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)

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, $\delta\lambda << \lambda$

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

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

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

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

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

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

((**Mathematica**))

WKB approximation

```
eq1 = -ℏ^2/(2 m) D[ψ[x], {x, 2}] + V[x] ψ[x] - ε ψ[x];

rule1 = {ψ → (Exp[ⅈ/ℏ S[#]] &)};

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

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

```
rule2 =
  {S →
    (S0[#] + ℏ S1[#] + ℏ^2/2! S2[#] + ℏ^3/3! S3[#] + ℏ^4/4! 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	$2 S0'[x] S1'[x]-i S0''[x]$
2	$S1'[x]^2+S0'[x] S2'[x]-i S1''[x]$
3	$S1'[x] S2'[x]+\frac{1}{3} S0'[x] S3'[x]-\frac{1}{2} i S2''[x]$
4	$\frac{1}{12}\left(3 S2'[x]^2+4 S1'[x] S3'[x]+S0'[x] S4'[x]-2 i S3''[x]\right)$
5	$\frac{1}{24}(4 S2'[x] S3'[x]+2 S1'[x] S4'[x]-i S4''[x])$
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 $S_0(x)$

Suppose that $\varepsilon > V(x)$. Then we have

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

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

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

(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

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

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

$$\begin{aligned} \psi(x) &= \frac{A'}{\sqrt{\hbar k(x)}}\exp[i\int_{x_0}^{x} k(x)dx] + \frac{B'}{\sqrt{\hbar k(x)}}\exp[-i\int_{x_0}^{x} k(x)dx] \\ &= \frac{A}{\sqrt{k(x)}}\exp[i\int_{x_0}^{x} k(x)dx] + \frac{B}{\sqrt{k(x)}}\exp[-i\int_{x_0}^{x} k(x)dx] \end{aligned}.$$

or

$$\psi(x) = \frac{A_1}{\sqrt{k(x)}}\cos[\int_{x_0}^{x} k(x)dx] + \frac{B_1}{\sqrt{k(x)}}\sin[\int_{x_0}^{x} k(x)dx]$$ for for $\varepsilon > V(x)$,

where we put

$$A = \frac{A'}{\sqrt{\hbar}}, \qquad B = \frac{B'}{\sqrt{\hbar}}, \qquad A_1 = A + B, \qquad B_1 = i(A - B)$$

We now assume that

Suppose that $\varepsilon < V(x)$. $k(x)$ is replaced by

$$k(x) \to i\kappa(x)$$

where

$$\kappa(x) = \sqrt{2m[V(x) - \varepsilon]}$$

Then we have the wave function

$$\psi(x) = \frac{A''}{\sqrt{\kappa(x)}}\exp[-\int_{x_0}^{x} \kappa(x)dx] + \frac{B''}{\sqrt{\kappa(x)}}\exp[\int_{x_0}^{x} \kappa(x)dx]$$ for $\varepsilon < V(x)$.

where A'' and B'' are constants.

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

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

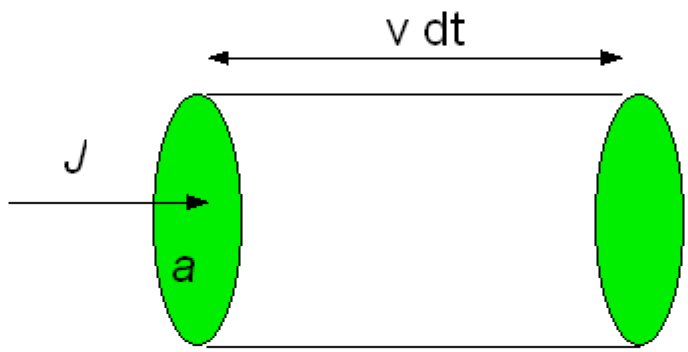
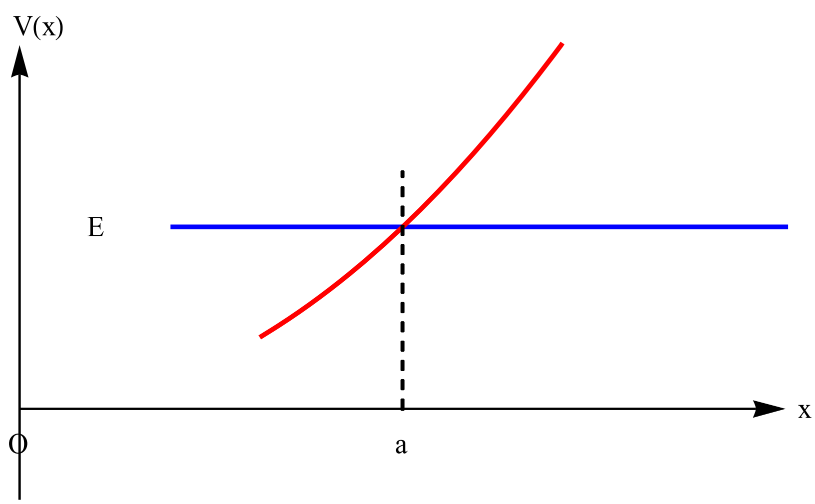


Fig. $Jadt = avdt|\psi|^2$, or $J = v|\psi|^2$

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 $V(x) > \varepsilon$,

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

where A_1 and B_1 are constants, and

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

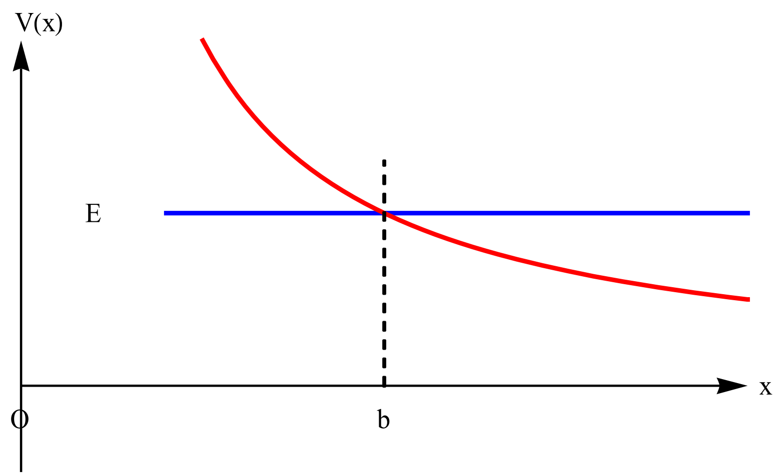
(ii) For $x<a$ where $V(x)<\varepsilon$,

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

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

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

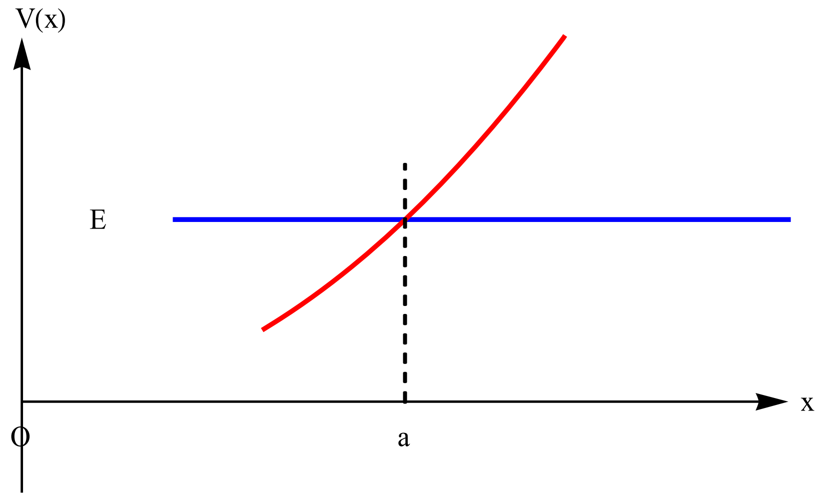
(ii) For $x>b$ where $V(x)<\varepsilon$,

$$\psi_{II}(x) = \frac{C}{\sqrt{k(x)}}\cos(\int_b^x k(x)dx) + \frac{D}{\sqrt{k(x)}}\sin(\int_b^x k(x)dx))$$

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

$$V(x) - \varepsilon = g(x - a)$$

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**))

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

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

Then we get

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

The solution of this equation is given by

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

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

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

and

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

where

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

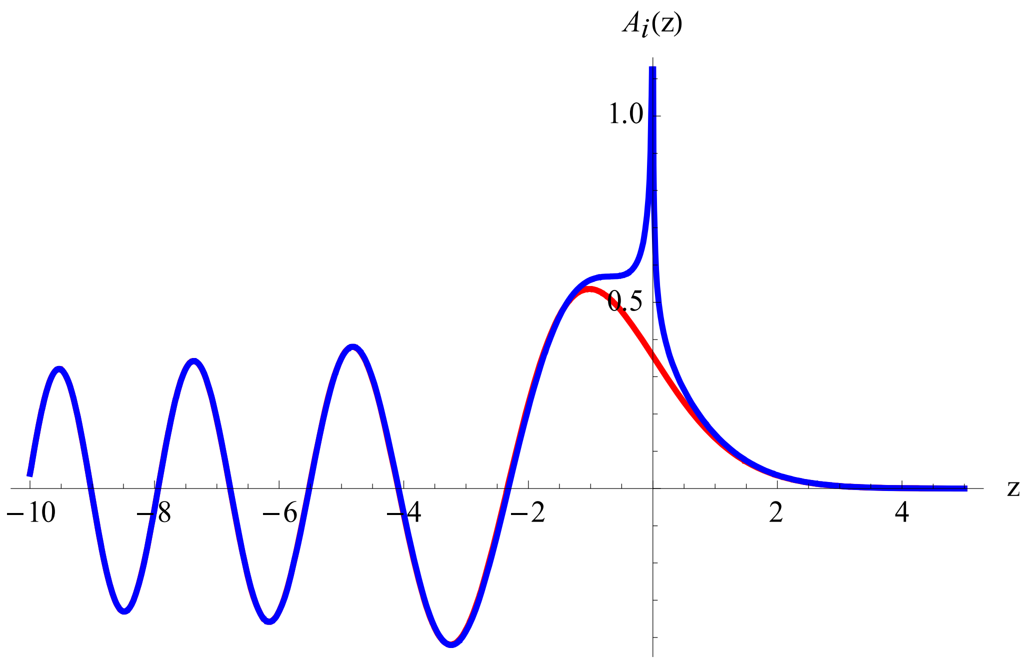


Fig. Plot of the $A_i(z)$ (red) and its asymptotic form (blue) as a function of z for $z<0$.

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

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

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

with

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

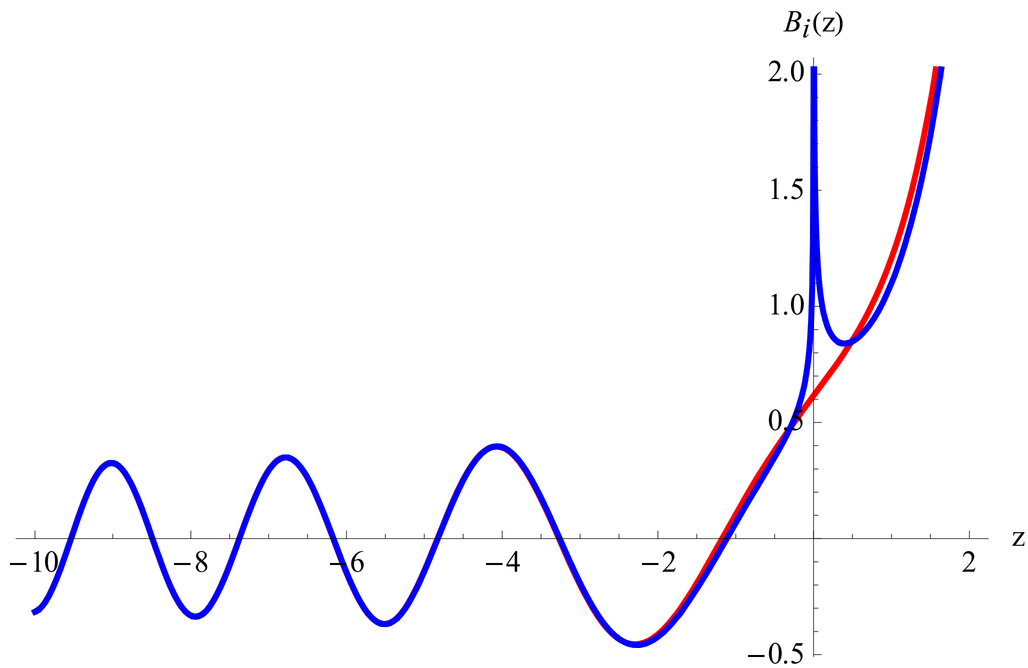


Fig. Plot of the $B_i(z)$ (red) and its asymptotic form (blue) as a function of z for $z<0$.

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 $z>0$,

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

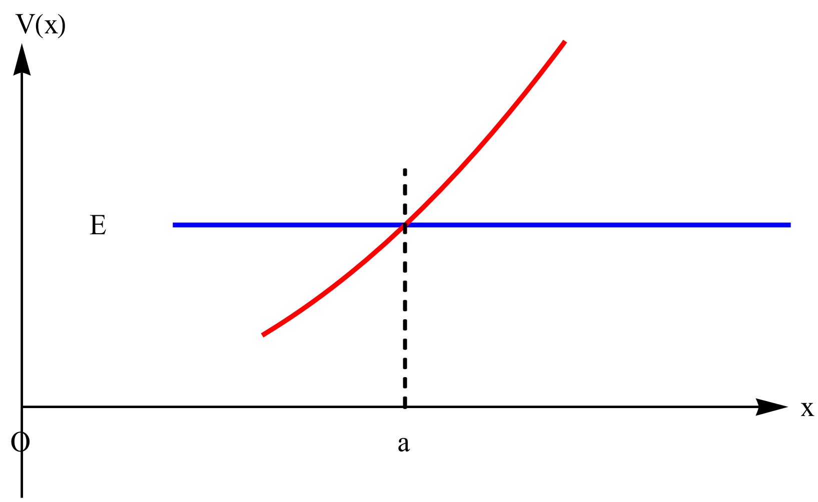
we have

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

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

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

6. Connection formula (I; upward)



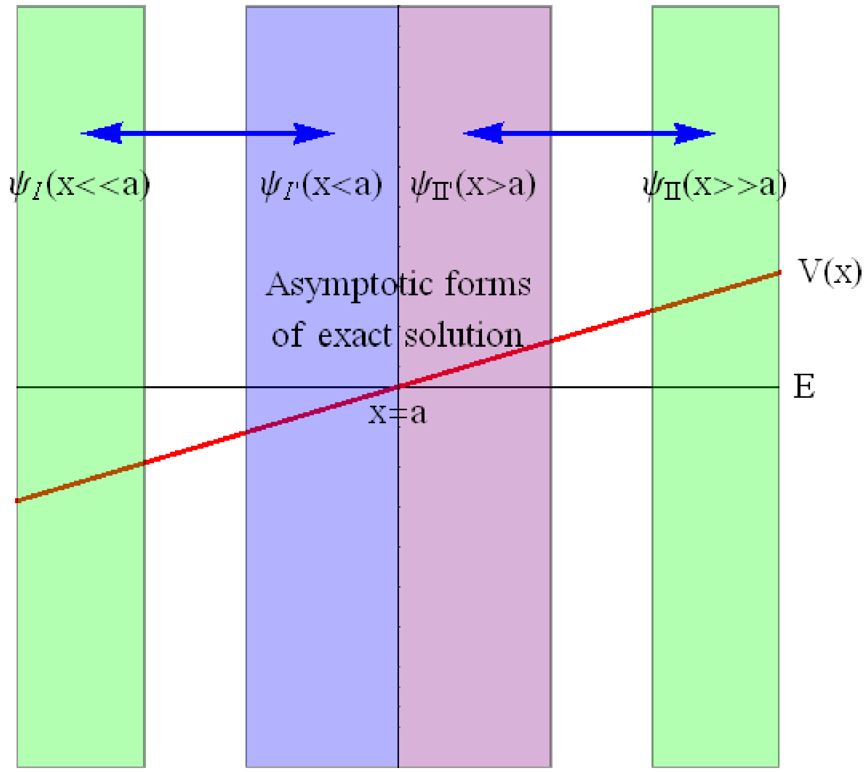


Fig. Connection formula (I; upward). The condition $\left|\frac{d\lambda}{dx}\right| << 1$ for the WKB approximation is not satisfied in the vicinity of $x = a$. We need the asymptotic form the exact solution of the Schrödinger equation. Note that $\psi_{II}(x > a) \approx \psi_{II}(x >> a)$ and $\psi_{II}(x < a) \approx \psi_{II}(x << a)$. The forms of $\psi_{II}(x >> b)$ and $\psi_{II}(x << b)$ are determined, depending on the nature of travelling waves, and the convergence of wave function at the infinity.

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

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

$$
\begin{aligned}
2C_1 A_i(z) + C_2 B_i(z) &= 2C_1 \pi^{-1/2} |z|^{-1/4} \cos(\varsigma - \frac{\pi}{4}) - C_2 \pi^{-1/2} |z|^{-1/4} \sin(\varsigma - \frac{\pi}{4}) \\
&= \pi^{-1/2} \left(\frac{2mg}{\hbar^2}\right)^{1/6} [2C_1 \frac{1}{\sqrt{k(x)}} \cos(\int_x^a k(x)dx - \frac{\pi}{4}) \\
&\quad - C_2 \frac{1}{\sqrt{k(x)}} \sin(\int_x^a k(x)dx - \frac{\pi}{4})]
\end{aligned}
\tag{1}
$$

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

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

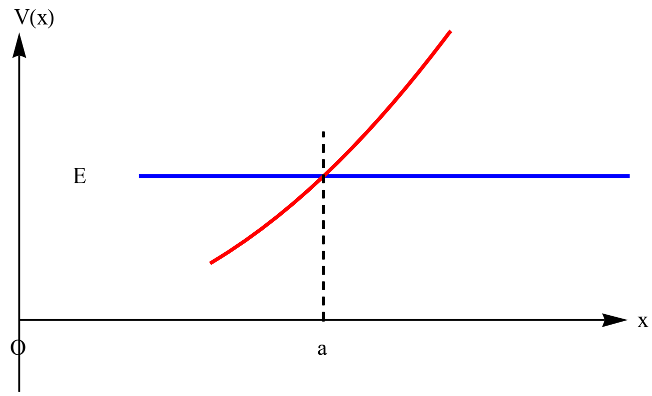
From Eqs.(1) and (2) we have the connection rule (I; upward) as follows.

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

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

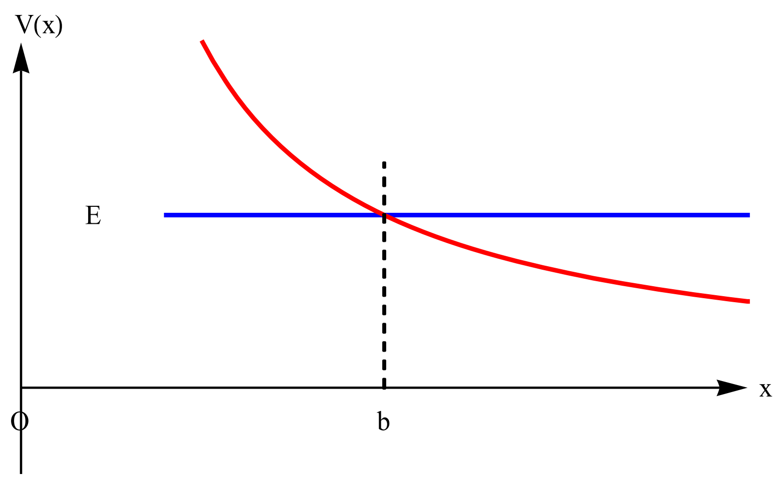
$$\frac{A}{\sqrt{\kappa(x)}} \exp[-\int_a^x \kappa(x)dx] + \frac{B}{\sqrt{\kappa(x)}} \exp[\int_a^x \kappa(x)dx]$$

at the boundary of $x = a$.



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

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)

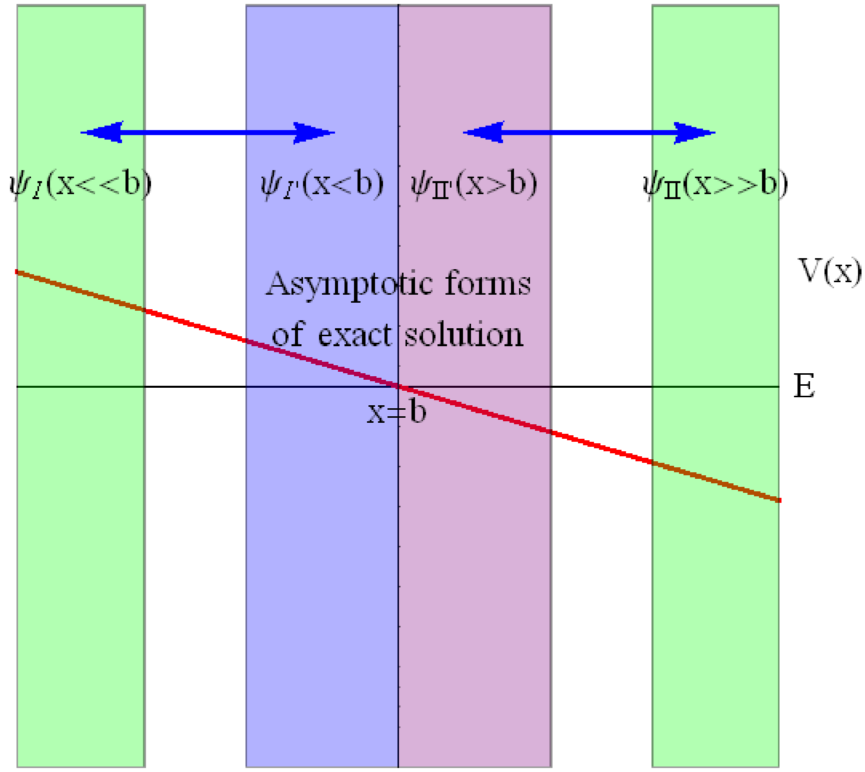


Fig. Connection formula (II; downward). The condition $\left|\frac{d\lambda}{dx}\right| << 1$ for the WKB approximation is not satisfied in the vicinity of $x = b$. We need the asymptotic form the exact solution of the Schrödinger equation. Note that $\psi_{II}(x > b) \approx \psi_{II}(x >> b)$ and $\psi_{II}(x < b) \approx \psi_{II}(x << b)$. The forms of $\psi_{II}(x >> b)$ and $\psi_{II}(x << b)$ are determined, depending on the nature of travelling waves, and the convergence of wave function at the infinity.

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;

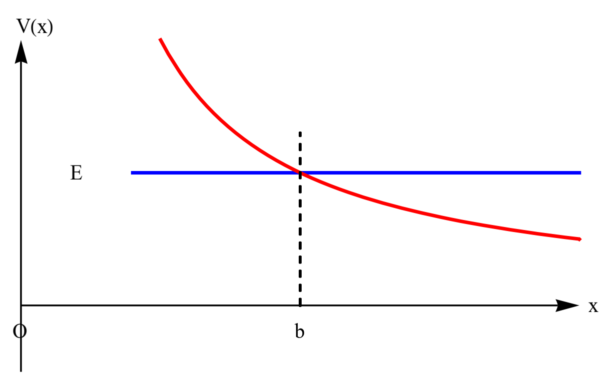
$$2C_1A_i(z)+C_2B_i(z)=C_1\pi^{-1/2}\left|z\right|^{-1/4}e^{-\varsigma}+C_2\pi^{-1/2}z^{-1/4}e^{\varsigma}$$
$$=\pi^{-1/2}\left(\frac{2mg}{\hbar^2}\right)^{1/6}[C_1\frac{1}{\sqrt{\kappa(x)}}\exp(-\int_x^b\kappa(x)dx)$$
$$+C_2\frac{1}{\sqrt{\kappa(x)}}\exp(\int_x^b\kappa(x)dx)]$$

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

$$\frac{A}{\sqrt{\kappa(x)}}\exp[-\int_x^b\kappa(x)dx]+\frac{B}{\sqrt{\kappa(x)}}\exp[\int_x^b\kappa(x)dx]$$
$$\Downarrow$$
$$\frac{2A}{\sqrt{k(x)}}\cos[\int_b^x k(x)dx-\frac{\pi}{4}]-\frac{B}{\sqrt{k(x)}}\sin[\int_b^x k(x)dx-\frac{\pi}{4}]$$

(**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.

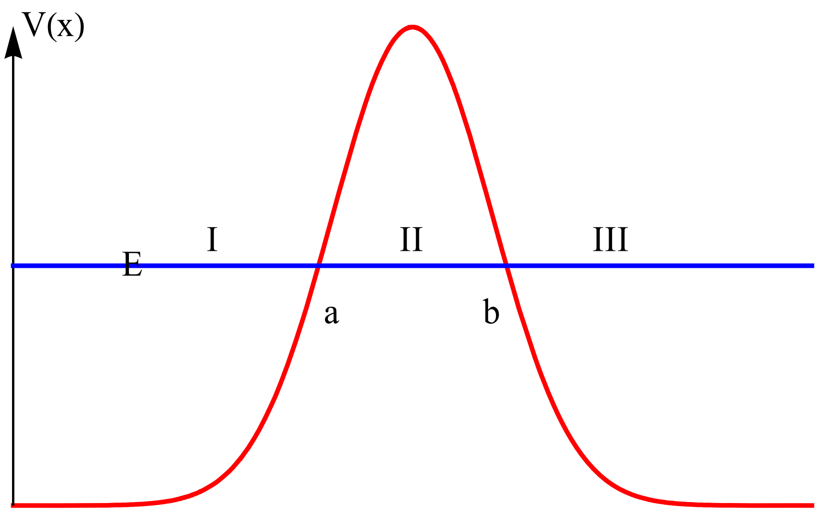


Fig. The connection formula I (upward) is used at $x = a$ and the connection formula II (downward) is used at $x = b$.

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

$$k_1(x) = \sqrt{\frac{2m}{\hbar^2}(\varepsilon - V(x))} \qquad \text{for } x>b$$

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

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

$$\Downarrow \qquad \text{(II, downward)}$$

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

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

$$\begin{aligned}\psi_{II} &= \frac{A}{2\sqrt{\kappa(x)}} \exp[-\int_a^b \kappa(x)dx + \int_a^x \kappa(x)dx] - \frac{iA}{\sqrt{\kappa(x)}} \exp[\int_a^b \kappa(x)dx - \int_a^x \kappa(x)dx] \\ &= \frac{-iA}{\sqrt{\kappa(x)}} \frac{1}{r} \exp[-\int_a^x \kappa(x)dx] + \frac{A}{\sqrt{\kappa(x)}} \frac{r}{2} \exp[\int_a^x \kappa(x)dx]\end{aligned}$$

where

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}[V(x) - \varepsilon]}, \qquad \text{for } a<x<b$$

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.

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

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

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

Here we get

$$C=-iA\frac{1}{r},$$

$$D=\frac{A}{2}r.$$

$$k_2(x)=\sqrt{\frac{2m}{\hbar^2}[\varepsilon-V(x)]} \qquad \text{for } x<a$$

Then we have the wave function of the region I,

$$\begin{aligned}
\psi_I &= \frac{-2iA}{\sqrt{k_2(x)}}\frac{1}{r}\cos[\int_x^a k_2(x)dx-\frac{\pi}{4}] \\
&\quad -\frac{A}{2\sqrt{k_2(x)}}r\sin[\int_x^a k_2(x)dx-\frac{\pi}{4}] \\
&= \frac{-iA}{\sqrt{k_2(x)}}\frac{1}{r}\{\exp[i(\int_x^a k_2(x)dx-\frac{\pi}{4})]+\exp[-i(\int_x^a k_2(x)dx-\frac{\pi}{4})]\} \\
&\quad +\frac{A}{\sqrt{k_2(x)}}\frac{ir}{4}\{\exp[i(\int_x^a k_2(x)dx-\frac{\pi}{4})]-\exp[-i(\int_x^a k_2(x)dx-\frac{\pi}{4})]\}
\end{aligned}$$

or

$$\begin{aligned}
\psi_I &= \frac{iA}{\sqrt{k_2(x)}}\{(\frac{r}{4}-\frac{1}{r})\exp[i(\int_x^a k_2(x)dx-\frac{\pi}{4})]-(\frac{r}{4}+\frac{1}{r})\exp[-i(\int_x^a k_2(x)dx-\frac{\pi}{4})]\} \\
&= \frac{-iA}{\sqrt{k_2(x)}}\{(\frac{1}{r}-\frac{r}{4})\exp[-i(\int_a^x k_2(x)dx+\frac{\pi}{4})]+(\frac{1}{r}+\frac{r}{4}))\exp[i(\int_a^x k_2(x)dx+\frac{\pi}{4})]\}
\end{aligned}$$

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

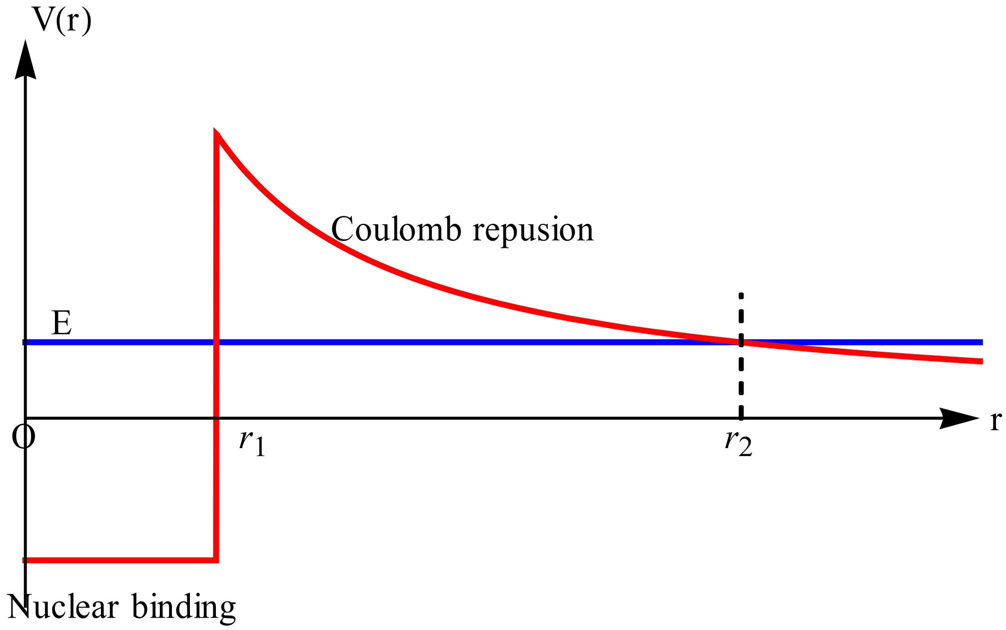


Fig. Gamov's model for the potential energy of an alpha particle in a radioactive nucleus.

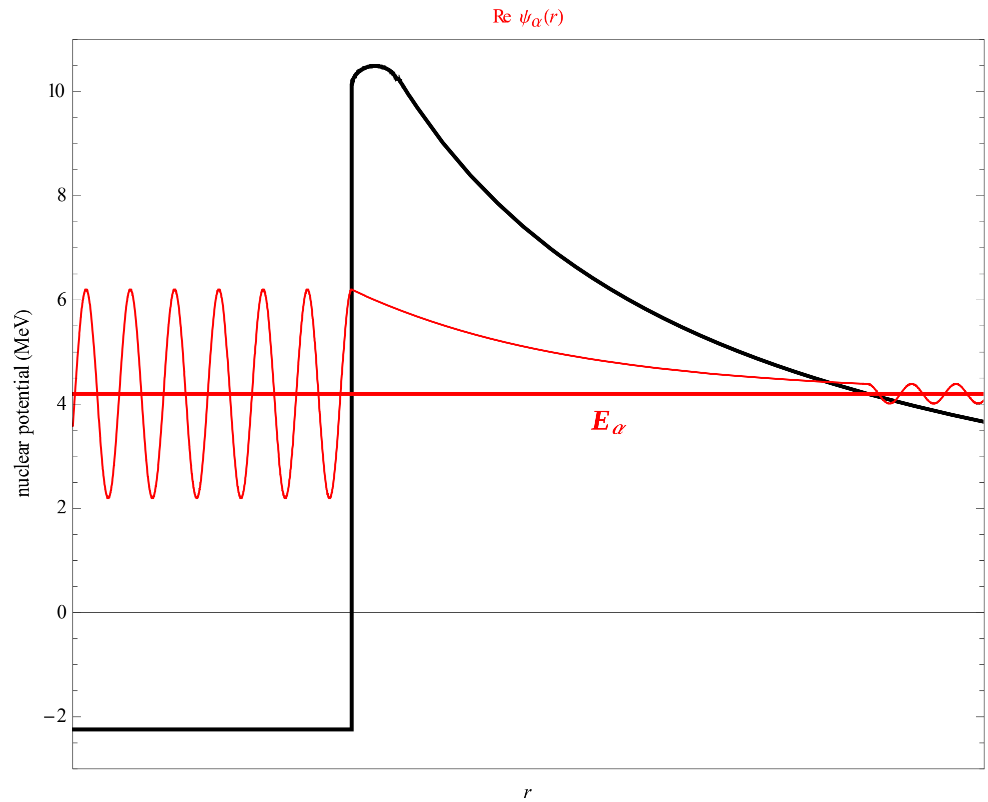


Fig. The tunneling of a particle from the ^{238}U ($Z = 92$). The kinetic energy 4.2 MeV. http://demonstrations.wolfram.com/GamowModelForAlphaDecayTheGeigerNuttallLaw/

For $r_1<r<r_2$.

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

At $r = r_2$,

$$\varepsilon=\frac{2Z_1e^2}{4\pi\varepsilon_0 r_2}.$$

The tunneling probability is

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

where

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

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

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

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

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

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 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_α = 4.001506179 u, we get

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

(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:

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

((**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 == (2 Z1 qe^2)/(4 π ϵ0 r) //. rule1
```

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

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

6.30842×10^{-14}

```
r2/fm /. rule1
```

63.0842

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

1.42318×10^{7}

```
γ = Sqrt[2 Ma K1]/ℏ (r2 ArcCos[Sqrt[r1/r2]] - Sqrt[r1 (r2 - r1)]) //.
  rule1
```

51.8796

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

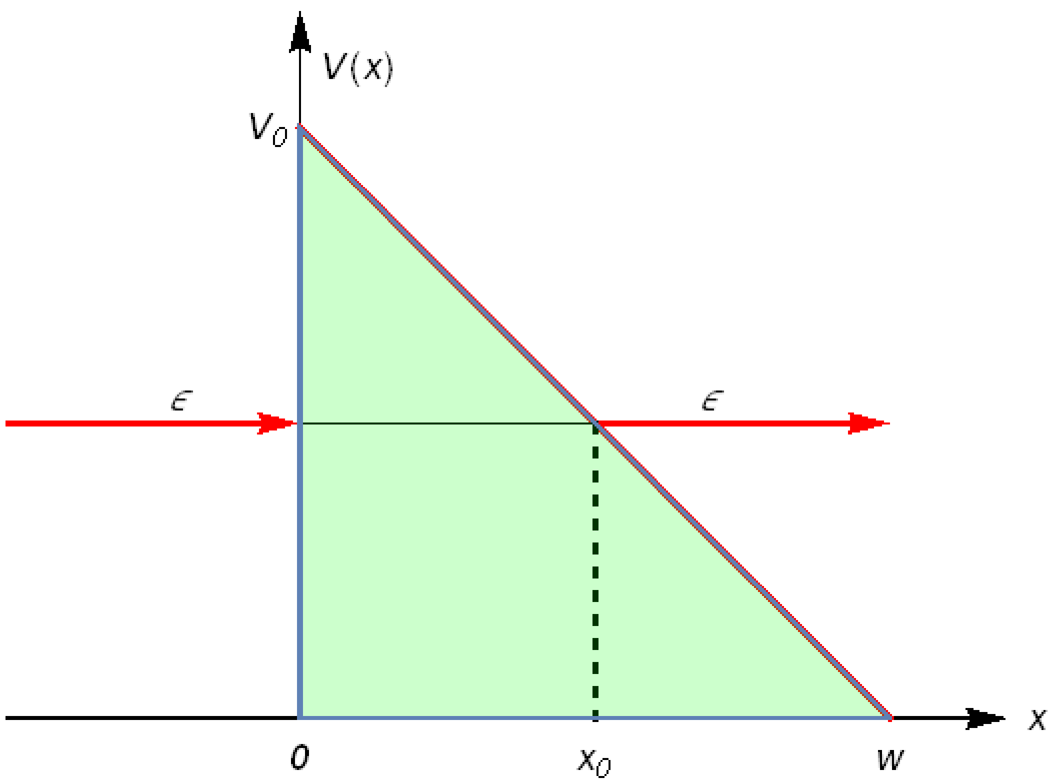
8.81282×10^{-25}

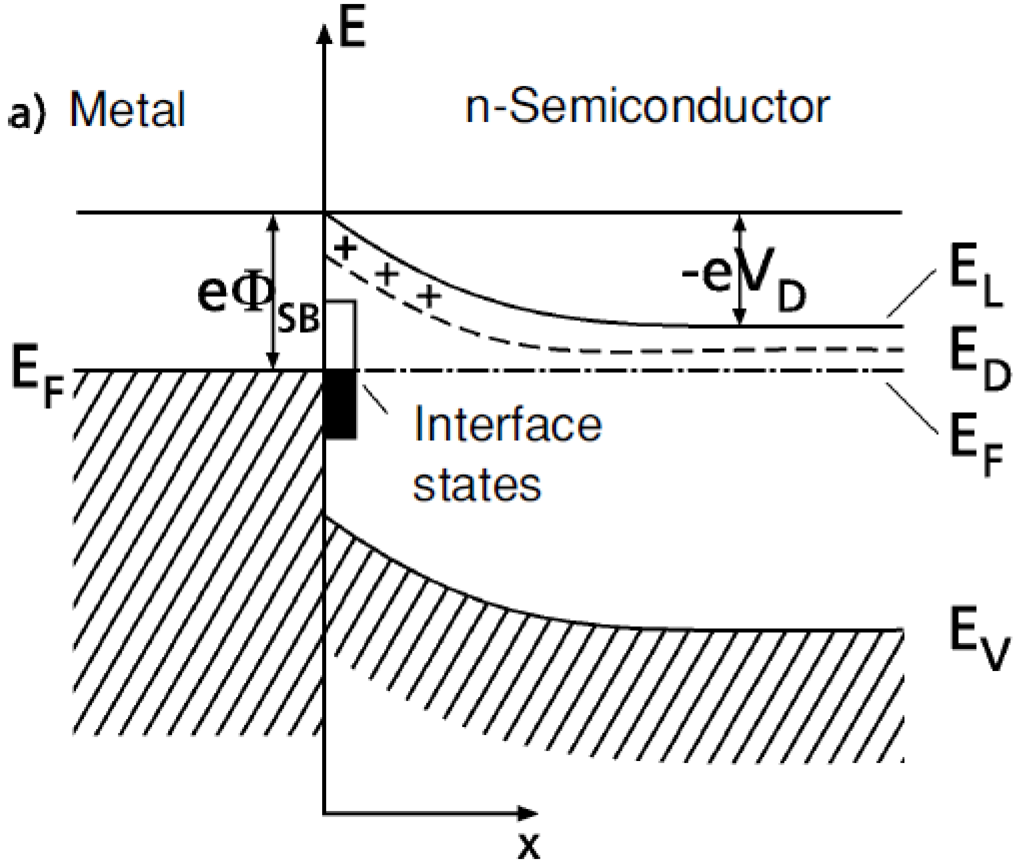
10. Schottky barrier

We consider the Schottky barrier which exists on the junction between a metal surface and a n-typed semiconductor surface. The form of the potential energy $V(x)$ for an electron can be determined from a Poisson equation with appropriate boundary condition. The parabolic form for $V(x)$ is expected. For simplicity, here, we assume that $V(x)$ has a triangular form given by

$$V(x) = V_0(1 - \frac{x}{w})$$

where w is the width of the depletion layer in the Schottky barrier (see a Fig. below)




E
a) Metal
n-Semiconductor
eΦSB
-eVD
EL
EF
ED
Interface
states
EF
EV
x

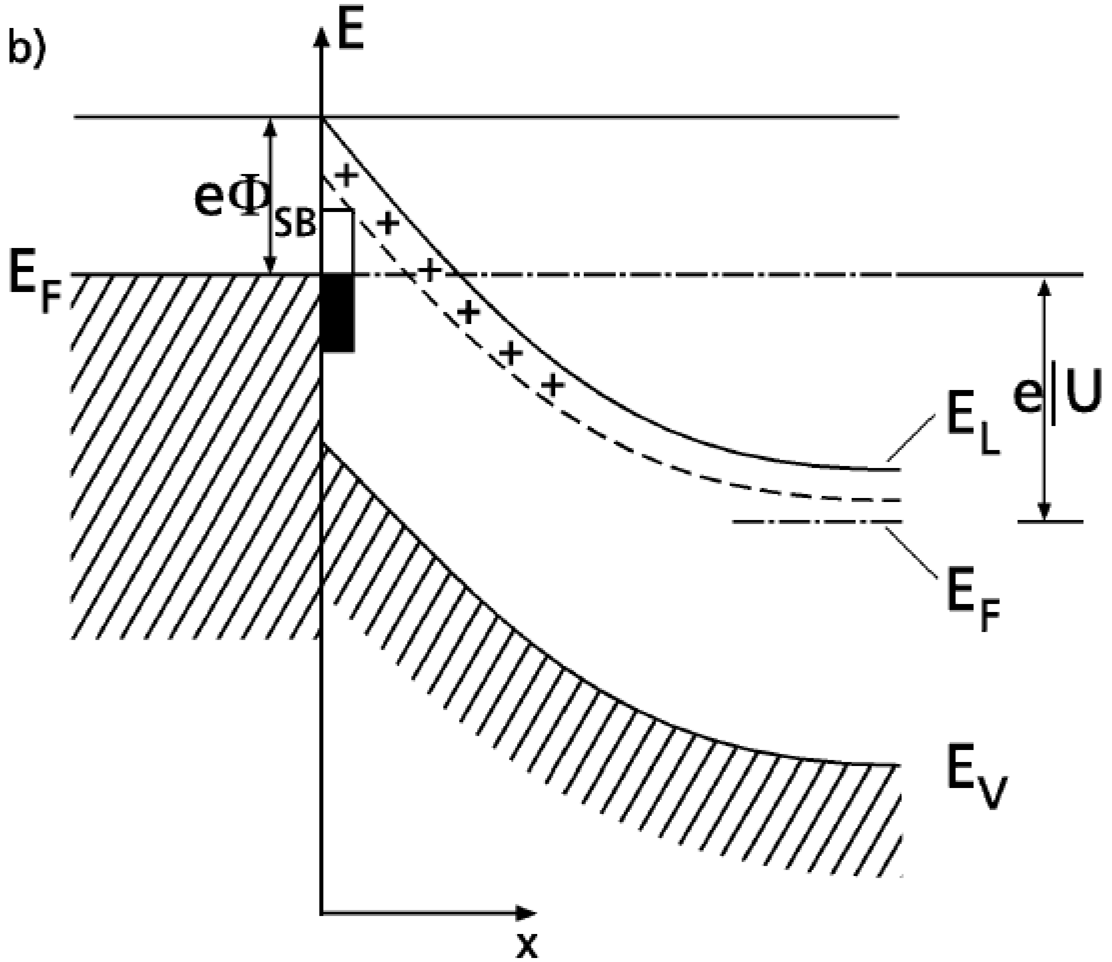


Fig. Electronic band scheme of a metal/semiconductor (n-doped) junction: pinning of the Fermi-level E_F in interface states near the neutrality level causes the formation of a Schottky-barrier $e\phi_{SB}$ and a depletion space charge layer within the semiconductor. VD is the built-in diffusion voltage. (a) In thermal equilibrium, (b) under external bias U.

When $V(x) = \varepsilon$, we have the value of x0

$$x = x_0 = w(1 - \frac{\varepsilon}{V_0})$$

where ε is the energy of electron with a mass m. The transition probability can be expressed by

$$T = \exp[-2\int_0^{x_0} \kappa(x)dx]$$

where

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}[V(x) - \varepsilon]} \qquad \text{for } 0 < x < x_0 .$$

Using the Mathematica we calculate the integral as

$$\begin{aligned}\int_0^{x_0} \kappa(x)dx &= \int_0^{x_0} \sqrt{\frac{2m}{\hbar^2}[V(x) - \varepsilon]}dx \\ &= \sqrt{\frac{2m}{\hbar^2}} \int_0^{x_0} \sqrt{V_0 - \varepsilon - V_0 \frac{x}{w}}dx \\ &= \sqrt{\frac{2m}{\hbar^2}} \frac{2(V_0 - \varepsilon)^{3/2}}{3V_0} w\end{aligned}$$

where $V(x) = V_0(1 - \frac{x}{w})$. Then we have

$$T(\varepsilon) = \exp[-\sqrt{\frac{2m}{\hbar^2}} \frac{4(V_0 - \varepsilon)^{3/2}}{3V_0} w]$$

Suppose that ε=0.

$$T(\varepsilon = 0) = \exp[-\frac{4}{3}\sqrt{\frac{2mV_0}{\hbar^2}} w]$$

or

$$T(\varepsilon = 0) = \exp[-6.83089\sqrt{V_0(eV)}w(nm)]$$

when V_0 = 0.7 eV,

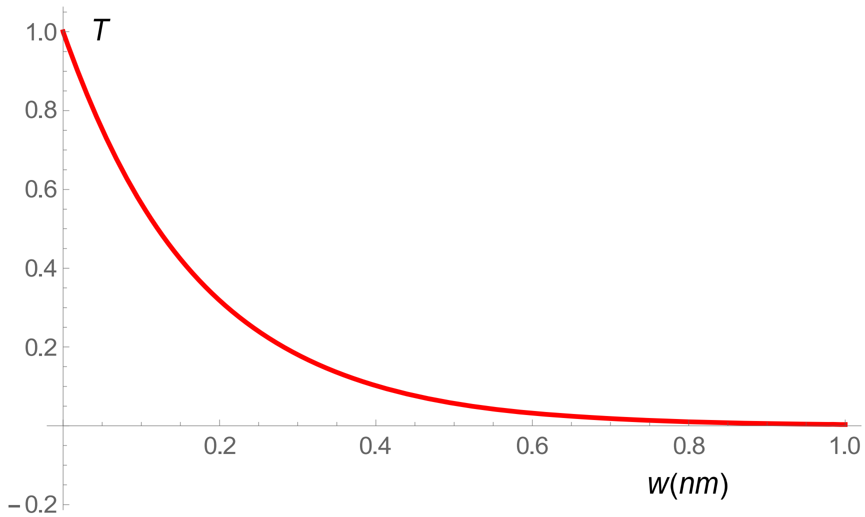
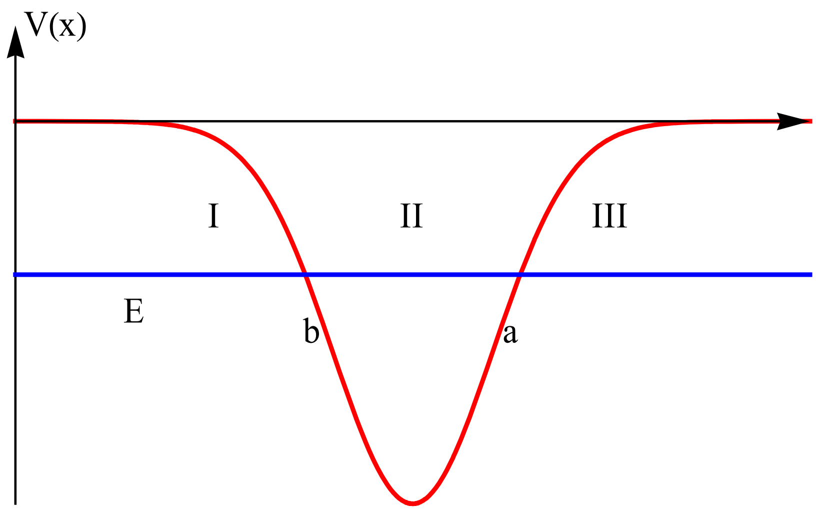


Fig. Transition probability T as a function of the width of the depletion layer. V0 = 0.7 eV. 1nm = 10 Å

9. Bound state: Bohr-Sommerfeld condition.



For $x<b$ (region I), the un-normalized 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

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

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

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

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

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

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

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

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

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

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

$$\oint p(x)dx = (n+\frac{1}{2})2\pi\hbar = (n+\frac{1}{2})h.$$

$\oint$ is an area inside the trajectory of the particle in the phase space.

10. Eample-1 (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

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

11. Example-2: linear potential

We consider a particle moving in 1D potential of the form

$$V(x) = \beta|x|$$

$$p(x) = \sqrt{2m(\varepsilon - \beta|x|)}$$

$$x_0 = \frac{\varepsilon}{\beta}.$$

$$\int_{-x0}^{x_0} p(x)dx = 2\int_0^{x_0} p(x)dx = (n_{odd} + \frac{1}{2})\pi\hbar$$

or

$$2\int_0^{x_0} \sqrt{2m(\varepsilon - \beta|x|)}dx = 2\int_0^{x_0} \sqrt{2m(\beta x_0 - \beta x)}dx$$

$$= 2\sqrt{2m\beta}\int_0^{x_0} \sqrt{x_0 - x}dx$$

$$= 2\sqrt{2m\beta}\frac{2}{3}x_0^{3/2}$$

or

$$2\sqrt{2m\beta}\frac{2}{3}x_0^{3/2} = (n_{odd} + \frac{1}{2})\pi\hbar .$$

because of the odd parity states. Then we get the energy as

$$\varepsilon = [\frac{3\beta}{4}(\frac{\hbar^2}{2m})^{1/2}(n_{odd} + \frac{1}{2})\pi]^{2/3}$$

When $\beta = mg$

$$\varepsilon = (\frac{3}{4}\pi)^{2/3}(n_{odd} + \frac{1}{2})^{2/3}\frac{1}{(2m)^{1/3}}(mg\hbar)^{2/3}$$

$$= p_n(\frac{mg^2\hbar^2}{2})^{1/3}$$

We now calculate the value

$$p_n = (\frac{3}{4}\pi)^{2/3}(2n - 1 + \frac{1}{2})^{2/3} = (\frac{3}{2}\pi)^{2/3}(n - \frac{1}{4})^{2/3},$$

where n_{odd}= $2n$ -1 (n = 1, 2, 3, 4,…),

and

$$-z_n$$

for n = 1, 2, 3,….. Note that z_n is the n-th zero points of the Airy function $A_i(z)$ with odd parity. The value of z_n can be obtained from the exact solution of the Schrödinger equation. The value pm is obtained from the WKB approximation. It is surprising that in spite of the approximation, the value of p_n is so close to that of -z_n

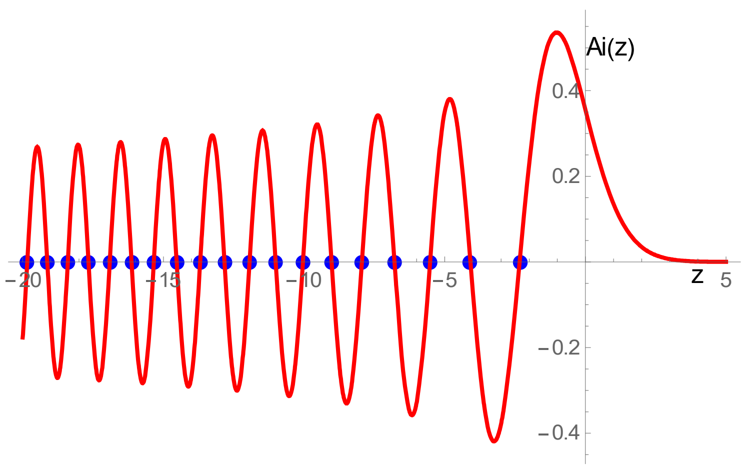


Fig. The Airyfunction Ai(z). The values of z at which Ai(z) becomes zero are denoted by blue circles. $z = z_n$.

Table

n	p_n	$-z_n$
1.	2.32025	2.33811
2.	4.08181	4.08795
3.	5.51716	5.52056
4.	6.78445	6.78671
5.	7.94249	7.94413
6.	9.02137	9.02265
7.	10.0391	10.0402
8.	11.0077	11.0085
9.	11.9353	11.936
10.	12.8281	12.8288
11.	13.6909	13.6915
12.	14.5273	14.5278
13.	15.3403	15.3408
14.	16.1323	16.1327
15.	16.9053	16.9056
16.	17.661	17.6613
17.	18.4008	18.4011
18.	19.1261	19.1264
19.	19.8379	19.8381
20.	20.5371	20.5373
21.	21.2246	21.2248
22.	21.9012	21.9014
23.	22.5674	22.5676
24.	23.224	23.2242
25.	23.8714	23.8716
26.	24.5101	24.5103
27.	25.1407	25.1408
28.	25.7634	25.7635
29.	26.3787	26.3788
30.	26.9868	26.987

31.	27.5883	27.5884
32.	28.1832	28.1833
33.	28.7719	28.772
34.	29.3546	29.3548
35.	29.9316	29.9318
36.	30.5032	30.5033
37.	31.0694	31.0695
38.	31.6305	31.6306
39.	32.1866	32.1867
40.	32.738	32.7381
41.	33.2848	33.2849
42.	33.8271	33.8272
43.	34.3651	34.3652
44.	34.899	34.8991
45.	35.4288	35.4289
46.	35.9546	35.9547
47.	36.4767	36.4767
48.	36.995	36.9951
49.	37.5097	37.5098
50.	38.0209	38.021

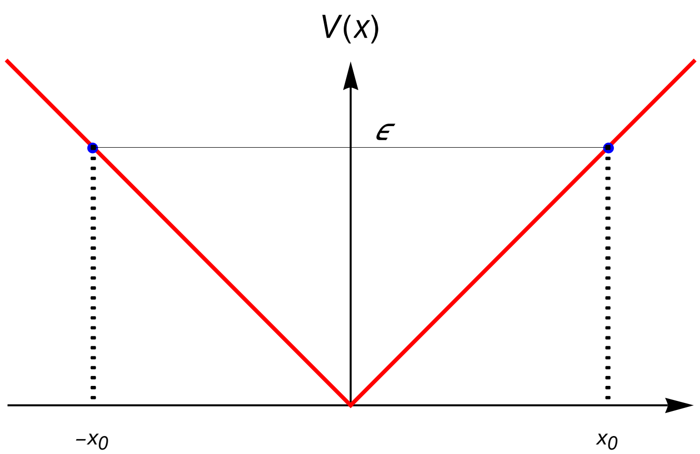


Fig. The potential energy $V(x) = \beta|x|$. $x_0 = \dfrac{\varepsilon}{\beta}$. Because of the symmetric potential, the wave function should have either the even parity or the odd parity.

((Note)) Solution with the even parity

$$\varepsilon = (\frac{3}{4}\pi)^{2/3}(n_{even} + \frac{1}{2})^{2/3}\frac{1}{(2m)^{1/3}}(mg\hbar)^{2/3}$$
$$= q_n(\frac{mg^2\hbar^2}{2})^{1/3}$$

where $n_{even} = 2n$ $(n = 0, 1, 2, 3,\ldots)$,

$$q_n = (\frac{3}{4}\pi)^{2/3}(2n + \frac{1}{2})^{2/3}$$

Note that q_n is nearly equal to $-y_n$, where the derivative of the Airy function Ai(z) with respect to z, becomes zero at $z = y_n$.

n	q_n	$-y_n$
0	1.11546	1.01879
1	3.26163	3,2482
2	4.82632	4.8201
3	6.16713	6.16331
4	7.37485	7.37218
5	8.49051	8.48849
6	9.53705	9.53545
7	10.529	10.5277
8	11.4762	11.4751
9	12.3857	12.3848
10	13.263	13.2622

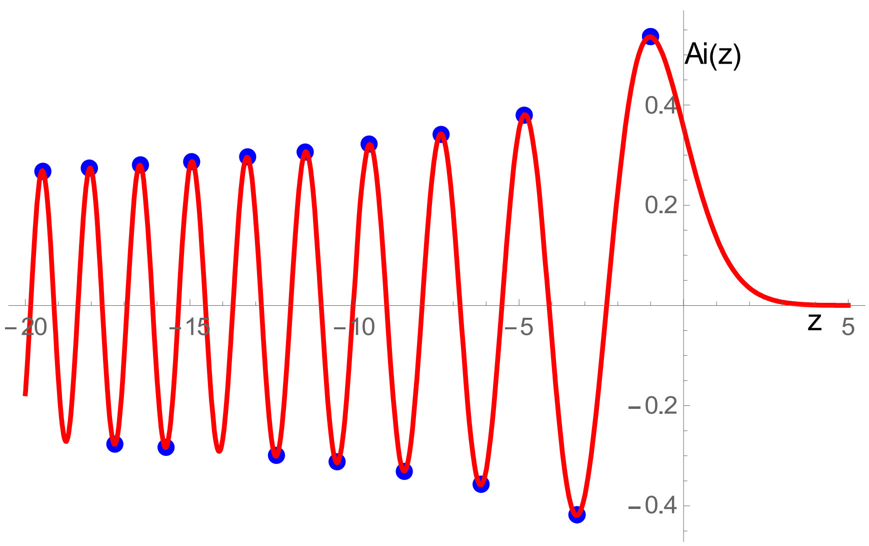
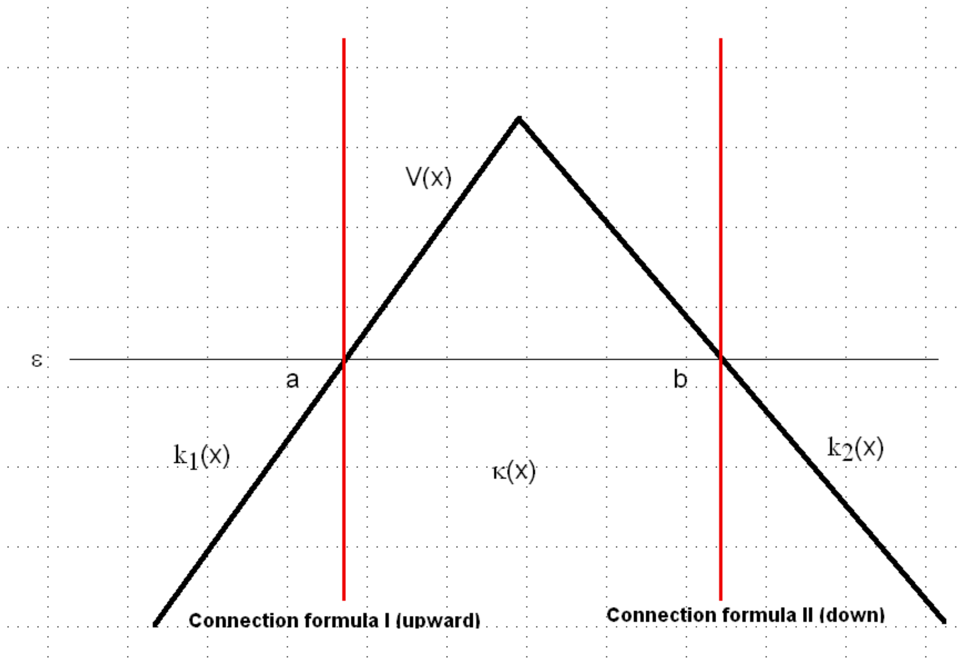


Fig. The Airyfunction Ai(z). The values of z at which the derivative of Ai(z) with respect to z becomes zero are denoted by blue circles. $z = y_n$.

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)

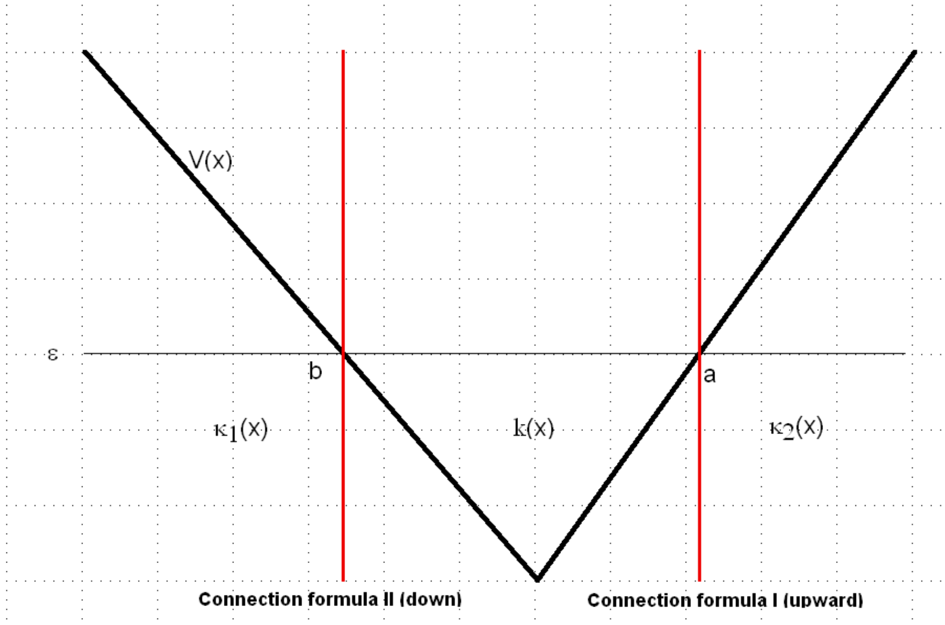
$$\frac{2A}{\sqrt{k_1(x)}}\cos(\int_x^a k_1(x)dx - \frac{\pi}{4}) - \frac{B}{\sqrt{k_1(x)}}\sin(\int_x^a k_1(x)dx - \frac{\pi}{4})]$$
$$\Downarrow$$
$$\frac{A}{\sqrt{\kappa(x)}}\exp(-\int_a^x \kappa(x)dx) + \frac{B}{\sqrt{\kappa(x)}}\exp(\int_a^x \kappa(x)dx)]$$

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 $x = a$

$$\frac{2A}{\sqrt{k(x)}}\cos[\int_x^a k(x)dx - \frac{\pi}{4}] - \frac{B}{\sqrt{k(x)}}\sin[\int_x^a k(x)dx - \frac{\pi}{4}]$$
$$\Downarrow$$
$$\frac{A}{\sqrt{\kappa_2(x)}}\exp[-\int_a^x \kappa_2(x)dx] + \frac{B}{\sqrt{\kappa_2(x)}}\exp[\int_a^x \kappa_2(x)dx]$$

formula I (upward)