WKB approximation: α particle decay
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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)

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Gregor Wentzel (February 17, 1898 – August 12, 1978) 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 (2 February 1894 – 24 April 1952) was a Dutch physicist who worked with Niels Bohr to understand how electromagnetic waves interact with matter.
http://en.wikipedia.org/wiki/Hans_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

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1. Classical limit

Change in the wavelength over the distance δx

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

When $\delta x = \lambda$

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

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

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

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

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

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

$$\left|\frac{mh}{p^3}\frac{dV(x)}{dx}\right| << 1 \qquad\qquad \text{(classical approximation)}$$

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If dV/dx is small, the momentum is large, or both, the above inequality is likely to be satisfied. <u>Around the turning point, $p(x) = 0$. $|$dV/d$x|$ is very small when $V(x)$ is a slowly changing function of x.</u> 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

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

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

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((**Mathematica**))

WKB approximation

```
eq1 = - ℏ²/(2 m) D[ψ[x], {x, 2}] + V[x] ψ[x] - ε ψ[x];
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```
rule1 = {ψ → (Exp[ⅈ/ℏ S[#]] &)};
```

```
eq2 = eq1 /. rule1 // Simplify
```

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

```
rule2 =
  {S →

    (S0[#] + ℏ S1[#] + ℏ²/2! S2[#] + ℏ³/3! S3[#] + ℏ⁴/4! S4[#] &)};
```

```
eq3 = (-2 ε m + 2 m V[x] + S'[x]² - ⅈ ℏ S''[x]);
```

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

```
list1 = Table[{n, Coefficient[eq4, ℏ, n]}, {n, 0, 6}] //
    Simplify;
```

```
% // TableForm
```

0    $-2\, m\, \varepsilon + 2\, m\, V[x] + S0'[x]^2$

1    $2\, S0'[x]\, S1'[x] - \mathrm{i}\, S0''[x]$

2    $S1'[x]^2 + S0'[x]\, S2'[x] - \mathrm{i}\, S1''[x]$

3    $S1'[x]\, S2'[x] + \frac{1}{3} S0'[x]\, S3'[x] - \frac{1}{2}\,\mathrm{i}\, S2''[x]$

4    $\frac{1}{12} \left(3\, S2'[x]^2 + 4\, S1'[x]\, S3'[x] + S0'[x]\, S4'[x] - 2\,\mathrm{i}\, S3''[x]\right)$

5    $\frac{1}{24} \left(4\, S2'[x]\, S3'[x] + 2\, S1'[x]\, S4'[x] - \mathrm{i}\, S4''[x]\right)$

6    $\frac{1}{72} \left(2\, S3'[x]^2 + 3\, S2'[x]\, S4'[x]\right)$

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 $S_1(x)$

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

$$S_1{}'(x) = \frac{iS_0{}''(x)}{2S_0{}'(x)} = \frac{i}{2}\frac{\dfrac{d}{dx}S_0{}'(x)}{S_0{}'(x)},$$

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

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

or

$$e^{iS_1(x)} = \frac{1}{\sqrt{\hbar k(x)}}.$$

(c) Derivation of $S_2(x)$

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

$$S_2'(x) = \frac{iS_1''(x) - [S_1'(x)]^2}{S_0'(x)}.$$

Then the WKB solution is given by

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

$$= \pm\hbar\int_{x_0}^{x} k(x)dx - \frac{\hbar}{2i}\ln[\hbar k(x)] + ...$$

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

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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

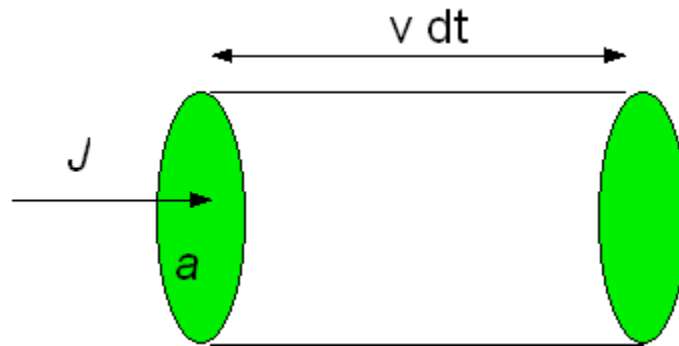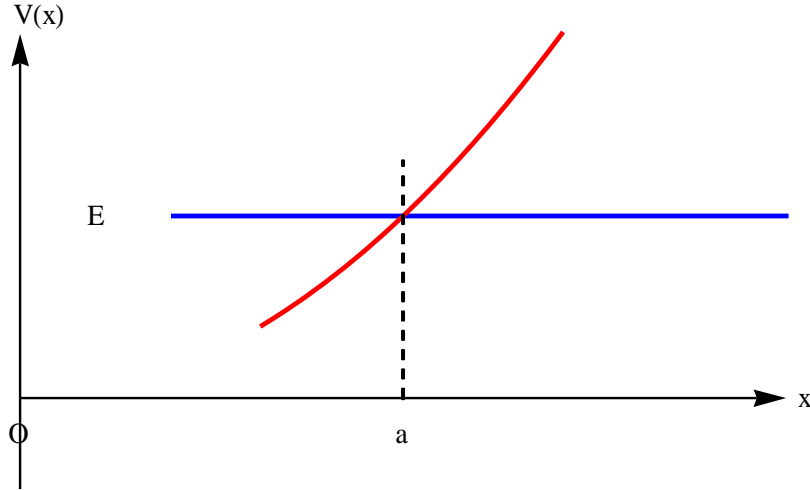$$J = v|\psi|^2 = v\frac{|A|^2}{v}\frac{\hbar}{m} = \frac{\hbar}{m}|A|^2.$$

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 $k(x) \to 0$ 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

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

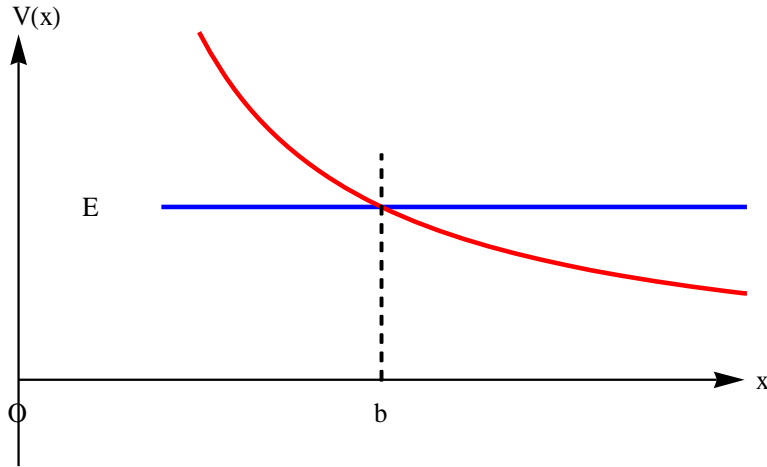(ii)   For $x<a$ where $V(x)<\varepsilon$,

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

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 $V(x)>\varepsilon$,

$$\psi_I(x) = \frac{A}{\sqrt{\kappa(x)}}\exp(\int_x^b \kappa(x)dx) + \frac{B}{\sqrt{\kappa(x)}}\exp(\int_x^b \kappa(x)dx),$$
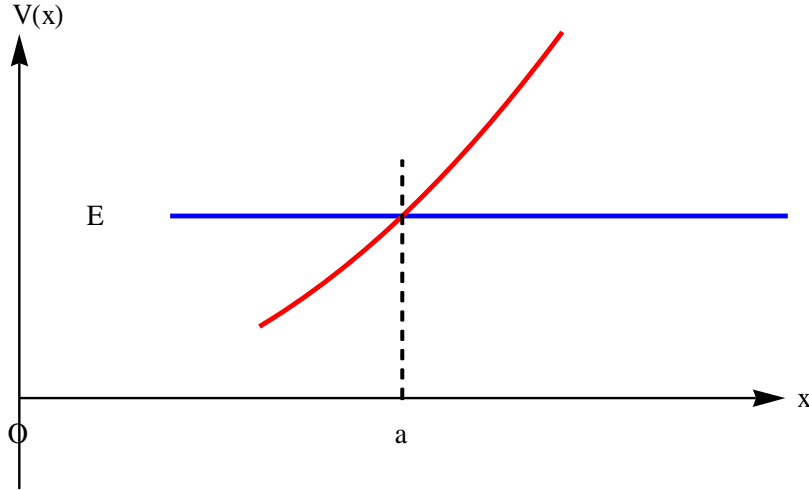
with

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

(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

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

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

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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

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

((Note))

$$\frac{d}{dx} = \frac{dz}{dx}\frac{d}{dz} = \left(\frac{2mg}{\hbar^2}\right)^{1/3}\frac{d}{dz},$$

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$$\frac{d^2}{dx^2} = \left(\frac{2mg}{\hbar^2}\right)^{2/3} \frac{d^2}{dz^2}.$$

Then we get

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

The solution of this equation is given by

$$\psi(z) = 2C_1 A_i(z) + C_2 B_i(z),$$

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

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

and

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

where

$$\varsigma = \frac{2}{3}|z|^{3/2}$$
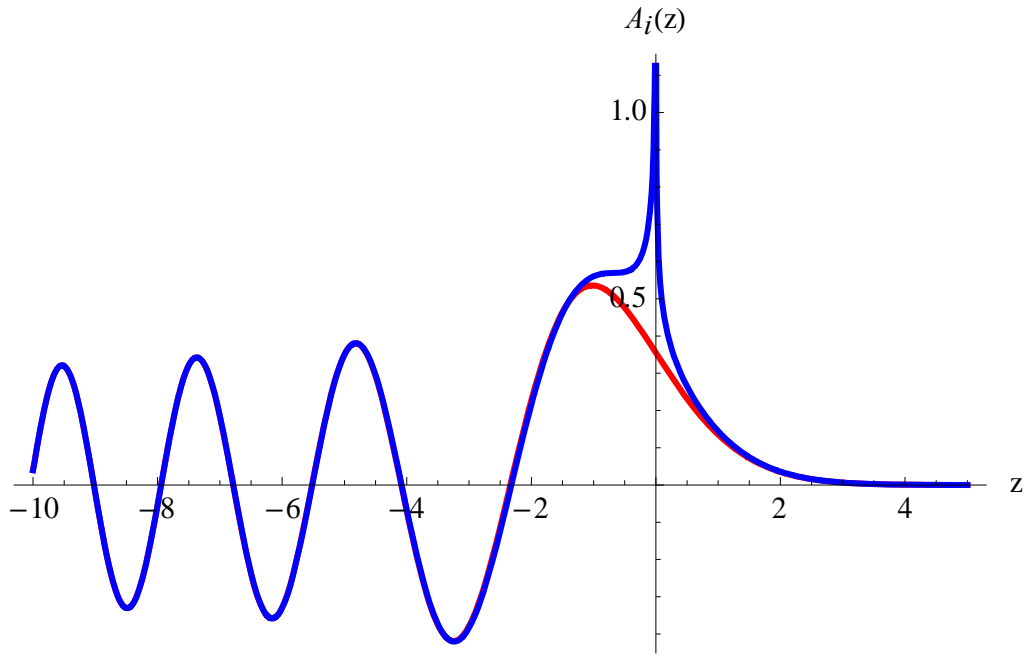
Fig. Plot of the $A_i(z)$ (red) and its asymptotic form (blue) as a function of z for $z<0$.

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

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

$$B_i(z) = \pi^{-1/2} z^{-1/4} e^{\varsigma}, \qquad\qquad \text{for } z>0$$
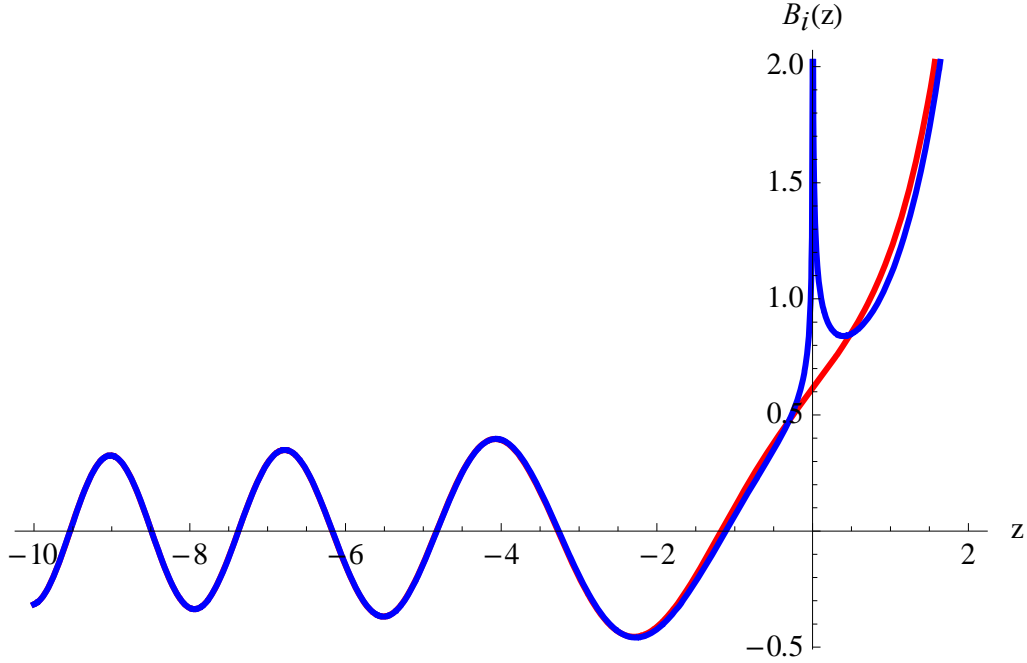
with

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

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 $z<0$,

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

Then we have

$$\int_x^a k(x)dx = \left(\frac{2mg}{\hbar^2}\right)^{1/2} \int_x^a \sqrt{a-x}dx$$

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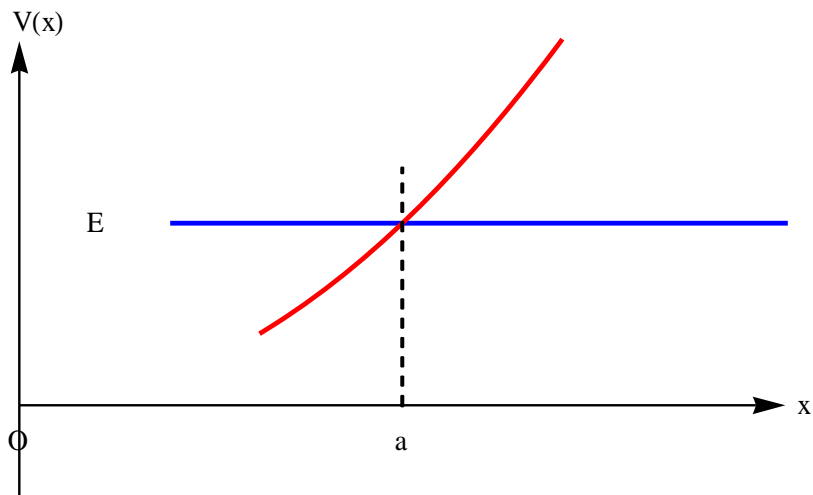
$$= \frac{2}{3}|z|^{3/2} = \varsigma$$

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

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$$\int_a^x \kappa(x) dx = \left(\frac{2mg}{\hbar^2}\right)^{1/2} \int_a^x \sqrt{x-a}\, dx$$

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

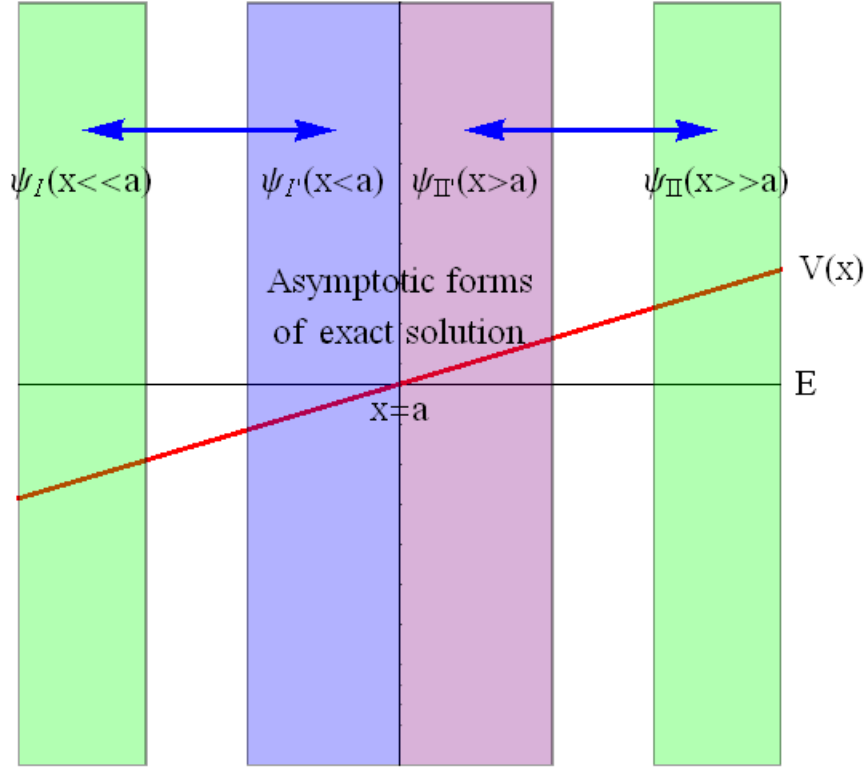$$= \frac{2}{3}|z|^{3/2} = \varsigma$$

6. Connection formula (I; upward)

Fig. Connection formula (I; upward). The condition $\left|\dfrac{d\lambda}{dx}\right| \ll 1$ for the WKB approximation is not satisfied in the vicinity of $x = a$. We need the asymptotic form the exact solution of the Schrödinger equation.

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

The asymptotic form of the wave function for $z<0$ ($x<a$) can be expressed by

$$2C_1 A_i(z) + C_2 B_i(z) = 2C_1 \pi^{-1/2} |z|^{-1/4} \cos(\varsigma - \frac{\pi}{4}) - C_2 \pi^{-1/2} |z|^{-1/4} \sin(\varsigma - \frac{\pi}{4})$$

$$= \pi^{-1/2} \left(\frac{2mg}{\hbar^2}\right)^{1/6} [2C_1 \frac{1}{\sqrt{k(x)}} \cos(\int_x^a k(x)dx - \frac{\pi}{4}) \tag{1}$$

$$- C_2 \frac{1}{\sqrt{k(x)}} \sin(\int_x^a k(x)dx - \frac{\pi}{4})]$$

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 $z>0$ ($x>a$) can be expressed by

$$2C_1 A_i(z) + C_2 B_i(z) = C_1 \pi^{-1/2}|z|^{-1/4} e^{-\varsigma} + C_2 \pi^{-1/2} z^{-1/4} e^{\varsigma}$$

$$= \pi^{-1/2}\left(\frac{2mg}{\hbar^2}\right)^{1/6} [C_1 \frac{1}{\sqrt{\kappa(x)}} \exp(-\int_a^x \kappa(x)dx) \qquad (2)$$

$$+ C_2 \frac{1}{\sqrt{\kappa(x)}} \exp(\int_a^x \kappa(x)dx)]$$

where

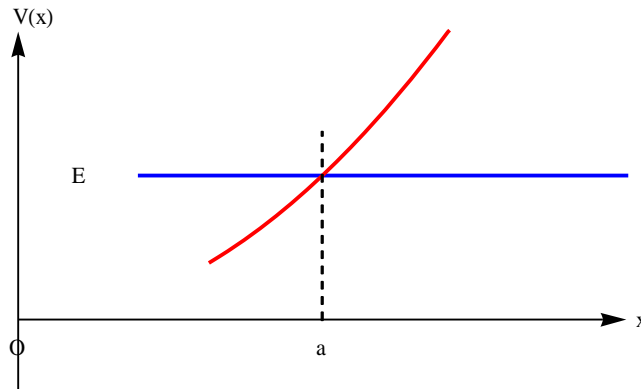$$\varsigma = \int_a^x \kappa(x)dx = \frac{2}{3}|z|^{3/2}, \qquad \kappa(x) = \left(\frac{2mg}{\hbar^2}\right)^{1/3}|z|^{1/2}.$$
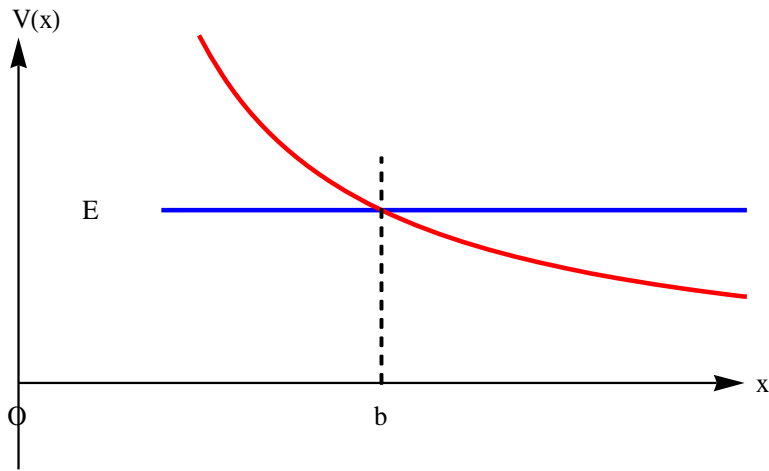
From Eqs.(1) and (2) we have the connection rule (I; upward) as follows.

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

$$\Rightarrow \qquad\qquad\qquad\qquad\qquad\qquad\qquad\text{(I; upward)}$$

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

at the boundary of $x = a$.

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

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7. Exact solution of wave function around the turning point $x = b$

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

$$\psi(z) = 2C_1 A_i(z) + C_2 B_i(z).$$

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

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}[\varepsilon - V(x)]} = \sqrt{\frac{2m}{\hbar^2} g(b-x)}$$

$$= \left(\frac{2mg}{\hbar^2}\right)^{1/3} |z|^{1/2}$$

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

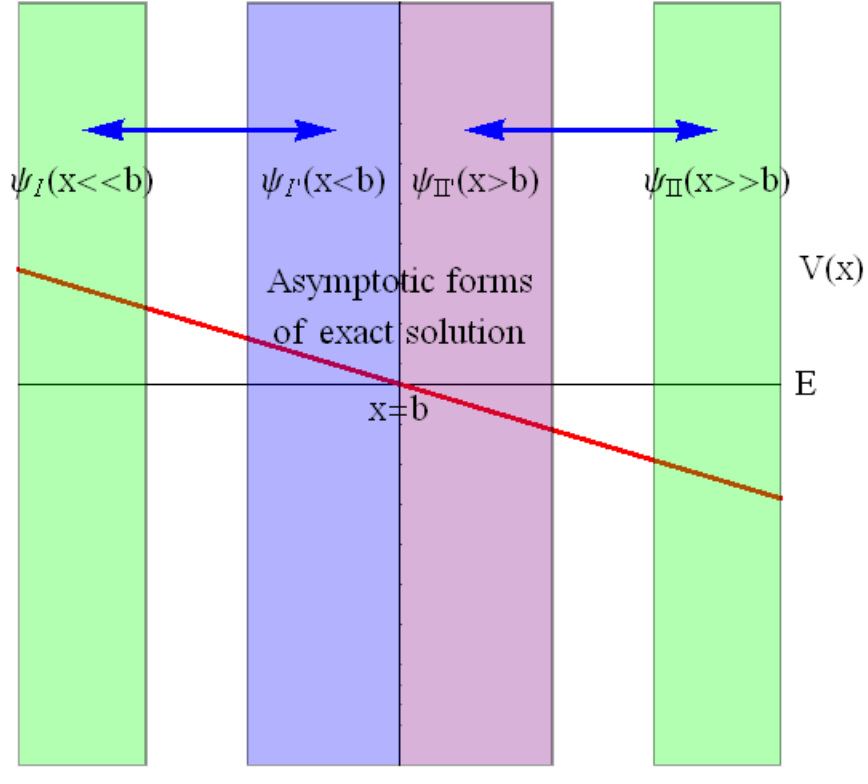## 8.   Connection formula-II (downward)

Fig. Connection formula (II; downward). The condition $\left|\dfrac{d\lambda}{dx}\right| << 1$ for the WKB approximation is not satisfied in the vicinity of $x = b$. We need the asymptotic form the exact solution of the Schrödinger equation.

The asymptotic form for $z<0$;

$$2C_1 A_i(z) + C_2 B_i(z) = 2C_1 \pi^{-1/2} |z|^{-1/4} \cos(\varsigma - \frac{\pi}{4}) - C_2 \pi^{-1/2} |z|^{-1/4} \sin(\varsigma - \frac{\pi}{4})$$

$$= \pi^{-1/2} \left(\frac{2mg}{\hbar^2}\right)^{1/6} [2C_1 \frac{1}{\sqrt{k(x)}} \cos(\int_b^x k(x)dx - \frac{\pi}{4})$$

$$- C_2 \frac{1}{\sqrt{k(x)}} \sin(\int_b^x k(x)dx - \frac{\pi}{4})]$$

The asymptotic form for $z>0$;

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$$2C_1 A_i(z) + C_2 B_i(z) = C_1 \pi^{-1/2} |z|^{-1/4} e^{-\varsigma} + C_2 \pi^{-1/2} z^{-1/4} e^{\varsigma}$$

$$= \pi^{-1/2} \left(\frac{2mg}{\hbar^2} \right)^{1/6} [C_1 \frac{1}{\sqrt{\kappa(x)}} \exp(-\int_x^b \kappa(x)dx)$$

$$+ C_2 \frac{1}{\sqrt{\kappa(x)}} \exp(\int_x^b \kappa(x)dx)]$$

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

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

$\Downarrow$ \qquad\qquad (II, downward)

$$\frac{2A}{\sqrt{k(x)}} \cos[\int_b^x k(x)dx - \frac{\pi}{4}] - \frac{B}{\sqrt{k(x)}} \sin[\int_b^x k(x)dx - \frac{\pi}{4}]$$
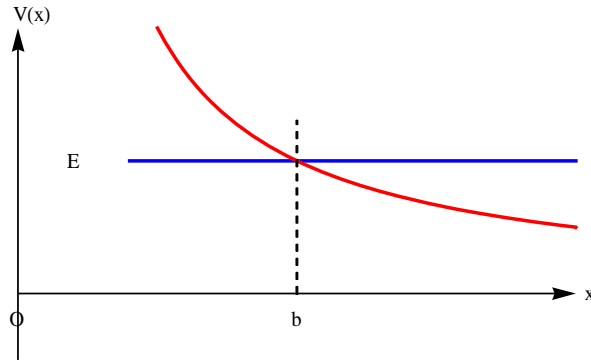
with

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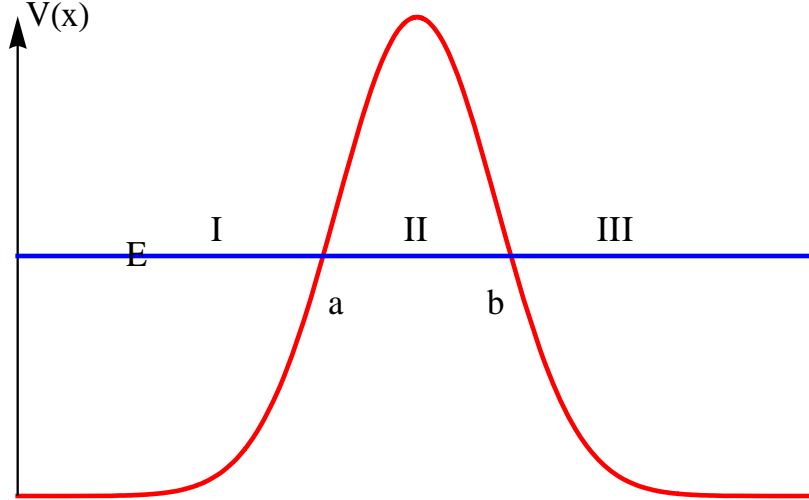
Fig.   The connection formula I (upward) is used at $x = a$ and the connection formula II (downward) is used at $x = b$.

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.

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

$\Downarrow$ (II, downward)

$$\frac{A}{\sqrt{k_1(x)}} \cos[\int_b^x k_1(x)dx - \frac{\pi}{4}] - \frac{B}{2\sqrt{k_1(x)}} \sin[\int_b^x k_1(x)dx - \frac{\pi}{4}]$$

Here we get

$B = -2iA$.

Then we get the wave function of the region II,

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

$\Downarrow$

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

or

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

$$= \frac{-iA}{\sqrt{\kappa(x)}} \frac{1}{r} \exp[-\int_a^x \kappa(x)dx] + \frac{A}{\sqrt{\kappa(x)}} \frac{r}{2} \exp[\int_a^x \kappa(x)dx]$$

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.

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

$$\Rightarrow$$ (I; upward)

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

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

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

where

$$r = \exp(-\int_a^b \kappa(x)dx).$$

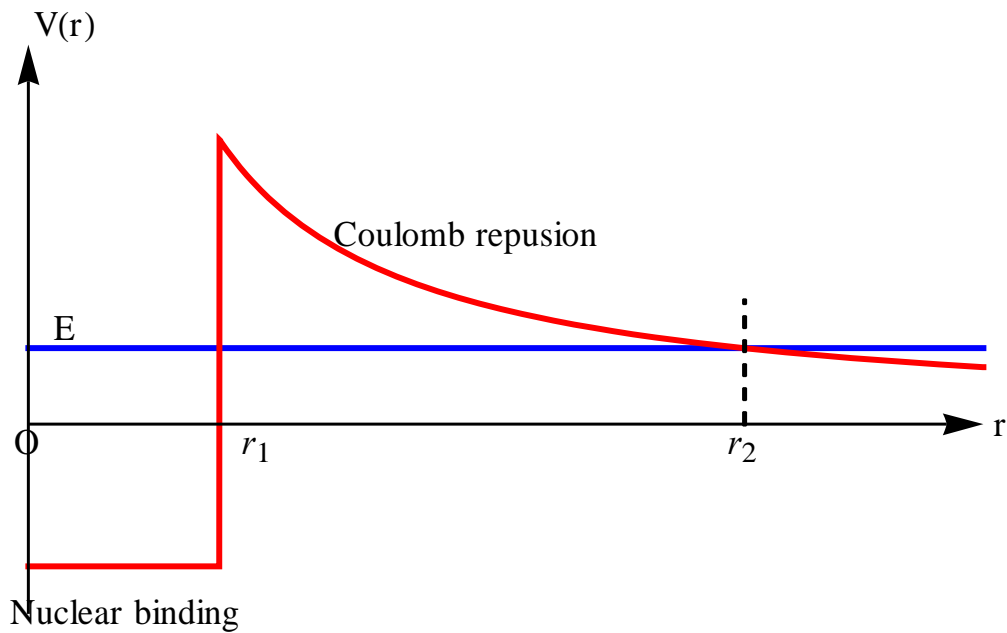## 9. α-particle decay: quantum tunneling

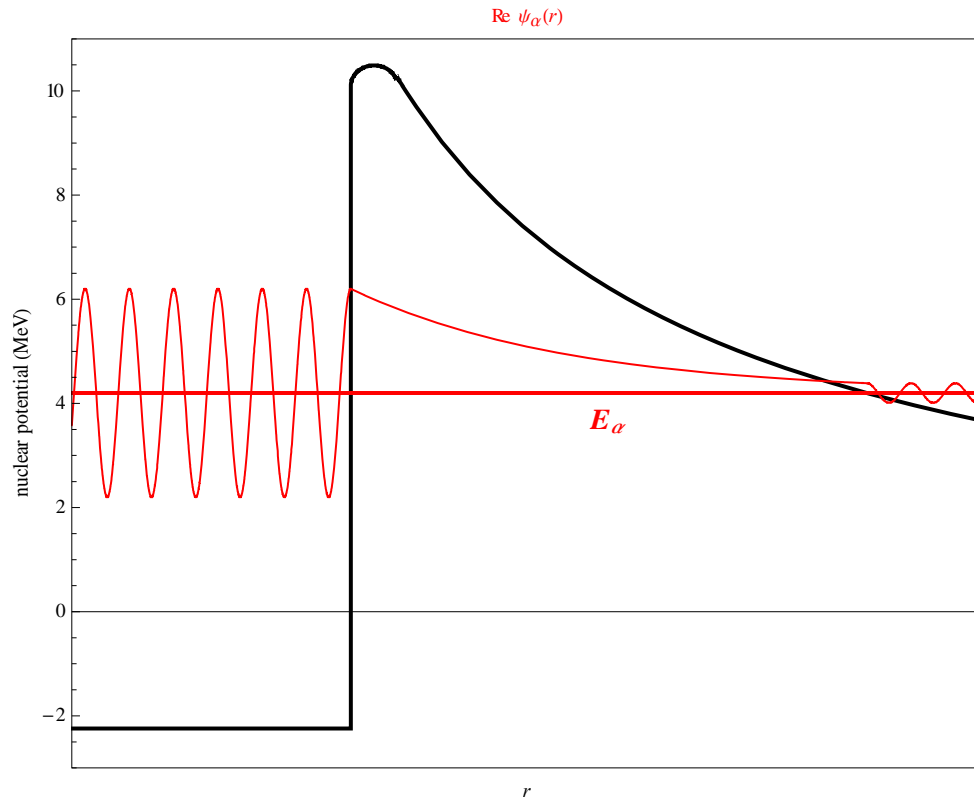**Fig.** Gamov's model for the potential energy of an alpha particle in a radioactive nucleus.

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

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

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

where

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$$\gamma = \int_{r_1}^{r_2} \kappa(r)\,dr$$

$$= \frac{\sqrt{2m}}{\hbar} \int_{r_1}^{r_2} \sqrt{V(r) - \varepsilon}\,dr$$

$$= \frac{\sqrt{2m\varepsilon}}{\hbar} \int_{r_1}^{r_2} \sqrt{\frac{r_2}{r} - 1}\,dr$$

$$= \frac{\sqrt{2m\varepsilon}}{\hbar} [r_2 \arccos\sqrt{\frac{r_1}{r_2}} - \sqrt{r_1(r_2 - r_1)}]$$

$$= \frac{\sqrt{2m\varepsilon}}{\hbar} r_2 [\arccos\sqrt{\frac{r_1}{r_2}} - \sqrt{\frac{r_1}{r_2}(1 - \frac{r_1}{r_2})}]$$

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

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

((**Example**))
We consider the α particle emission from ^{238}U 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

$$r_2 = 63.08 \text{ fm.}$$

(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

$v = 1.42318 \times 10^7$ 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:

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

((**Mathematica**))

```
Clear["Global`*"];
rule1 = {u → 1.660538782 × 10^-27, eV → 1.602176487 × 10^-19,
    qe → 1.602176487 × 10^-19, c → 2.99792458 × 10^8,
    ℏ → 1.05457162853 × 10^-34, ϵ0 → 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};
```

$$eq0 = K1 == \frac{2\ Z1\ qe^2}{4\ \pi\ \epsilon0\ r} \ //. \ rule1$$

$$6.72914 \times 10^{-13} == \frac{4.24502 \times 10^{-26}}{r}$$

```
eq01 = Solve[eq0, r]; r2 = r /. eq01[[1]]
```

$$6.30842 \times 10^{-14}$$

```
r2
── /. rule1
fm
```

$$63.0842$$

```
eq1 = 1/2 Ma v^2 == K1 //. rule1; eq2 = Solve[eq1, v];
v1 = v /. eq2[[2]]
```

$$1.42318 \times 10^7$$

$$\gamma = \frac{\sqrt{2\ Ma\ K1}}{\hbar} \left(r2\ ArcCos\left[\sqrt{\frac{r1}{r2}}\right] - \sqrt{r1\ (r2 - r1)} \right) \ //.$$
$$rule1$$

$$51.8796$$

```
R1 = v1/(2 r1) Exp[-2 γ] //. rule1
```

$$8.81282 \times 10^{-25}$$

9. Bound state: Bohr-Sommerfeld condition.
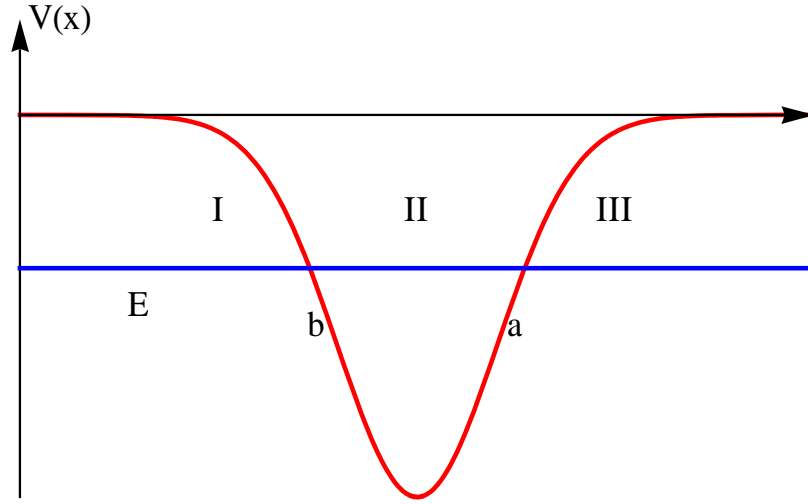
For $x<b$ (region I), the unnormalized wave function is

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

Using the connection rule (II; downward)

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

$\Downarrow$ (II; downward)

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

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

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

$$= \frac{2}{\sqrt{k(x)}} \cos[\int_b^a k(x)dx - \int_x^a k(x)dx + \frac{\pi}{4} - \frac{\pi}{2}]$$

$$= \frac{2}{\sqrt{k(x)}} \sin[\int_b^a k(x)dx - \int_x^a k(x)dx + \frac{\pi}{4}]$$

$$= \frac{2}{\sqrt{k(x)}} \sin[\int_b^a k(x)dx] \cos[\int_x^a k(x)dx - \frac{\pi}{4}]$$

$$- \frac{2}{\sqrt{k(x)}} \cos[\int_b^a k(x)dx] \sin[\int_x^a k(x)dx - \frac{\pi}{4}]$$

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

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

$$\Rightarrow \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(I; upward)}$$

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

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

$$A = \sin[\int_b^a k(x)dx], \qquad B = -2\cos[\int_b^a k(x)dx].$$

Since ψ_{III} should have such a form

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$$\psi_{III} = \frac{A}{\sqrt{\kappa(x)}} \exp[-\int_a^x \kappa(x)dx].$$

for $x>a$. Then we need the condition that

$$B = -2\cos[\int_b^a k(x)dx] = 0,$$

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 $n = 0, 1, 2, ...$ (Bohr-Sommerfeld condition).

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

$$\int_{-x0}^{x_0} p(x)dx = (n+\frac{1}{2})\pi\hbar,$$

we have

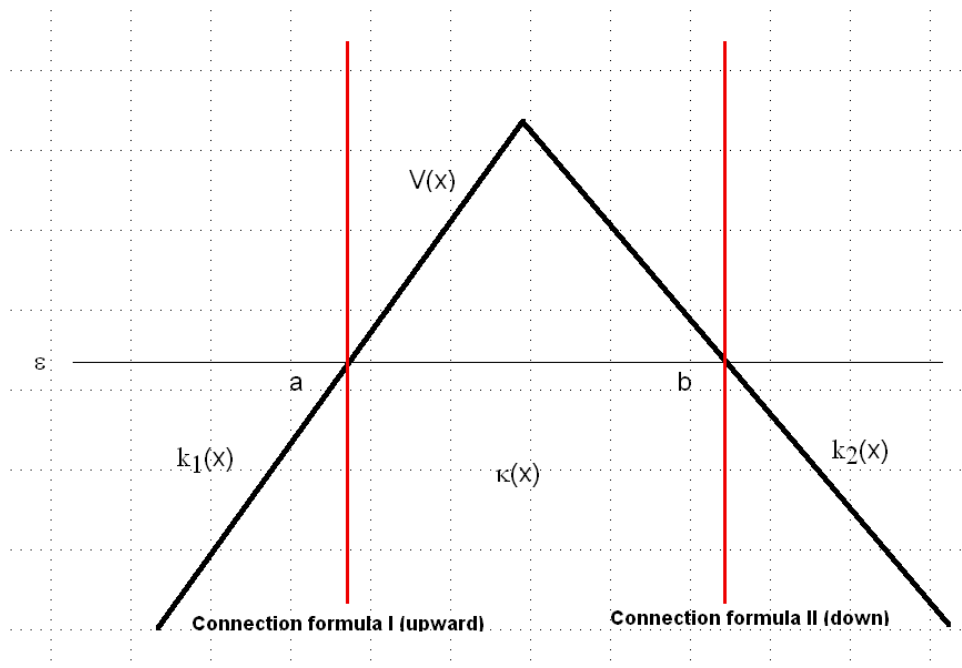$$\frac{\pi\varepsilon}{\omega_0} = (n + \frac{1}{2})\pi\hbar ,$$

or

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

APPENDIX

Connection formula

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

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

(i)   Connection formula at $x = a$ (upward)

$$\frac{2A}{\sqrt{k_1(x)}}\cos(\int_x^a k_1(x)dx - \frac{\pi}{4}) - \frac{B}{\sqrt{k_1(x)}}\sin(\int_x^a k_1(x)dx - \frac{\pi}{4})]$$

$$\Downarrow$$

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

formula I (upward)
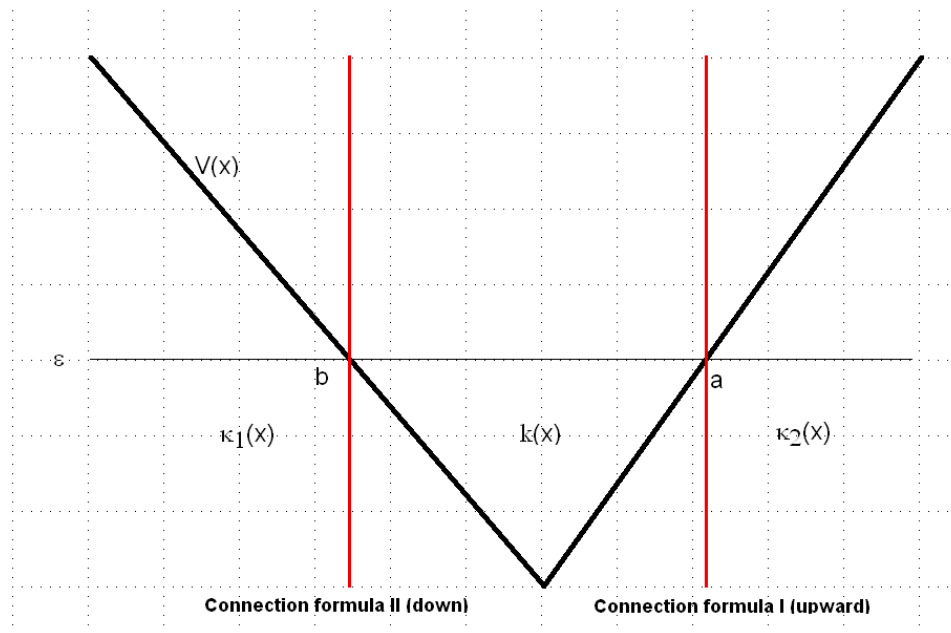
(ii) Connection formula at $x = b$ (downward)

$$\frac{C}{2\sqrt{\kappa(x)}}\exp(-\int_x^b \kappa(x)dx) + \frac{D}{2\sqrt{\kappa(x)}}\exp(\int_x^b \kappa(x)dx)]$$

$$\Downarrow$$

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

formula II (downward)

(i) Connection formula at $x = b$

$$\frac{C}{2\sqrt{\kappa_1(x)}}\exp[-\int_x^b \kappa_1(x)dx] + \frac{D}{2\sqrt{\kappa_1(x)}}\exp[\int_x^b \kappa_1(x)dx]$$

$$\Downarrow$$

$$\frac{C}{\sqrt{k(x)}}\cos[\int_b^x k(x)dx - \frac{\pi}{4}] - \frac{D}{2\sqrt{k(x)}}\sin[\int_b^x k(x)dx - \frac{\pi}{4}]$$

formula II (downward,)

(ii) Connection formula at $x = a$

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

$\Downarrow$ formula I (upward)

$$\frac{A}{\sqrt{\kappa_2(x)}}\exp[-\int_a^x \kappa_2(x)dx] + \frac{B}{\sqrt{\kappa_2(x)}}\exp[\int_a^x \kappa_2(x)dx]$$