbar}S(x)},$$

$$S(x) = S_0(x) + \frac{\hbar}{1!}S_1(x) + \frac{\hbar^2}{2!}S_2(x) + \frac{\hbar^3}{3!}S_3(x) + \dots$$

((Mathematica))

WKB approximation

$$eq1 = -\frac{\hbar^{2}}{2 m} D[\psi[x], \{x, 2\}] + V[x] \psi[x] - \varepsilon \psi[x];$$

$$rule1 = \left\{ \psi \rightarrow \left(Exp\left[\frac{i}{\hbar} S[\#]\right] \varepsilon \right) \right\};$$

$$eq2 = eq1 /. rule1 // Simplify$$

$$\frac{e^{\frac{i}{\hbar}} (-2 m \varepsilon + 2 m V[x] + S'[x]^{2} - i \hbar S''[x])}{2 m}$$

$$rule2 = \left\{ S \rightarrow \left[S 0[\#] + \hbar S1[\#] + \frac{\hbar^{2}}{2!} S2[\#] + \frac{\hbar^{3}}{3!} S3[\#] + \frac{\hbar^{4}}{4!} S4[\#] \varepsilon \right] \right\};$$

$$eq3 = \left(-2 \varepsilon m + 2 m V[x] + S'[x]^{2} - i \hbar S''[x] \right);$$

$$eq4 = eq3 /. rule2 // Expand;$$

$$list1 = Table[{n, Coefficient[eq4, \hbar, n]}, {n, 0, 6}] // simplify;$$

$$\% // TableForm$$

$$0 \quad -2 m \varepsilon + 2 m V[x] + S0'[x]^{2} \\ 1 \quad 2 S0'[x] S1'[x] - i S0''[x] \\ 2 \quad S1'[x]^{2} + S0'[x] S2'[x] - i S1''[x] \\ 3 \quad S1'[x] S2'[x] + \frac{1}{3} S0'[x] S3'[x] - \frac{1}{2} i S2''[x] \\ 4 \quad \frac{1}{12} (3 S2'[x]^{2} + 4 S1'[x] S3'[x] + S0'[x] - i S4''[x]) \\ 5 \quad \frac{1}{24} (4 S2'[x] S3'[x] + 2 S1'[x] S4'[x] - i S4''[x]) \\ 6 \quad \frac{1}{72} (2 S3'[x]^{2} + 3 S2'[x] S4'[x])$$

For each power of \hbar , we have

 $-2m\varepsilon+2mV(x)+[S_0'(x)]^2=0\,,$

$$2S_0'(x)S_1'(x) = iS_0''(x),$$

$$[S_1'(x)]^2 + S_0'(x)S_2'(x) = iS_1''(x),$$

.....

(a) **Derivation of** $S_0(x)$

$$[S_0'(x)]^2 = 2m[\varepsilon - V(x)] = p^2(x),$$

where

$$p^2(x) = 2m[\varepsilon - V(x)],$$

or

$$S_0'(x) = \pm p(x),$$

or

$$S_0(x) = \pm \int_{x_0}^x p(x) dx \, .$$

Since $p(x) = \hbar k(x)$,

$$S_0(x) = \pm \hbar \int_{x_0}^x k(x) dx \, .$$

(b) Derivation of $S_1(x)$

$$2S_0'(x)S_1'(x) = iS_0''(x),$$

$$S_{1}'(x) = \frac{iS_{0}''(x)}{2S_{0}'(x)} = \frac{i}{2} \frac{\frac{d}{dx} S_{0}'(x)}{S_{0}'(x)},$$

which is independent of sign.

$$S_1(x) = \int S_1'(x) dx = \frac{i}{2} \ln[S_0'(x)] = \frac{i}{2} \ln[\hbar k(x)],$$

or

$$iS_1(x) = -\frac{1}{2}\ln[\hbar k(x)] = \ln[\hbar k(x)]^{-1/2},$$

or

$$S_1(x) = \frac{1}{\sqrt{\hbar k(x)}}.$$

(c) **Derivation of** $S_2(x)$

$$[S_1'(x)]^2 + S_0'(x)S_2'(x) = iS_1''(x),$$
$$iS_2''(x) - [S_1'(x)]^2$$

$$S_{2}'(x) = \frac{iS_{1}''(x) - [S_{1}'(x)]^{-1}}{S_{0}'(x)}.$$

Then the WKB solution is given by

$$S(x) = S_0(x) + \frac{\hbar}{1!}S_1(x) + \frac{\hbar^2}{2!}S_2(x) + \frac{\hbar^3}{3!}S_3(x) + \dots$$
$$= \pm \hbar \int_{x_0}^x k(x)dx - \frac{\hbar}{2i}\ln[\hbar k(x)] + \dots$$

The wave function has the form

$$\psi(x) = \exp[-\frac{1}{2}\ln(\hbar k(x))][A'\exp(i\int_{x_0}^x k(x)dx) + B''\exp(-i\int_{x_0}^x k(x)dx)],$$

or

$$\psi(x) = \frac{A'}{\sqrt{\hbar k(x)}} \exp(i \int_{x_0}^x k(x) dx) + \frac{B'}{\sqrt{\hbar k(x)}} \exp(-i \int_{x_0}^x k(x) dx)$$
$$= \frac{A}{\sqrt{k(x)}} \exp(i \int_{x_0}^x k(x) dx) + \frac{B}{\sqrt{k(x)}} \exp(-i \int_{x_0}^x k(x) dx)$$

where we put

$$A = \frac{A'}{\sqrt{\hbar}}, \qquad B = \frac{B'}{\sqrt{\hbar}}$$

3. The probability current density

We now consider the case of B = 0.

$$\psi(x) = \frac{A}{\sqrt{k(x)}} \exp(i \int_{x_0}^x k(x) dx) \,.$$

The probability is obtained as

$$P(x) = \psi^{*}(x)\psi(x) = \frac{|A|^{2}}{k(x)} = \frac{|A|^{2}}{v}\frac{\hbar}{m},$$

where $\hbar k(x) = mv$.

The probability current density is



Fig. $Jadt = avdt |\psi|^2$, or $J = v |\psi|^2$

4. WKB approximation near the turning points

We consider the potential energy V(x) and the energy ε shown in the following figure. The inadequacy of the WKB approximation near the turning point is evident, since $k(x) \rightarrow 0$ implies an unphysical divergence of $\psi(x)$.

(a) V(x): increasing function of x around the turning point x = a



(i) For x >> a where $V(x) > \varepsilon$,

$$\psi_I(x) = \frac{A_1}{\sqrt{\kappa(x)}} \exp(-\int_a^x \kappa(x) dx) + \frac{B_1}{\sqrt{\kappa(x)}} \exp(\int_a^x \kappa(x) dx),$$

where A_1 and B_1 are constants, and

$$\kappa(x) = \frac{1}{\hbar} \sqrt{2m} \sqrt{V(x) - \varepsilon} ,$$

(ii) For x < a where $V(x) < \varepsilon$,

$$\psi_{II}(x) = \frac{A_2}{\sqrt{k(x)}} \cos(\int_x^a k(x) dx) + \frac{B_2}{\sqrt{k(x)}} \sin(\int_x^a k(x) dx),$$

where

$$k(x) = \frac{1}{\hbar} \sqrt{2m} \sqrt{\varepsilon - V(x)} \,.$$

(b) V(x): decreasing function of x around the turning point



(i) For x << b where $V(x) > \varepsilon$,

$$\psi_{I}(x) = \frac{A}{\sqrt{\kappa(x)}} \exp(\int_{x}^{b} \kappa(x) dx) + \frac{B}{\sqrt{\kappa(x)}} \exp(\int_{x}^{b} \kappa(x) dx),$$

with

$$\kappa(x) = \frac{1}{\hbar} \sqrt{2m} \sqrt{V(x) - \varepsilon} ,$$

(ii) For
$$x > b$$
 where $V(x) < \varepsilon$,

$$\psi_{II}(x) = \frac{2A}{\sqrt{k(x)}} \cos(\int_{b}^{x} k(x)dx) + \frac{B}{\sqrt{k(x)}} \sin(\int_{b}^{x} k(x)dx))$$

where

$$k(x) = \frac{1}{\hbar} \sqrt{2m} \sqrt{\varepsilon - V(x)}$$

5. Exact solution of wave function around the turning point x = a



The Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = \varepsilon\psi(x)$$

or

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + [V(x) - \varepsilon]\psi = 0$$

where ε is the energy of a particle with a mass *m*. We assume that

$$V(x) - E = g(x - a)$$

in the vicinity of x = a, where g > 0. Then the Schrödinger equation is expressed by

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}g(x-a)\psi = 0.$$

Here we put

$$z = \left(\frac{2mg}{\hbar^2}\right)^{1/3} (x-a) \, .$$

Then we get

$$\frac{d^2\psi(z)}{dz^2} - z\psi(z) = 0.$$

The solution of this equation is given by

$$\psi(z) = 2C_1A_i(z) + C_2B_i(z)$$

where we use $2C_1$ instead of C_1 . The asymptotic form of the Airy function $A_i(z)$ for large |z| is given by

$$A_i(z) = \pi^{-1/2} |z|^{-1/4} \cos(\zeta - \frac{\pi}{4}), \qquad \text{for } z < 0$$

and

$$A_{i}(z) = \frac{1}{2} \pi^{-1/2} |z|^{-1/4} e^{-\varsigma}, \qquad \text{for } z > 0$$

where



Fig. Plot of the $A_i(z)$ (red) and its asymptotic form (blue) as a function of z for z<0.

The asymptotic form of the Airy function $B_i(z)$ for large |z|,

$$B_i(z) = -\pi^{-1/2} |z|^{-1/4} \sin(\zeta - \frac{\pi}{4}), \qquad \text{for } z < 0$$

with
$$\varsigma = \frac{2}{3} |z|^{3/2}$$

$$B_i(z)$$

$$1.5$$

$$1.0$$

$$0.6$$

$$0.6$$

$$0.6$$

$$-10$$

$$-8$$

$$-6$$

$$-4$$

$$-2$$

$$-0.5$$

for *z*>0

Fig. Plot of the $B_i(z)$ (red) and its asymptotic form (blue) as a function of *z* for *z*<0. Here we note that

For *z*<0,

$$k(x) = \sqrt{\frac{2m}{\hbar^2}g(a-x)} = \left(\frac{2mg}{\hbar^2}\right)^{1/3} |z|^{1/2}$$

 $B_i(z) = \pi^{-1/2} z^{-1/4} e^{\varsigma},$

Then we have

$$\int_{x}^{a} k(x) dx = \left(\frac{2mg}{\hbar^{2}}\right)^{1/2} \int_{x}^{a} \sqrt{a - x} dx$$
$$= \frac{2}{3} \left(\frac{2mg}{\hbar^{2}}\right)^{1/2} (a - x)^{3/2}$$
$$= \frac{2}{3} |z|^{3/2} = \zeta$$

For *z*>0,

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}g(x-a)} = \left(\frac{2mg}{\hbar^2}\right)^{1/3} |z|^{1/2}$$

we have

$$\int_{a}^{x} \kappa(x) dx = \left(\frac{2mg}{\hbar^2}\right)^{1/2} \int_{a}^{x} \sqrt{x-a} dx$$
$$= \frac{2}{3} \left(\frac{2mg}{\hbar^2}\right)^{1/2} (x-a)^{3/2}$$
$$= \frac{2}{3} |z|^{3/2} = \varsigma$$



(i) Asymptotic form for z < 0 (x < a)

The asymptotic form of the wave function for z < 0 can be expressed by

$$2C_1A_i(z) + C_2B_i(z) = 2C_1\pi^{-1/2} |z|^{-1/4} \cos(\varsigma - \frac{\pi}{4}) - C_2\pi^{-1/2} |z|^{-1/4} \sin(\varsigma - \frac{\pi}{4})$$
$$= \pi^{-1/2} \left(\frac{2mg}{\hbar^2}\right)^{1/6} [2C_1\frac{1}{\sqrt{k(x)}}\cos(\int_x^a k(x)dx - \frac{\pi}{4}) - C_2\frac{1}{\sqrt{k(x)}}\sin(\int_x^a k(x)dx - \frac{\pi}{4})]$$

where

$$\varsigma = \int_{x}^{a} k(x) dx = \frac{2}{3} |z|^{3/2}, \qquad k(x) = \left(\frac{2mg}{\hbar^{2}}\right)^{1/3} |z|^{1/2}.$$

(ii) The asymptotic form for z>0;

The asymptotic form of the wave function for z>0 can be expressed by

$$2C_1A_i(z) + C_2B_i(z) = C_1\pi^{-1/2} |z|^{-1/4} e^{-\varsigma} + C_2\pi^{-1/2} z^{-1/4} e^{\varsigma}$$
$$= \pi^{-1/2} \left(\frac{2mg}{\hbar^2}\right)^{1/6} [C_1 \frac{1}{\sqrt{\kappa(x)}} \exp(-\int_a^x \kappa(x) dx) + C_2 \frac{1}{\sqrt{\kappa(x)}} \exp(\int_a^x \kappa(x) dx)]$$

where

$$\zeta = \int_{a}^{x} \kappa(x) dx = \frac{2}{3} |z|^{3/2}, \qquad \kappa(x) = \left(\frac{2mg}{\hbar^{2}}\right)^{1/3} |z|^{1/2}.$$

The we have the connection rule (I; upward) as follows.

$$\frac{2A}{\sqrt{k(x)}}\cos\left(\int_{x}^{a}k(x)dx - \frac{\pi}{4}\right) - \frac{B}{\sqrt{k(x)}}\sin\left(\int_{x}^{a}k(x)dx - \frac{\pi}{4}\right)\right]$$
$$\Rightarrow$$
$$\frac{A}{\sqrt{\kappa(x)}}\exp\left(-\int_{a}^{x}\kappa(x)dx\right) + \frac{B}{\sqrt{\kappa(x)}}\exp\left(\int_{a}^{x}\kappa(x)dx\right)\right]$$

(I; upward)

at the boundary of x = a.



where $C_1 = A$ and $C_2 = B$.



The Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=\varepsilon\psi(x)\,,$$

or

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+[V(x)-\varepsilon]\psi=0,$$

where ε is the energy of a particle with a mass *m*. We assume that

$$V(x) - \varepsilon = -g(x - b),$$

in the vicinity of x = b, where g > 0. The Schrödinger equation is expressed by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}g(x-b)\psi = 0.$$

Here we put

$$z = -\left(\frac{2mg}{\hbar^2}\right)^{1/3} (x-b) \,.$$

Then we get

$$\frac{d^2\psi(z)}{dz^2} - z\psi(z) = 0.$$

The solution of this equation is given by

$$\psi(z) = 2C_1A_i(z) + C_2B_i(z).$$

We note the following.

(i) For z < 0 (x > b) k(x) is expressed by

$$k(x) = \sqrt{\frac{2m}{\hbar^2}g(x-b)} = \left(\frac{2mg}{\hbar^2}\right)^{1/3} |z|^{1/2},$$

$$\int_{b}^{x} k(x)dx = \left(\frac{2mg}{\hbar^2}\right)^{1/2} \int_{b}^{x} \sqrt{x-b}dx = \frac{2}{3} \left(\frac{2mg}{\hbar^2}\right)^{1/2} (x-b)^{3/2} = \frac{2}{3} |z|^{3/2} = \varsigma.$$

(ii) For z>0 (x < b), where $\varepsilon > V(x)$ $\kappa(x)$ is expressed by

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}} [\varepsilon - V(x)] = \sqrt{\frac{2m}{\hbar^2}} g(b - x)$$
$$= \left(\frac{2mg}{\hbar^2}\right)^{1/3} |z|^{1/2}$$
$$\int_{x}^{b} \kappa(x) dx = \left(\frac{2mg}{\hbar^2}\right)^{1/2} \int_{x}^{b} \sqrt{b - x} dx = \frac{2}{3} \left(\frac{2mg}{\hbar^2}\right)^{1/2} (b - x)^{3/2} = \frac{2}{3} |z|^{3/2} = \zeta$$

8. Connection formula-II (downward) The asymptotic form for *z*<0;

$$2C_{1}A_{i}(z) + C_{2}B_{i}(z) = 2C_{1}\pi^{-1/2} |z|^{-1/4} \cos(\zeta - \frac{\pi}{4}) - C_{2}\pi^{-1/2} |z|^{-1/4} \sin(\zeta - \frac{\pi}{4})$$
$$= \pi^{-1/2} \left(\frac{2mg}{\hbar^{2}}\right)^{1/6} [2C_{1}\frac{1}{\sqrt{k(x)}}\cos(\int_{b}^{x} k(x)dx - \frac{\pi}{4})$$
$$-C_{2}\frac{1}{\sqrt{k(x)}}\sin(\int_{b}^{x} k(x)dx - \frac{\pi}{4})]$$

The asymptotic form for *z*>0;

$$2C_{1}A_{i}(z) + C_{2}B_{i}(z) = C_{1}\pi^{-1/2} |z|^{-1/4} e^{-\varsigma} + C_{2}\pi^{-1/2} z^{-1/4} e^{\varsigma}$$
$$= \pi^{-1/2} \left(\frac{2mg}{\hbar^{2}}\right)^{1/6} [C_{1} \frac{1}{\sqrt{\kappa(x)}} \exp(-\int_{x}^{b} \kappa(x) dx) + C_{2} \frac{1}{\sqrt{\kappa(x)}} \exp(\int_{x}^{b} \kappa(x) dx)]$$

Then we have the connection formula (II; downward) as

| $\frac{A}{\sqrt{\kappa(x)}} \exp\left(\frac{1}{2} - \frac{1}{2}\right)$ | $p(-\int_{x}^{b}\kappa(x)dx) + \frac{B}{\sqrt{\kappa(x)}}\exp(\int_{x}^{b}\kappa(x)dx)]$ |
|---|---|
| Ų | |
| $\frac{2A}{\sqrt{k(x)}}$ co | $s(\int_{b}^{x} k(x)dx - \frac{\pi}{4}) - \frac{B}{\sqrt{k(x)}}sin(\int_{b}^{x} k(x)dx - \frac{\pi}{4})]$ |

(II, downward)

with



where $C_1 = A$ and $C_2 = B$.

9. Tunneling probability

We apply the connection formula to find the tunneling probability. In order that the WKB approximation apply within a barrier, it is necessary that the potential V(x) does not change so rapidly. Suppose that a particle (energy ε and mass m) penetrates into a barrier shown in the figure. There are three regions, I, II, and III.



Fig. The connection formula I (upward) is used at x = a and the connection formula II (downward) is used at x = b.

For x > b, (region III)

$$\psi_{III} = \frac{A}{\sqrt{k_1(x)}} \exp[i(\int_{b}^{x} k_1(x)dx - \frac{\pi}{4})]$$
$$= \frac{A}{\sqrt{k_1(x)}} \cos(\int_{b}^{x} k_1(x)dx - \frac{\pi}{4}) + \frac{iA}{\sqrt{k_1(x)}} \sin(\int_{b}^{x} k_1(x)dx - \frac{\pi}{4})]$$

(we consider on the wave propagating along the positive *x* axis), where

$$k_1(x) = \sqrt{\frac{2m}{\hbar^2}(\varepsilon - V(x))} \ .$$

The connection formula (II, downward) is applied to the boundary between the regions III and II.

$$\frac{A}{2\sqrt{\kappa(x)}}\exp(-\int_{x}^{b}\kappa(x)dx) + \frac{B}{2\sqrt{\kappa(x)}}\exp(\int_{x}^{b}\kappa(x)dx)]$$

$$\Downarrow$$

$$\frac{A}{\sqrt{k_{1}(x)}}\cos(\int_{b}^{x}k_{1}(x)dx - \frac{\pi}{4}) - \frac{B}{2\sqrt{k_{1}(x)}}\sin(\int_{b}^{x}k_{1}(x)dx - \frac{\pi}{4})]$$
(4)

(II, downward)

Here we get

$$B = -2iA$$
.

Then we get the wave function of the region II,

$$\psi_{II} = \frac{A}{2\sqrt{\kappa(x)}} \exp(-\int_{x}^{b} \kappa(x) dx) - \frac{iA}{\sqrt{\kappa(x)}} \exp(\int_{x}^{b} \kappa(x) dx)]$$

₩

$$\psi_{III} = \frac{A}{\sqrt{k_1(x)}} \cos(\int_{b}^{x} k_1(x) dx - \frac{\pi}{4}) + \frac{iA}{\sqrt{k_1(x)}} \sin(\int_{b}^{x} k_1(x) dx - \frac{\pi}{4})]$$

or

$$\psi_{II} = \frac{A}{2\sqrt{\kappa(x)}} \exp(-\int_{a}^{b} \kappa(x)dx + \int_{a}^{x} \kappa(x)dx) - \frac{iA}{\sqrt{\kappa(x)}} \exp(\int_{a}^{b} \kappa(x)dx - \int_{a}^{x} \kappa(x)dx)]$$
$$= \frac{-iA}{\sqrt{\kappa(x)}} \frac{1}{r} \exp(-\int_{a}^{x} \kappa(x)dx) + \frac{A}{\sqrt{\kappa(x)}} \frac{r}{2} \exp(\int_{a}^{x} \kappa(x)dx) + \frac{A}{\sqrt{\kappa(x)}} \exp(\int_{a}^{x} \kappa(x)dx)$$

where

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}(V(x) - \varepsilon)},$$

and

$$r = \exp(-\int_{a}^{b} \kappa(x) dx),$$

Next, the connection formula (I; upward) is applied to the boundary between the regions II and I.

$$\frac{2C}{\sqrt{k_2(x)}} \cos\left(\int_x^a k_2(x)dx - \frac{\pi}{4}\right) - \frac{D}{\sqrt{k_2(x)}} \sin\left(\int_x^a k_2(x)dx - \frac{\pi}{4}\right)\right]$$

$$\Rightarrow \qquad (I; upward)$$

$$\frac{C}{\sqrt{\kappa(x)}} \exp\left(-\int_a^x \kappa(x)dx\right) + \frac{D}{\sqrt{\kappa(x)}} \exp\left(\int_a^x \kappa(x)dx\right)\right]$$

Here we get

$$C = -iA\frac{1}{r},$$
$$D = \frac{A}{2}r.$$

Then we have the wave function of the region I,

$$\psi_{I} = \frac{-2iA}{\sqrt{k_{2}(x)}} \frac{1}{r} \cos(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})$$

$$-\frac{A}{2\sqrt{k_{2}(x)}} r \sin(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})]$$

$$= \frac{-iA}{\sqrt{k_{2}(x)}} \frac{1}{r} \{ \exp[i(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})] + \exp[-i(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})] \}$$

$$+ \frac{A}{\sqrt{k_{2}(x)}} \frac{ir}{4} \{ \exp[i(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})] - \exp[-i(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})] \}$$

or

$$\psi_{I} = \frac{iA}{\sqrt{k_{2}(x)}} \{ (\frac{r}{4} - \frac{1}{r}) \exp[i(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})] - (\frac{r}{4} + \frac{1}{r}) \exp[-i(\int_{x}^{a} k_{2}(x)dx - \frac{\pi}{4})] \}$$
$$= \frac{-iA}{\sqrt{k_{2}(x)}} \{ (\frac{1}{r} - \frac{r}{4}) \exp[-i(\int_{a}^{x} k_{2}(x)dx + \frac{\pi}{4})] + (\frac{1}{r} + \frac{r}{4})) \exp[i(\int_{a}^{x} k_{2}(x)dx + \frac{\pi}{4})] \}$$

The first term corresponds to that of the reflected wave and the second term corresponds to that of the incident wave. Then the tunneling probability is

$$T = \frac{1}{\left(\frac{1}{r} + \frac{r}{4}\right)^2} \approx r^2 = \exp(-2\int_a^b \kappa(x) dx)$$

where

$$r = \exp(-\int_{a}^{b} \kappa(x) dx)$$



Fig. Gamov's model for the potential energy of an alpha particle in a radioactive nucleus.



Fig. The tunneling of a particle from the 238 U (Z = 92). The kinetic energy 4.2 MeV. <u>http://demonstrations.wolfram.com/GamowModelForAlphaDecayTheGeigerNutt</u><u>allLaw/</u>

For $r_1 < r < r_2$.

$$\kappa(r) = \frac{1}{\hbar} \sqrt{2m} \sqrt{V(r) - \varepsilon}$$

At $r = r_2$,

$$\varepsilon = \frac{2Z_1 e^2}{4\pi\varepsilon_0 r_2}$$

The tunneling probability is

$$P = e^{-2\gamma} = \exp[-2\int_{r_1}^r \kappa(r)dr]$$

where

$$\begin{split} \gamma &= \int_{r_1}^{r_2} \kappa(r) dr \\ &= \frac{\sqrt{2m}}{\hbar} \int_{r_1}^{r_2} \sqrt{V(r) - \varepsilon} dr \\ &= \frac{\sqrt{2m\varepsilon}}{\hbar} \int_{r_1}^{r_2} \sqrt{\frac{r_2}{r} - 1} dr \\ &= \frac{\sqrt{2m\varepsilon}}{\hbar} [r_2 \arccos \sqrt{\frac{r_1}{r_2}} - \sqrt{r_1(r_2 - r_1)}] \\ &= \frac{\sqrt{2m\varepsilon}}{\hbar} r_2 [\arccos \sqrt{\frac{r_1}{r_2}} - \sqrt{\frac{r_1}{r_2}(1 - \frac{r_1}{r_2})}] \end{split}$$

where *m* is the mass of α -particle (= 4.001506179125 u). fm = 10⁻¹⁵ m (fermi).

The quantity P gives the probability that in one trial an α particle will penetrate the barrier. The number of trials per second could estimated to be

$$N = \frac{v}{2r_1}$$

if it were assumed that a particle is bouncing back and forth with velocity v inside the nucleus of diameter $2r_1$. Then the probability per second that nucleus will decay by emitting a particle, called the decay rate *R*, would be

$$R = \frac{v}{2r_1} e^{-2\eta}$$

((Example))

We consider the α particle emission from ²³⁸U nucleus (Z = 92), which emits a K = 4.2 MeV α particle. The a particle is contained inside the nuclear radius $r_1 = 7.0$ fm (fm = 10^{-15} m).

(i) The distance r_2 : From the relation

$$K = \frac{2Ze^2}{4\pi\varepsilon_0 r_2}$$

we get

 $r_2 = 63.08$ fm.

(ii) The velocity of a particle inside the nucleus, *v*:

From the relation

$$K_1 = \frac{1}{2}m_{\alpha}v^2$$

where m_{α} is the mass of the a particle; $m_{\alpha} = 4.001506179$ u, we get

$$v = 1.42318 \ge 10^7 \text{ m/s}$$

(iii) The value of γ .

$$\gamma = \frac{\sqrt{2mK}}{\hbar} [r_2 \arccos \sqrt{\frac{r_1}{r_2}} - \sqrt{r_1(r_2 - r_1)}] = 51.8796$$

(iv) The decay rate *R*:

$$R = \frac{v}{2r_1}e^{-2\gamma} = 8.813 \text{ x } 10^{-25}.$$

((Mathematica))

Clear["Global`*"];
rule1 = {u → 1.660538782 × 10⁻²⁷, eV → 1.602176487 × 10⁻¹⁹,
qe → 1.602176487 × 10⁻¹⁹, c → 2.99792458 × 10⁸,

$$\hbar \to 1.05457162853 \times 10^{-34}$$
, e0 → 8.854187817 × 10⁻¹²,
MeV → 1.602176487 × 10⁻¹³, Ma → 4.001506179125 u,
fm → 10⁻¹⁵, Z1 → 92, r1 → 7 fm, K1 → 4.2 MeV};
eq0 = K1 == $\frac{2 Z1 qe^2}{4 \pi e0 r}$ //. rule1
6.72914 × 10⁻¹³ = $\frac{4.24502 \times 10^{-26}}{r}$
eq01 = Solve[eq0, r]; r2 = r /. eq01[[1]]
6.30842 × 10⁻¹⁴
 $\frac{r2}{fm}$ /. rule1
63.0842
eq1 = $\frac{1}{2}$ Ma v² = K1 //. rule1; eq2 = Solve[eq1, v];
v1 = v /. eq2[[2]]
1.42318 × 10⁷
 $\gamma = \frac{\sqrt{2 Ma K1}}{\hbar} (r2 \operatorname{ArcCos} [\sqrt{\frac{r1}{r2}}] - \sqrt{r1 (r2 - r1)}) //.$
rule1
51.8796
R1 = $\frac{v1}{2 r1}$ Exp[-2 γ] //. rule1

 8.81282×10^{-25}





For *x*<*b* (region I), the unnormalized wave function is

$$\psi_I = \frac{1}{\sqrt{\kappa(x)}} \exp(-\int_x^b \kappa(x) dx),$$

Using the connection rule (II; downward)

$$\psi_{II} = \frac{A}{2\sqrt{\kappa(x)}} \exp(-\int_{x}^{b} \kappa(x)dx) + \frac{B}{2\sqrt{\kappa(x)}} \exp(\int_{x}^{b} \kappa(x)dx)]$$

$$\Downarrow$$

$$\psi_{II} = \frac{A}{\sqrt{k(x)}} \cos(\int_{b}^{x} k(x)dx - \frac{\pi}{4}) - \frac{B}{2\sqrt{k(x)}} \sin(\int_{b}^{x} k(x)dx - \frac{\pi}{4})]$$

we get

$$A=2, \qquad B=0$$

Then we have

$$\psi_{II} = \frac{2}{\sqrt{k(x)}} \cos(\int_{b}^{x} k(x) dx - \frac{\pi}{4})] \qquad \text{for } b < x < a$$

This may also be written as

(II; downward)

$$\begin{split} \psi_{II} &= \frac{2}{\sqrt{k(x)}} \cos(\int_{b}^{x} k(x) dx - \frac{\pi}{4}) = \frac{2}{\sqrt{k(x)}} \cos(\int_{b}^{a} k(x) dx - \int_{x}^{a} k(x) dx - \frac{\pi}{4}) \\ &= \frac{2}{\sqrt{k(x)}} \cos[\int_{b}^{a} k(x) dx - \int_{x}^{a} k(x) dx) + \frac{\pi}{4} - \frac{\pi}{2}] \\ &= \frac{2}{\sqrt{k(x)}} \sin[\int_{b}^{a} k(x) dx - \int_{x}^{a} k(x) dx) + \frac{\pi}{4}] \\ &= \frac{2}{\sqrt{k(x)}} \sin[\int_{b}^{a} k(x) dx] \cos[\int_{x}^{a} k(x) dx) - \frac{\pi}{4}] \\ &- \frac{2}{\sqrt{k(x)}} \cos[\int_{b}^{a} k(x) dx] \sin[\int_{x}^{a} k(x) dx) - \frac{\pi}{4}] \end{split}$$

Here we use the connection rule (I, upward),

$$\frac{2A}{\sqrt{k(x)}}\cos(\int_{x}^{a}k(x)dx - \frac{\pi}{4}) - \frac{B}{\sqrt{k(x)}}\sin(\int_{x}^{a}k(x)dx - \frac{\pi}{4})$$

$$\Rightarrow \qquad (I; upward)$$

$$\frac{A}{\sqrt{\kappa(x)}}\exp(-\int_{a}^{x}\kappa(x)dx) + \frac{B}{\sqrt{\kappa(x)}}\exp(\int_{a}^{x}\kappa(x)dx)]$$

From this we have

$$\psi_{II} = \frac{2}{\sqrt{k(x)}} \sin[\int_{b}^{a} k(x)dx] \cos[\int_{x}^{a} k(x)dx) - \frac{\pi}{4}] - \frac{2}{\sqrt{k(x)}} \cos[\int_{b}^{a} k(x)dx] \sin[\int_{x}^{a} k(x)dx) - \frac{\pi}{4}]$$

with

$$A = \sin\left[\int_{b}^{a} k(x)dx\right], \qquad B = -2\cos\left[\int_{b}^{a} k(x)dx\right].$$

Since ψ_{III} should have such a form

$$\psi_{III} = \frac{A}{\sqrt{\kappa(x)}} \exp(-\int_{a}^{x} \kappa(x) dx)$$

for x > a. Then we need the condition that

$$B = -2\cos\left[\int_{b}^{a} k(x)dx\right] = 0,$$

or

$$\int_{b}^{a} k(x)dx = (n+\frac{1}{2})\pi$$

or

$$\int_{b}^{a} p(x)dx = (n+\frac{1}{2})\hbar\pi,$$

where n = 0, 1, 2, ...

10. Simple harmonics

We consider a simple harmonics,

$$p(x) = \sqrt{2m(\varepsilon - V(x))} = \sqrt{2m(\varepsilon - \frac{1}{2}m\omega^2 x^2)} = 2m\omega_0\sqrt{x_0^2 - x^2}$$

where

$$x_0 = \sqrt{\frac{2\varepsilon}{m\omega_0^2}} \,.$$

Then we get

$$\int_{-x_0}^{x_0} p(x) dx = 2m\omega_0 \int_{0}^{x_0} \sqrt{x_0^2 - x^2} dx = 2m\omega_0 \frac{\pi x_0^2}{4} = \frac{1}{2}m\omega_0 \pi \frac{2\varepsilon}{m\omega_0^2} = \frac{\pi\varepsilon}{\omega_0}$$

When

$$\int_{-x0}^{a} p(x) dx = (n + \frac{1}{2})\pi \hbar$$

we have

$$\frac{\pi\varepsilon}{\omega_0} = (n + \frac{1}{2})\pi\hbar ,$$

or

$$\varepsilon = (n + \frac{1}{2})\hbar\omega$$

APPENDIX

Connection formula

$$k(x) = \frac{1}{\hbar} \sqrt{2m} \sqrt{\varepsilon - V(x)}$$
$$\kappa(x) = \frac{1}{\hbar} \sqrt{2m} \sqrt{V(x) - \varepsilon}$$





