(2)

WKB approximation.

Consider the one-dimensional Schrödinger equation

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

For a free particle, $V(x) = \text{constant} = V_0$ and the solution of Eq. (1) is of the form

$$\psi(x) = e^{\pm i p_0 x/\hbar} \quad \cdots\cdots (2)$$

where

$$p_0 = \sqrt{2m(E - V_0)} = \text{constant}. \quad \cdots\cdots (3)$$

This suggests that when $V(x)$ is slowly varying, we try a solution of the form

$$\psi(x) = e^{iS(x)/\hbar} \quad \cdots\cdots (4)$$

$$\therefore \quad \frac{d\psi(x)}{dx} = \frac{i}{\hbar}\frac{dS(x)}{dx}\, e^{iS(x)/\hbar} \quad \cdots\cdots (5)$$

$$\frac{d^2\psi(x)}{dx^2} = \frac{i}{\hbar}\frac{d^2S}{dx^2}\, e^{iS(x)/\hbar} - \frac{1}{\hbar^2}\left(\frac{dS}{dx}\right)^2 e^{iS(x)/\hbar} \quad \cdots (6)$$

Substituting (4) and (6) in Eq. (1) we obtain

$$\frac{i}{\hbar}\frac{d^2S}{dx^2} - \frac{1}{\hbar^2}\left(\frac{dS}{dx}\right)^2 + \frac{2m}{\hbar^2}(E - V(x)) = 0$$

or, multiplying by $-\hbar^2$, we get

$$\left(\frac{ds}{dx}\right)^2 - i\hbar\frac{d^2s}{dx^2} - 2m\left(E - V(x)\right) = 0.$$

Defining

$$p(x) = \sqrt{2m\left(E - V(x)\right)} \quad \cdots\cdots (7)$$

the above equation can be written as

$$\left(\frac{ds}{dx}\right)^2 = p^2(x) + i\hbar\frac{d^2s}{dx^2} \quad \cdots\cdots (8)$$

Note that for a free particle $\frac{d^2s}{dx^2} = 0$, since $S = \text{const} \times x$. This suggests that for a slowly varying potential $\frac{d^2s}{dx^2}$ is small. Thus we may set up a successive approximation scheme for solving Eq. (8). The zeroth order, i.e., the dominant term of $S(x)$ is obtained by setting the second term on the right hand side of Eq. (8) to zero, i.e., by setting $\hbar = 0$. The correction to $S(x)$ is of the order of $\hbar$. Thus we write $S(x)$ as a series involving successive higher powers of $\hbar$:

$$S(x) = S_0(x) + \frac{\hbar}{i} S_1(x) + \left(\frac{\hbar}{i}\right)^2 S_2(x) + \cdots \qquad (9)$$

The WKB approximation consists of retaining only the first two terms of Eq. (9), i.e.,

$$S_{WKB}(x) \cong S_0(x) + \frac{\hbar}{i} S_1(x) \quad \cdots \cdots (10)$$

The WKB approximation is also called semi classical approximation. If we did set $\hbar = 0$, i.e., if we took $S(x) = S_0(x)$ we would have the classical limit of the quantum mechanical problem. However, we retain terms which are linear in $\hbar$, neglecting terms of higher orders in $\hbar$. In this sense, the WKB approximation is semiclassical.

Next, we substitute Eq. (9) in Eq. (8) and equate the coefficients of equal powers of $\hbar$ on both sides of the resulting equation. We obtain

Zeroth order in $\hbar$

$$\left(\frac{dS_0(x)}{dx}\right)^2 = p^2(x) \qquad (11)$$

First-order in $\hbar$

$$\frac{2\hbar}{i}\frac{dS_0}{dx}\cdot\frac{dS_1}{dx} = i\hbar\frac{d^2S_0}{dx^2}$$

or

$$\frac{d^2S_0}{dx^2} + 2\frac{dS_0}{dx}\frac{dS_1}{dx} = 0 \qquad \text{- - - - - -} (12).$$

From Eq. (11) we obtain

$$S_0(x) = \pm\int^x p(x')dx'. \qquad (13)$$

Substituting (13) in (12) we can now solve for $S_1(x)$.
First, we rewrite (12) in the form

$$\frac{dS_1}{dx} = -\frac{1}{2}\frac{S_0''(x)}{S_0'(x)}$$

where the prime means derivative with respect to x.
Integrating the above equation we get

$$S_1(x) = -\frac{1}{2}\ln|S_0'(x)| + \ln C \qquad (14)$$

where C is an arbitrary constant. We can cast

Eq. (14) in the form

$$S_1(x) = \ln \frac{c}{\sqrt{|S_0'(x)|}} \qquad \text{.......... (14a)}$$

Since we have

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

from Eq. (13), we can write Eq. (14a) as

$$S_1(x) = \ln \frac{c}{\sqrt{|p(x)|}} \,. \qquad (15)$$

The wavefunction in the WKB approximation can now be written as

$$\psi_{WKB}(x) = e^{\frac{i}{\hbar}\left(S_0(x) + \frac{\hbar}{i} S_1(x)\right)}$$

$$= e^{\frac{i}{\hbar} S_0(x) + S_1(x)}$$

or

$$\psi_{WKB}(x) = \frac{c}{\sqrt{|p(x)|}}\, e^{\pm \frac{i}{\hbar}\int^{x} p(x')\,dx'} \qquad \text{..... (16)}$$

Thus there are two linearly independent WKB wavefunctions. They are

$$\psi_+(x) = \frac{1}{\sqrt{|p(x)|}}\, e^{+\frac{i}{\hbar}\int^x p(x')\,dx'} \qquad (17)$$

$$\psi_-(x) = \frac{1}{\sqrt{|p(x)|}}\, e^{-\frac{i}{\hbar}\int^x p(x')\,dx'} \qquad (18)$$

A general solution of the Schrödinger equation in the WKB approximation is a linear combination of $\psi_+(x)$ and $\psi_-(x)$.

Validity of WKB approximation.

The WKB approximation consists of treating the second term on the right hand side of Eq. (8) to be small:

$$\left| i\hbar \frac{d^2 S}{dx^2} \right| << |p^2(x)|. \quad \text{------} \quad (19)$$

Since $S(x) = S_0(x) + O(\hbar)$, the above equation can be written approximately as

$$\left| i\hbar \frac{d^2 S_0}{dx^2} \right| + O(\hbar^2) << |p^2(x)| \quad \text{-----} \quad (20)$$

Since

$$S_0(x) = \pm \int^x p(x')dx'$$

we have

$$\frac{dS_0(x)}{dx} = \pm p(x)$$

Therefore, Eq. (20) can be written as

$$\left| \hbar \frac{dp(x)}{dx} \right| << |p^2(x)| \quad (\text{up to first order in } \hbar)$$

or

$$\hbar \left| \frac{1}{p(x)} \frac{dp(x)}{dx} \right| << |p(x)| . \quad (21)$$

Now, introducing the 'wavelength' $\lambda(x)$ as

$$\lambda(x) = \frac{h}{p(x)} = \frac{2\pi\hbar}{p(x)}$$

Eq. (21) can be written as

$$\hbar \frac{|\lambda(x)|}{2\pi\hbar} \left|\frac{dp(x)}{dx}\right| << |p(x)|$$

or,

$$|\lambda(x)| \left|\frac{dp(x)}{dx}\right| << 2\pi |p(x)| \quad \cdots\cdots (22)$$

The left hand side of this equation is the ~~fractional~~ change of $|p(x)|$ within the distance $|\lambda(x)|$, i.e.,

$$|\Delta p(x)| = |\lambda(x)| \left|\frac{dp(x)}{dx}\right|.$$

Therefore Eq. (22) is written as

$$|\Delta p(x)| << 2\pi |p(x)|$$

or

$$\frac{1}{|p(x)|} |\Delta p(x)| << 2\pi \quad \cdots\cdots (23)$$

i.e., the fractional change of $|p(x)|$ within the distance $|\lambda(x)|$ must be small.

We can also write Eq. (22) as

$$\left|\frac{d\lambda(x)}{dx}\right| << 2\pi . \qquad (24)$$

Therefore, the change of $|\lambda(x)|$ within the distance $|\lambda(x)|$ is

$$|\Delta\lambda(x)| = |\lambda(x)|\left|\frac{d\lambda(x)}{dx}\right| .$$

Hence we write Eq. (24) as

$$\left|\frac{\Delta\lambda(x)}{\lambda(x)}\right| << 2\pi \qquad (25)$$

i.e., fractional change of $|\lambda(x)|$ is also very small.

Now, we have shown that the WKB approximation to the wave function can be written as

$$\psi_{WKB}(x) = \frac{C}{\sqrt{|P(x)|}} e^{\pm\frac{i}{\hbar}\int^{x} P(x')dx'}$$

The condition that $|P(x)|$ changes slowly implies that both amplitude $A(x) \propto \frac{1}{\sqrt{|P(x)|}}$ and the 'wavelength' $|\lambda(x)|$ changes slowly.

Connection formulas

The WKB solutions given in Eqs. (17) and (18) break down near classical turning points. At a turning point $E = V(x)$, therefore $p(x) = 0$, and the WKB solutions become infinity.

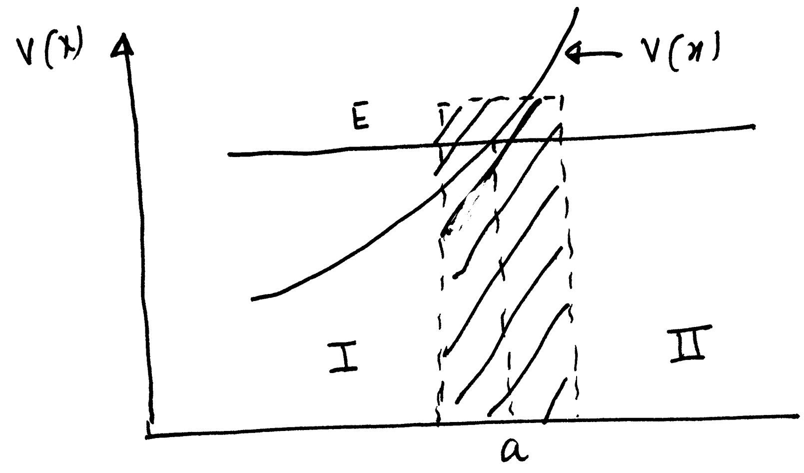


Figure 1

The figure shows a turning point at $x = a$. We have considered the case in which $V(x)$ is increasing at the turning point. In region I, i.e., to the far left of the turning point, $E > V(x)$, $p(x)$ is real and positive and the WKB solution is oscillatory. In region I we can write the WKB wavefunction in the form

$$\psi_{I,\,WKB}(x) = \frac{A_1}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_x^a p(x')dx' + \pi/4\right]$$

$$+ \frac{A_2}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' + \pi/4\right] \qquad (26)$$

where A_1 and A_2 are arbitrary constants. The phase $\pi/4$ is chosen purely for convenience as we will see later.

Next, to the far right of the turning point, i.e., in region II, we have $E < V(x)$, therefore $p(x)$ is purely imaginary. In this region we have

$$p(x) = \sqrt{2m(E - V(x))} = i\sqrt{2m(V(x) - E)}$$

$$= i\,|p(x)|\,.$$

The WKB wavefunction in this region is exponential. We write

$$\psi_{\text{II},WKB}(x) = \frac{B_1}{\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar}\int_a^x |p(x)|\,dx\right]$$

$$+ \frac{B_2}{\sqrt{|p(x)|}} \exp\left[+\frac{1}{\hbar}\int_a^x |p(x)|\,dx\right] \qquad (27)$$

Since Eqs. (26) and (27) are expressions of the same wavefunctions in different regions, the constants (A_1, A_2) and (B_1, B_2) cannot be arbitrarily chosen. This is because there must be a connection between the WKB solutions in regions I and II.

In order to discover this connection, we must follow the variation of the wavefunction from region I to region II. In doing so it is necessary to pass through the hatched region in figure 1 where the WKB solution is not valid. In order to find the behaviour of $\psi(x)$ in this region, we make a linear approximation of the potential and solve the Schrödinger equation exactly.

This 'exact' solution when extrapolated to regions I and II will resemble the WKB solution there and hence will provide a link between the WKB solutions in region I and region II.

To find a solution near the turning point a, we assume $V(x)$ to be linear near a. So we can write

$$V(x) = V(a) + \left(\frac{\partial V}{\partial x}\right)_{x=a} (x-a)$$

or

$$V(x) = V(a) + A(x-a) \quad \cdots\cdots (28)$$

where A is the slope of $V(x)$ at A. For the case under consideration $V(x)$ is rising at $x = a$ and so A is a positive number. With this linear approximation for $V(x)$, the Schrödinger equation near the turning point becomes

$$\frac{d^2\psi(x)}{dx^2} - \frac{2mA}{\hbar^2}(x-a)\,\psi(x) = 0. \qquad (29)$$

Now, making the change of variable

$$z = \left(\frac{2mA}{\hbar^2}\right)^{1/3}(x-a) \qquad (30)$$

the equation transforms to

$$\frac{d^2\psi}{dz^2} - z\psi = 0. \qquad (31)$$

This equation is standard in mathematical physics. The solutions are known as Airy functions and are given by the following integral formulas:

$$Ai(z) = \frac{1}{\pi}\int_0^\infty \cos(s^3/3 + sz)\,ds, \qquad (32)$$

and

$$Bi(z) = \frac{1}{\pi}\int_0^\infty \left[\exp(-s^3/3 - sz) + \sin(s^3/3 + sz)\right]ds.$$

$$\cdots (33)$$

We are only interested in the asymptotic forms of the Airy functions. Defining

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

the asymptotic forms are

$$\begin{aligned} Ai(z) &\underset{z\to\infty}{\sim} \frac{1}{2\sqrt{\pi}} z^{-1/4} \exp(-\xi) \\ &\underset{z\to-\infty}{\sim} \frac{1}{\sqrt{\pi}} |z|^{-1/4} \sin(\xi + \pi/4) \end{aligned} \tag{34}$$

and

$$\begin{aligned} Bi(z) &\underset{z\to\infty}{\sim} \frac{1}{\sqrt{\pi}} z^{-1/4} \exp(\xi) \\ &\underset{z\to-\infty}{\sim} \frac{1}{\sqrt{\pi}} \cos(\xi + \pi/4) . \end{aligned} \tag{35}$$

In figure 2 below, we have plotted Airy functions of both types. Both $Ai(z)$ and $Bi(z)$ are oscillatory for negative z, while for positive z, $Ai(z)$ is exponentially falling and $Bi(z)$ is exponentially rising.

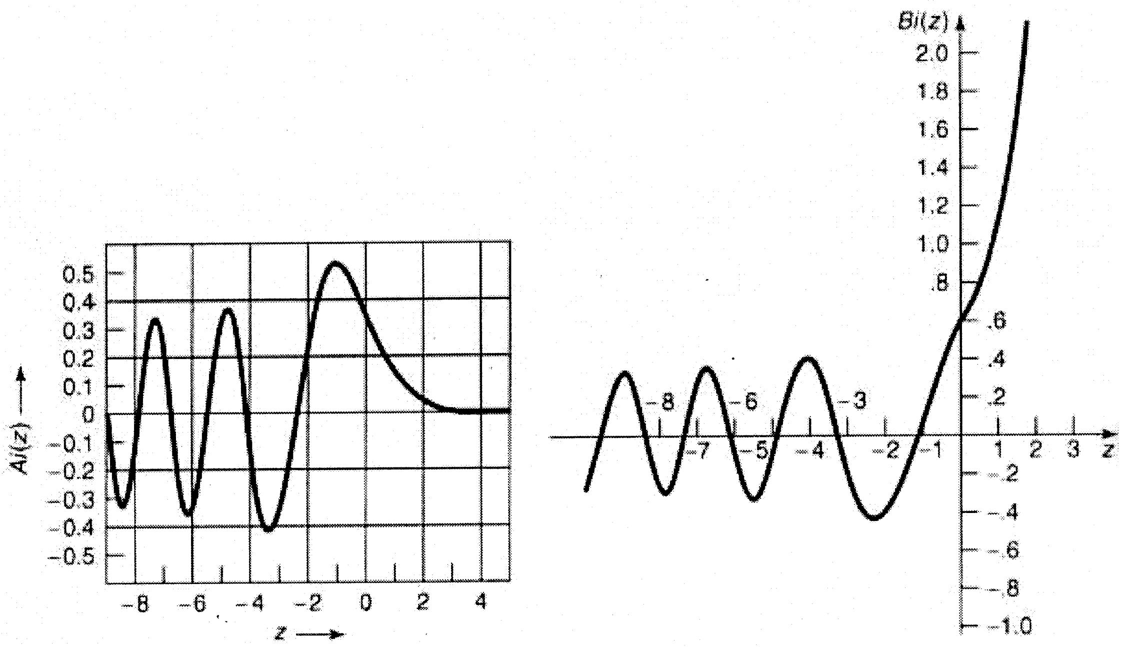


Figure 2 - Airy functions, of both types.

Now, to the left of the turning point, z is negative and

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

is positive (figure 1). Furthermore,

$$\frac{1}{\hbar}\int_x^a p(x)\,dx = \frac{1}{\hbar}\int_x^a \sqrt{2m(E - V(x))}\,dx$$

$$= \frac{\sqrt{2mA}}{\hbar}\int_x^a (a-x)^{1/2}\,dx$$

$V(x) = E + A(x-a)$

$\therefore\ E - V(x) = -A(x-a)$

$= A(a-x)$

$(+ve)$

$$= \frac{\sqrt{2mA}}{\hbar}\cdot\frac{2}{3}(a-x)^{3/2}$$

$$= \frac{2}{3}\sqrt{\frac{2mA}{\hbar^2}}\,(a-x)^{3/2}$$

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

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

$$= \xi .$$

i.e.,

$$\frac{1}{\hbar}\int_x^a p(x)\,dx = \xi \quad \cdots\cdots (36)$$

To the left of the turning point we also have

$$|z|^{-1/4} = \left(\frac{2mA}{\hbar^2}\right)^{-1/12} (a-x)^{-1/4} .$$

But

$$p(x) = \sqrt{2m(E-V(x))} = (2mA)^{1/2}(a-x)^{-1/2}$$

Therefore

$$|z|^{-1/4} = \frac{\alpha}{\sqrt{p(x)}} \quad \cdots\cdots\cdots (37)$$

where α is a constant which can be determined.

Similarly, we see from figure 1 that to the right of the turning point, z is positive and $p(x)$ is ~~po~~ purely imaginary

$$p(x) = i\,|p(x)| = i\sqrt{2m(V(x)-E)} .$$

Proceeding exactly as we did in case of $x < a$, we can show that for $x > a$

$$\frac{1}{\hbar}\int_a^x |p(x)|\,dx = \xi \quad \cdots\cdots\cdots (38)$$

and

$$z^{-1/4} = \frac{\alpha}{\sqrt{|p(x)|}} \quad \text{-------} \quad (39)$$

Thus, the asymptotic forms of $Ai(z)$ and $Bi(z)$ can be written as

$$Ai(z) \underset{z\to-\infty}{\sim} \frac{1}{\sqrt{\pi}} \frac{\alpha}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_x^a p(x)\,dx + \pi/4\right]$$

$$\underset{z\to\infty}{\sim} \frac{1}{2\sqrt{\pi}} \frac{\alpha}{\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar}\int_a^x |p(x)|\,dx\right] \qquad (40)$$

and

$$Bi(z) \underset{z\to-\infty}{\sim} \frac{1}{\sqrt{\pi}} \frac{\alpha}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x)\,dx + \frac{\pi}{4}\right]$$

$$\underset{z\to\infty}{\sim} \frac{1}{\sqrt{\pi}} \frac{\alpha}{\sqrt{|p(x)|}} \exp\left[\frac{1}{\hbar}\int_a^x |p(x)|\,dx\right]. \qquad (41)$$

From Eqs. (40) and (41), the connection formulas between the WKB wavefunctions in regions I and II are apparent. If the wavefunction near the turning point is $Ai(z)$, it goes over to oscillatory sine function (first of Eq. (40)) to the left of the turning point, and to the right of the turning point $Ai(z)$ goes over into an exponentially decaying function (the second of Eq. (40)). Hence the sine function in region I matches with the exponentially decaying function in region II.

Similarly, if we take $Bi(z)$ as the solution near the turning point, we can deduce from Eq. (41) that cosine function in region I matches with the exponentially rising function in region II.

To be specific, the connection formulas are:

$$\frac{1}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_x^a p(x)dx + \pi/4\right] \Longleftarrow\!\longrightarrow \frac{1}{2\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar}\int_a^x |p(x)|dx\right] \quad (a)$$

$$\frac{1}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x)dx + \pi/4\right] \longleftarrow\!\Longrightarrow \frac{1}{\sqrt{|p(x)|}} \exp\left[\frac{1}{\hbar}\int_a^x |p(x)|dx\right] \quad (b)$$

$$\cdots (42)$$

For these connection formulas to be valid, V(x) should be a rising function through the turning point, as shown in figure 1. Referring to Eqs. (26) and (27) we must therefore have

$$B_1 = \frac{A_1}{2} \text{ and } B_2 = A_2 .$$

Using the same procedure, we can obtain the connection formulas when the potential is falling at the turning point as shown in the figure below

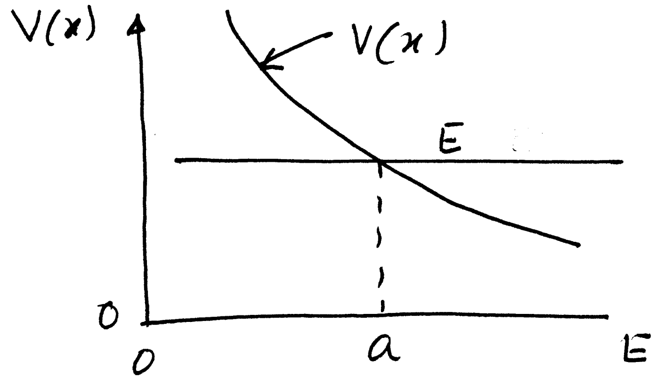


Figure 3: Turning point at $x = a$ where V is falling.

We have

$$\frac{1}{\sqrt{|P(x)|}} \exp\left[-\frac{1}{\hbar}\int_x^a |P(x)|dx\right] \longleftrightarrow\!\!\!> \frac{2}{\sqrt{P(x)}} \sin\left[\frac{1}{\hbar}\int_a^x P(x)dx + \pi/4\right] \quad (a)$$

$$\frac{1}{\sqrt{|P(x)|}} \exp\left[\frac{1}{\hbar}\int_x^a |P(x)|dx\right] <\!\!\!\longleftrightarrow \frac{1}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar}\int_a^x P(x)dx + \pi/4\right]. \quad (b)$$

$$\cdots (43)$$

Caution must be applied in the use of the connection formulas. Referring to figure 1 and Eq. (42), suppose that the wavefunction is adequately represented to the far right by an increasing potential (Eq. 42b). It is then in general not legitimate to infer that the wavefunction is given by the oscillatory cosine function $\frac{1}{\sqrt{p}} \cos\left[\frac{1}{\hbar}\int_x^a p(x)dx + \pi/4\right]$ to the far left. After all, an admixture of decreasing exponential would be considered negligible to the far right of the turning point, although it might, according to Eq. (42a) contribute an appreciable amount of the oscillatory sine function $\frac{1}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_x^a p(x)dx + \pi/4\right]$ to the wavefunction on the left.

Conversely, a minute admixture of $\frac{1}{\sqrt{p}} \cos\left[\frac{1}{\hbar}\int_x^a p(x)dx + \pi/4\right]$ to $\frac{1}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_x^a p(x)dx + \pi/4\right]$ on the left might be negligible there, but might lead to a very appreciable exponentially increasing portion to the right.

Thus, we see that unless we have assured ourselves properly of the absence of the other linearly independent component in the wavefunction, connection formulas are to be used only in the direction of the double arrows if considerable error is to be avoided.

Application to bound state problems

The WKB approximation can be applied to derive an equation for energies of bound states. Consider a simple well-shaped potential with two classical turning points as shown in figure 4 below.

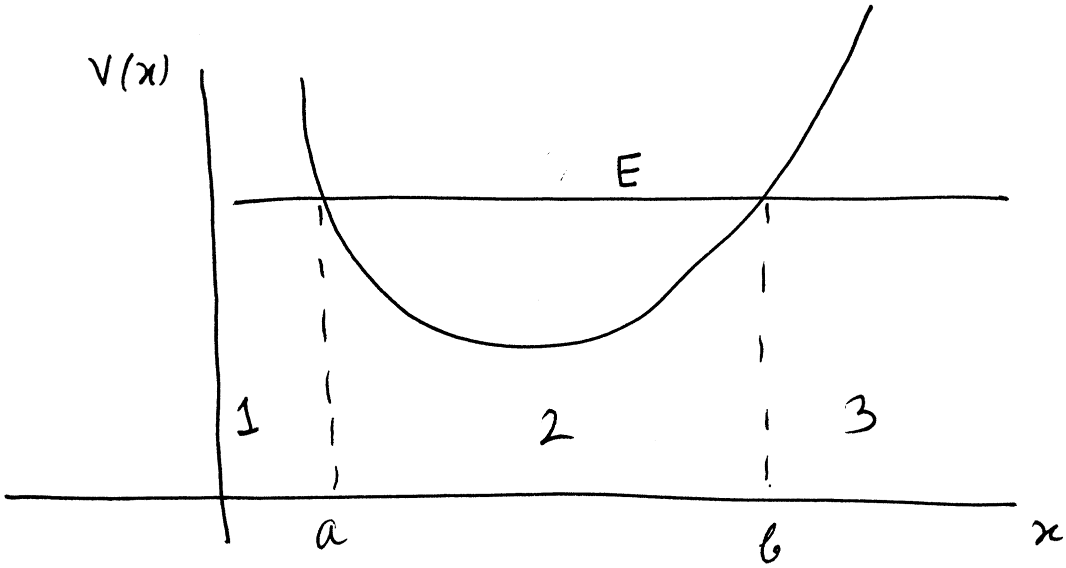


Fig. 4 A potential well.

The WKB approximation will be used in regions 1, 2 and 3 away from the turning points and connection formulas would serve near $x = a$ and $x = b$. The usual requirement that $\psi(x)$ must be finite dictates that solutions which increase exponentially as one moves outwards from the turning points must vanish rigorously.

In region 1, i.e., $x < a$, the wavefunction is exponentially decaying, i.e.,

$$\psi_1(x) = \frac{A}{\sqrt{|k(x)|}} \exp\left[-\int_x^a |k(x)|\,dx\right] \quad (1)$$

where we have used the wave ~~vector~~ number

$$k(x) = \frac{p(x)}{\hbar}.$$

Using the connection formulas, the wavefunction in region 2 is

$$\psi_2(x) = A\frac{2}{\sqrt{k(x)}} \sin\left[\int_a^x k(x)\,dx + \pi/4\right]$$

$$= \frac{2A}{\sqrt{k(x)}} \sin\left[\int_a^b k(x)\,dx - \int_x^b k(x)\,dx + \pi/4\right]$$

$$= \frac{2A}{\sqrt{k(x)}} \cos\left[\int_a^b k(x)\,dx - \int_x^b k(x)\,dx - \pi/4\right]$$

$\because \sin\theta = \cos(\theta - \pi/2)$

$$= \frac{2A}{\sqrt{k(x)}} \cos\left[\theta - \int_x^b k(x)\,dx - \pi/4\right] \quad (2)$$

where we have defined

$$\theta = \int_a^b k(x)\,dx .$$

Note that θ is a positive number. We can now expand Eq. (2) to get

$$\psi_2(x) = \frac{2A}{\sqrt{k(x)}} \cos\theta \cos\left[\int_x^b k(x)\,dx + \pi/4\right]$$

$$+ \frac{2A}{\sqrt{k(x)}} \sin\theta \sin\left[\int_x^b k(x)\,dx + \pi/4\right] \qquad (3).$$

Now, in region 3, the wavefunction is exponentially decreasing. But the $\cos\left[\int_x^b k(x)\,dx + \pi/4\right]$ term in ψ_2 goes over to an exponentially increasing function in region 3. Hence the term in ψ_2 which involves the cosine function must be made exactly zero.

We therefore put

$$\cos\theta = 0$$

i.e.,

$$\theta = \left(n + \tfrac{1}{2}\right)\pi \; ; \quad n = 0, 1, 2, \ldots$$

i.e.,

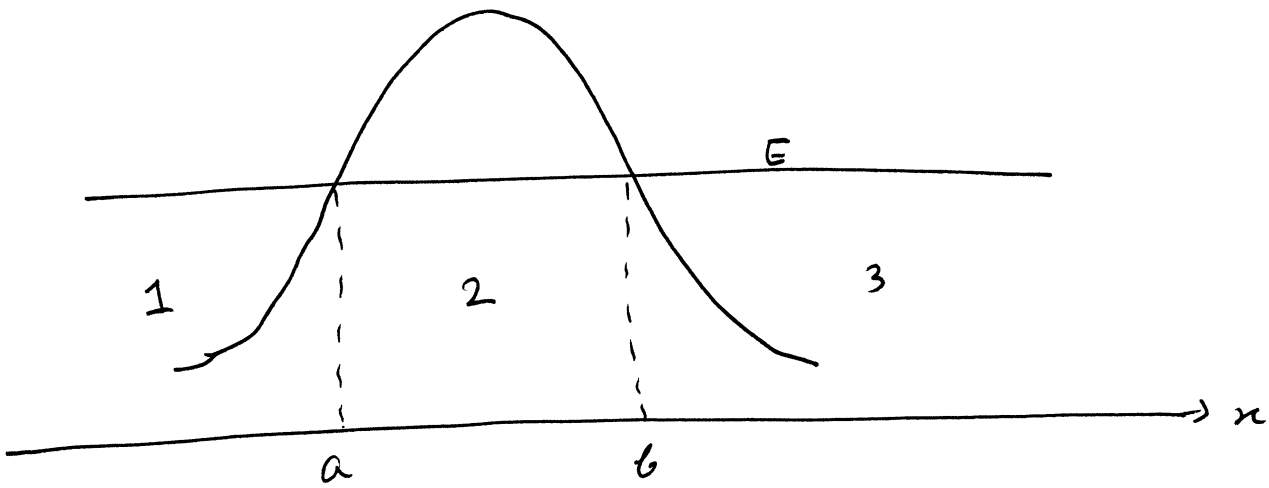
$$\boxed{\int_a^b k(x)\,dx = \left(n + \tfrac{1}{2}\right)\pi \; ; \quad n = 0, 1, 2, \ldots} \qquad (4)$$

In terms of $p(x)$ we can write

$$\int_a^b p(x)\,dx = \left(n + \tfrac{1}{2}\right)\pi\hbar \; ; \quad n = 0, 1, 2, \ldots \qquad (5)$$

Equations (4) & (5) are called Bohr-Sommerfeld quantization condition. Using this we can find the energy of the bound states of a particle in a potential well.

Transmission through a barrier



We assume that the particle is incident on the barrier from the left. In region 3, i.e., $x > b$, we have only the transmitted wave, so, the wavefunction in this region is of the form

$$\psi_3(x) = \frac{A}{\sqrt{k(x)}} \exp\left[i \int_b^x k(x)\,dx + \pi/4 \right] \qquad (1)$$

where A is a constant and the phase factor $\pi/4$ has been included to facilitate the application of the connection formulas. In terms of trigonometric functions, Eq. (1) can be written as

$$\psi_3(x) = \frac{A}{\sqrt{k(x)}}\left[\cos\left(\int_b^x k(x)dx + \pi/4\right) + i\sin\left(\int_b^x k(x)dx + \pi/4\right)\right] \tag{2}$$

Using the connection formulas, the WKB wavefunction in region 2 is

$$\psi_2(x) = \frac{A}{\sqrt{|k(x)|}}\left[\exp\left(\int_x^b |k(x)|dx\right) + \frac{i}{2}\exp\left(-\int_x^b |k(x)|dx\right)\right] \tag{3}$$

In order to find the appropriate wavefunction in region 1, we rewrite the integrals in the last expression using

$$\int_x^b |k(x)|dx = \int_a^b |k(x)|dx - \int_a^x |k(x)|dx. \tag{4}$$

Thus,

$$\psi_2(x) = \frac{A}{\sqrt{|k(x)|}}\left[\exp\left(\int_a^b |k(x)|dx\right)\exp\left(-\int_a^x |k(x)|dx\right)\right.$$
$$\left.+ \frac{i}{2}\exp\left(-\int_a^b |k(x)|dx\right)\exp\left(\int_a^x |k(x)|dx\right)\right]. \tag{5}$$

Using the connection formulas across the turning point a, we can now write the WKB wavefunction in region 1. We have

$$\psi_1(x) = \frac{A}{\sqrt{k(x)}}\left[\exp\left(\int_a^b |k(x)|dx\right).\, 2\sin\left(\int_x^a k(x)dx + \pi/4\right)\right.$$
$$\left. + \frac{i}{2}\exp\left(-\int_a^b |k(x)|dx\right)\cos\left(\int_x^a k(x)dx + \pi/4\right)\right] \quad (6)$$

Let

$$\theta = \exp\left(-\int_a^b |k(x)|dx\right). \quad \cdots\cdots \quad (7)$$

Therefore,

$$\psi_1(x) = \frac{A}{\sqrt{k(x)}}\left[2\theta^{-1}\sin\left(\int_x^a k(x)dx + \pi/4\right)\right.$$
$$\left. + \frac{i}{2}\theta\cos\left(\int_x^a k(x)dx + \pi/4\right)\right] \quad (8)$$

We now express $\psi_1(x)$ in terms of exponential functions using the identities

$$\sin\alpha = \frac{e^{i\alpha} - e^{-i\alpha}}{2i}$$

$$\cos\alpha = \frac{e^{i\alpha} + e^{-i\alpha}}{2}.$$

We get

$$\psi_1(x) = \frac{A}{i\sqrt{k(x)}} \left\{ \left(\theta^{-1} - \frac{\theta}{4}\right) \exp\left[i\left(\int_x^a k(x)dx + \pi/4 \right)\right] - \left(\theta^{-1} + \frac{\theta}{4}\right) \exp\left[-i\left(\int_x^a k(x)dx + \pi/4 \right)\right] \right\}. \tag{9}$$

The first term of this equation is identified with the reflected wave and the second term is identified with the incident wave.

Now, the incident flux is

$$S_i = \frac{|A|^2}{k(x)} \left(\theta^{-1} + \frac{\theta}{4}\right)^2 \frac{\hbar k(x)}{m}$$

or

$$S_i = |A|^2 \left(\theta^{-1} + \frac{\theta}{4}\right)^2 \frac{\hbar}{m} \quad \cdots\cdots (10).$$

The transmitted flux is obtained from $\psi_3(x)$ given in Eq. (1). We have

$$S_t = \frac{|A|^2}{k(x)} \frac{\hbar k(x)}{m} = |A|^2 \frac{\hbar}{m}. \quad \cdots\cdots (11)$$

Thus, the transmission probability is

$$T = \frac{\text{transmitted flux}}{\text{Incident flux}} = \frac{S_t}{S_i}$$

or

$$\boxed{T = \frac{1}{\left(\theta^{-1} + \frac{\theta}{4}\right)^2}} \quad \cdots\cdots (12)$$

We can rewrite T in the form

$$T = \left(\frac{\theta}{1 + \theta^2/4}\right)^2 .$$

Now,
$$\theta = \exp\left[-\int_a^b |k(x)|\,dx\right]$$
is small, since for WKB approximation to be valid $|k(x)|$ must be large. We can therefore neglect all powers of θ higher than the first, so that

$$T = \theta^2$$

or
$$T = \left[\exp\left(-\int_a^b |k(x)|\,dx\right)\right]^2$$

i.e.,
$$\boxed{T = \exp\left[-2\int_a^b |k(x)|\,dx\right]} \quad \cdots\cdots (13)$$

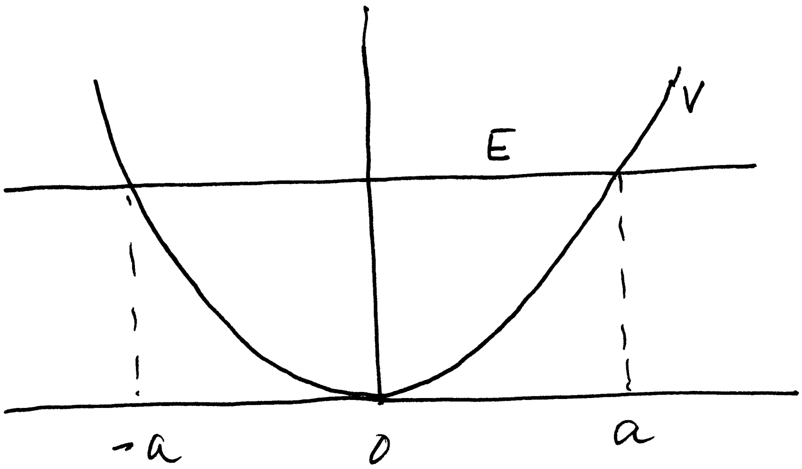
Examples

1. Determine the energy levels of the potential

$$V(x) = \frac{1}{2} m \omega^2 x^2$$

using the WKB method.

Ans.



The turning points are at $x = \pm a$. At the turning points

$$E = \frac{1}{2} m \omega^2 a^2$$

i.e., $$a = \sqrt{\frac{2E}{m\omega^2}} .$$

Now the quantization condition is

$$\int_{-a}^{a} k(x)\, dx = \left(n + \tfrac{1}{2}\right)\pi \, ; \quad n = 0, 1, 2, \ldots \quad (1)$$

where

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

Therefore,

$$\sqrt{\frac{2m}{\hbar^2}} \int_{-a}^{a} \left(E - \frac{1}{2} m \omega^2 x^2\right)^{1/2} dx = \left(n + \frac{1}{2}\right)\pi$$

or $$\sqrt{\frac{2mE}{\hbar^2}} \int_{-a}^{a} \left(1 - \frac{m\omega^2 x^2}{2E}\right)^{1/2} dx = (n + 1/2)\pi$$

or $$\sqrt{\frac{2mE}{\hbar^2}} \int_{-a}^{a} \left(1 - \frac{x^2}{a^2}\right)^{1/2} dx = (n + 1/2)\pi \qquad (2)$$

Now, consider the integral on the left hand side of this equation.

$$I \equiv \int_{-a}^{a} \left(1 - \frac{x^2}{a^2}\right) dx = a \int_{-1}^{+1} (1 - y^2)^{1/2} dy \quad \Big| \; \frac{x}{a} = y$$

$$= a \int_{\pi}^{0} (1 - \cos^2\theta)^{1/2} d(\cos\theta) \qquad \Big| \; y = \cos\theta$$

$$= a \int_{\pi}^{0} \sin\theta \, (-\sin\theta \, d\theta)$$

or $$I = a\int_0^{\pi} \sin^2\theta \, d\theta = a \cdot \frac{1}{2}\int_0^{\pi} (1 - \cos 2\theta)\, d\theta$$

or, $$I = a \cdot \frac{1}{2}\pi$$

i.e., $$I = \pi a/2 .$$

Hence, Eq. (2) becomes

$$\sqrt{\frac{2mE}{\hbar^2}} \cdot \frac{\pi a}{2} = (n + 1/2)\pi$$

or $$\sqrt{\frac{2mE}{\hbar^2}} \cdot \frac{\pi}{2} \cdot \sqrt{\frac{2E}{m\omega^2}} = (n + 1/2)\pi \qquad \Bigg| \quad a = \sqrt{\frac{2E}{m\omega^2}}$$

or $$\frac{2E}{\hbar\omega} \cdot \frac{\pi}{2} = (n + 1/2)\pi$$

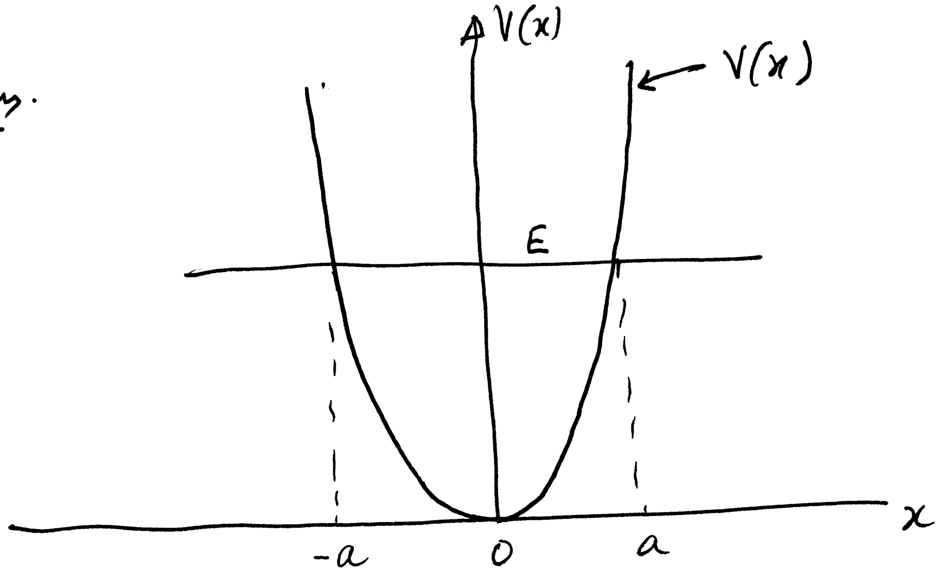
or $$\boxed{E = (n + 1/2)\hbar\omega, \quad n = 0, 1, 2, \cdots .}$$

Ex Determine the energy levels of the potential

$$V(x) = \lambda x^4 \quad (\lambda > 0)$$

using WKB method.

Ans.



The turning points are at $x = \pm a$, where

$$\lambda a^4 = E$$

or

$$a = \left(\frac{E}{\lambda}\right)^{1/4}.$$

Now, the Bohr-Sommerfeld quantization condition is

$$\int_{-a}^{a} k(x)\,dx = (n + 1/2)\pi \;;\; n = 0, 1, 2, \ldots.$$

i.e.,

$$\sqrt{\frac{2mE}{\hbar^2}} \int_{-a}^{a} \sqrt{1 - \frac{\lambda x^4}{E}}\, dx = (n + 1/2)\pi$$

or

$$\sqrt{\frac{2mE}{\hbar^2}} \int_{-a}^{a} \sqrt{1 - \frac{x^4}{a^4}}\, dx = (n + 1/2)\pi. \qquad (1)$$

Let

$$y = \frac{x}{a}.$$

$$\therefore \sqrt{\frac{2mE}{\hbar^2}} \cdot a \int_{-1}^{1} \sqrt{1 - y^4}\, dy = (n + 1/2)\pi$$

or

$$\sqrt{\frac{2mE}{\hbar^2}}\, a\, 2\int_{0}^{1} \sqrt{1 - y^4}\, dy = (n + 1/2)\pi$$

or

$$\sqrt{\frac{2mE}{\hbar^2}} \cdot \left(\frac{E}{\lambda}\right)^{1/4} 2\int_{0}^{1} \sqrt{1 - y^4}\, dy = (n + 1/2)\pi \qquad (2)$$

Now, consider the integral

$$I = \int_{0}^{1} \sqrt{1 - y^4}\, dy$$

Let $y^4 = z$

$$\therefore \quad 4y^3\,dy = dZ$$

or $$dy = \frac{dZ}{4y^3} = \frac{dZ}{4\,Z^{3/4}}$$

Hence

$$I = \frac{1}{4}\int_0^1 (1-Z)^{1/2} Z^{-3/4}\,dZ$$

$$= \frac{1}{4}\int_0^1 Z^{1/4-1}(1-Z)^{3/2-1}\,dZ .$$

Now, the beta function $B(\alpha,\beta)$ is defined by

$$B(\alpha,\beta) = \int_0^1 x^{\alpha-1}(1-x)^{\beta-1}\,dx$$

The β-function is related to the gamma function as

$$B(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} .$$

Some properties of the gamma function are:

$$\Gamma(\alpha+1) = \alpha\,\Gamma(\alpha)$$

$$\Gamma(n) = (n-1)! \quad (n = \text{integer})$$

$$\Gamma(1) = \Gamma(2) = 1$$

$$\Gamma(3/2) = \sqrt{\pi}/2 , \quad \Gamma(1/2) = \sqrt{\pi}$$

In terms of the beta function, the integral I is

$$I = \frac{1}{4} B\left(\frac{1}{4}, \frac{3}{2}\right).$$

Hence Eq (2) becomes

$$\sqrt{\frac{2mE}{\hbar^2}} \left(\frac{E}{\lambda}\right)^{1/4} 2 \cdot \frac{1}{4} B(1/4, 3/2) = (n + 1/2)\pi$$

or

$$\left(\frac{2mE}{\hbar^2}\right)^2 \frac{E}{\lambda} \cdot \frac{1}{16} B^4(1/4, 3/2) = (n + 1/2)^4 \pi^4$$

or

$$E^3 = \frac{16 \lambda \hbar^4 \pi^4}{4 m^2 B^4(1/4, 3/2)} (n + 1/2)^4$$

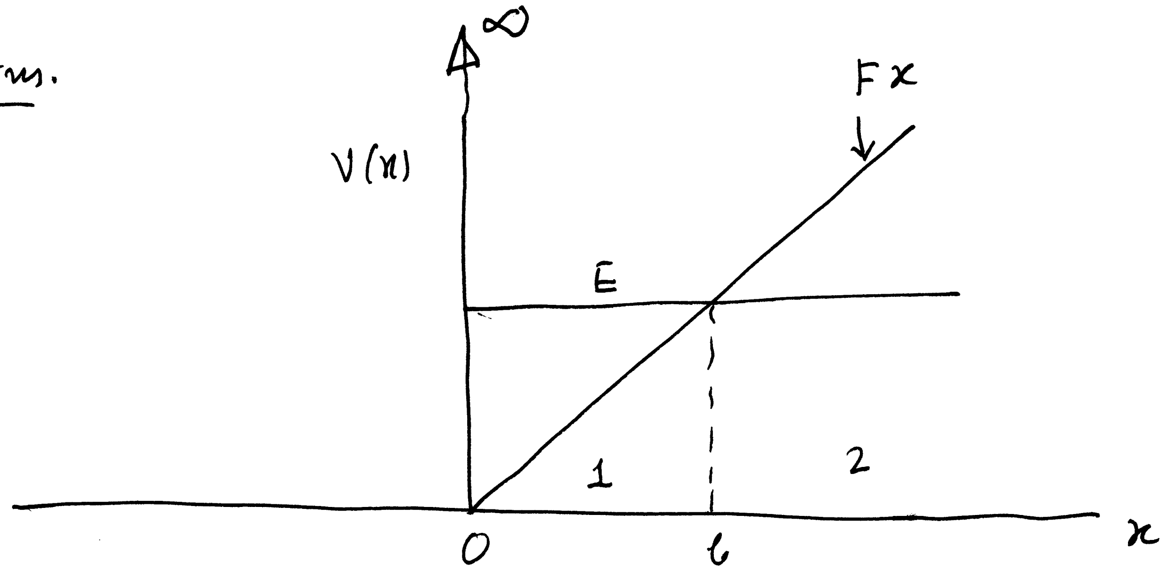
or

$$E = \left[\frac{4 \lambda \hbar^4 \pi^4}{m^2 B^4(1/4, 3/2)}\right]^{1/3} (n + 1/2)^{4/3}; \quad n = 0, 1, 2, \ldots$$

Ex Find the bound state eigenvalues for a particle of mass m in the potential

$$V(x) = \begin{cases} Fx & \text{for } x > 0 \quad (F>0) \\ \infty & \text{for } x \le 0. \end{cases}$$

Ans.



There are two turning points, one at $x=0$ and the other at $x=b$. Since at the turning point $x=0$, V goes to infinity, the wavefunction goes to zero. So the Bohr-Sommerfeld quantization condition has to be modified.

At the turning point $x = b$, we have

$$E = Fb$$

i.e., $\quad b = \dfrac{E}{F}$.

Now, to the far right of the turning point, the wavefunction must be exponentially decaying. Therefore, we can write

$$\psi_2(x) = \frac{A}{\sqrt{|k(x)|}} \exp\left[-\int_b^x |k(x)|\, dx \right].$$

By using the connection formulas, the WKB wavefunction in region 1 can be written as

$$\psi_1(x) = \frac{2A}{\sqrt{k(x)}} \sin\left[\int_x^b k(x)\, dx + \pi/4 \right]$$

Now,

$$\psi_1(x = 0) = 0 .$$

Therefore, we must have

$$\sin\left[\int^{b} k(x)\,dx + \pi/4\right] = 0$$

i.e.,

$$\int_0^b k(x)\,dx + \pi/4 = m\pi \; ; \quad m = 1, 2, 3, \ldots$$

or

$$\int_0^b k(x)\,dx = (m - 1/4)\pi \; ; \quad m = 1, 2, 3, \ldots .$$

We can write this equation as

$$\boxed{\int_0^b k(x)\,dx = (n + 3/4)\pi \; ; \quad n = 0, 1, 2, \ldots .}$$

This is the Bohr-Sommerfeld quantization condition modified for the situation when the wavefunction tends to zero at a turning point.

For our particular problem we have

$$\int_0^b \sqrt{\frac{2m}{\hbar^2}(E - Fx)}\, dx = (n + 3/4)\pi$$

$$\text{or} \quad \sqrt{\frac{2mF}{\hbar^2}} \int_0^b \sqrt{\frac{E}{F} - x}\, dx = (n + 3/4)\pi$$

$$\text{or} \quad \sqrt{\frac{2mF}{\hbar^2}} \int_0^b \sqrt{b - x}\, dx = (n + 3/4)\pi$$

$$\text{or} \quad \sqrt{\frac{2mF}{\hbar^2}}\, \frac{2}{3} \left[- (b - x)^{3/2} \right]_0^b = (n + 3/4)\pi$$

$$\text{or} \quad \sqrt{\frac{2mF}{\hbar^2}} \cdot \frac{2}{3}\, b^{3/2} = (n + 3/4)\pi$$

$$\text{or} \quad \sqrt{\frac{2mF}{\hbar^2}} \cdot \frac{2}{3} \cdot \left(\frac{E}{F}\right)^{3/2} = (n + 3/4)\pi$$

$$\text{or} \quad E^{3/2} = \frac{3\hbar F}{2\sqrt{2m}} (n + 3/4)\pi$$

$$\text{or} \quad \boxed{E^3 = \frac{9\pi^2\hbar^2 F^2}{8m} (n + 3/4)^2 ; \quad n = 0, 1, 2, \ldots}$$

The positive cube root of this equation gives the required eigenvalues.

Example.

Cold emission of electrons from a metal surface in an electric field.

Bransden and Joachain p400

Let us suppose that the electrons in the metal are bound in a square well potential.

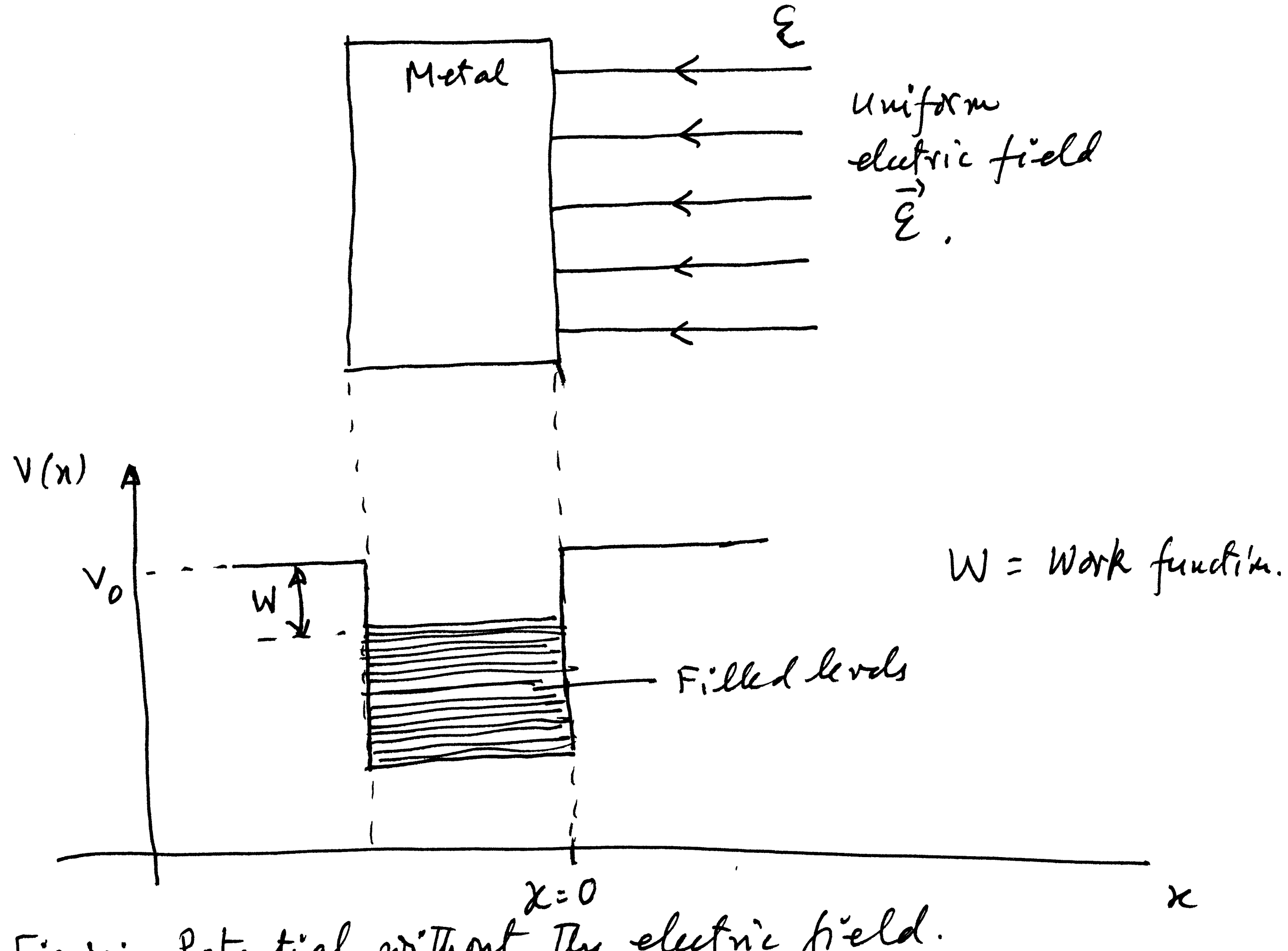


Figure: Potential without the electric field.

Let us impose an electric field $\mathcal{E}$ perpendicular to the metal surface as shown in the first figure. The potential energy function for $x > 0$ is now

$$V(x) = V(x=0) - |\vec{F}|\,x$$

$$= V_0 - e\mathcal{E}x \qquad \Big|\; e = \text{magnitude of charge of an electron. } (+ve)$$

The new potential energy is graphed below:

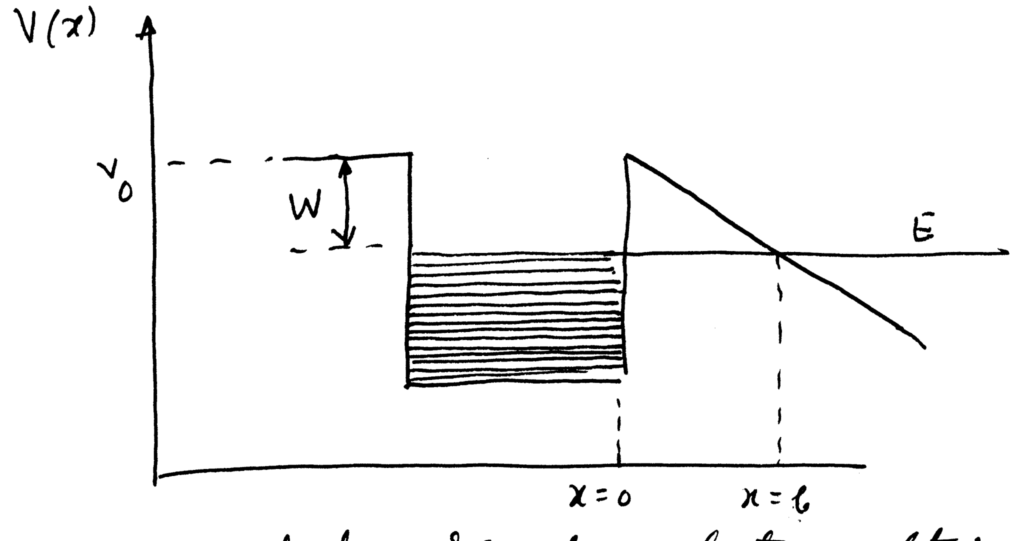


Fig 2: Potential energy of an electron after the electric field is imposed.

Now the potential barrier has a finite width, and the electrons are able to escape. The transmission coefficient for the most energetic electron is

$$T = \exp\left[-2\int_0^b |k(x)|\,dx\right]$$

$$= \exp\left[-2\int_0^b \sqrt{\frac{2m}{\hbar^2}(V(x)-E)}\;dx\right]$$

The turning point at $x = b$ is found from

$$V(x=b) = E$$

i.e

$$V_0 - e\mathcal{E}b = E$$

or

$$V_0 - e\mathcal{E}b = V_0 - W$$

or

$$b = \frac{W}{e\mathcal{E}}.$$

Here W is the work function of the metal. Also,

$$V(x) - E = V_0 - e\mathcal{E}x - E$$

$$= V_0 - e\mathcal{E}x - (V_0 - W)$$

$$= W - e\mathcal{E}x$$

$$\therefore \quad T = \exp\left[-\frac{2}{\hbar}\sqrt{2m} \int_0^{W/e\mathcal{E}} \sqrt{W - e\mathcal{E}x}\, dx \right]$$

i.e.,

$$\boxed{T = \exp\left[-\frac{4}{3}\frac{\sqrt{2m}}{\hbar e \mathcal{E}} W^{3/2} \right]}.$$

This expression, known as the Fowler-Nordheim formula, is in qualitative agreement with experiment.