# 1 WKB Approximation

This approximation method is particularly useful when one is dealing with s-lowly - varying potential. Let's suppose we are interested in solving the 1D TISE:

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

or

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

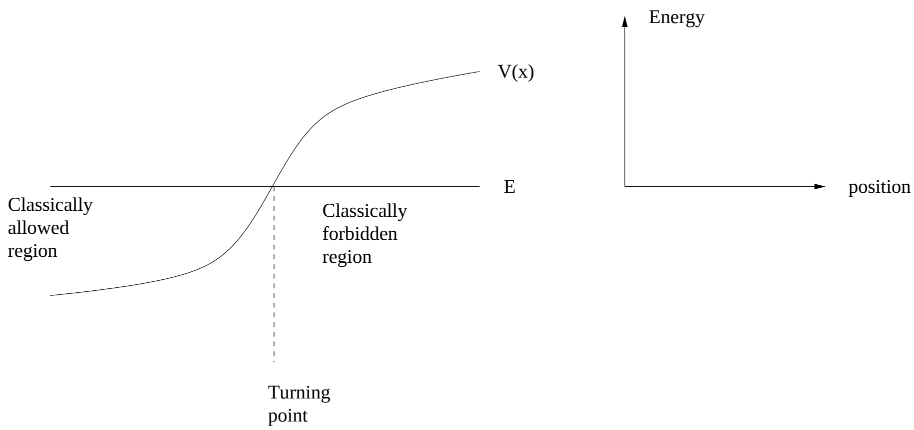


Figure 1: Arbitrary potential

**(A) Classically - allowed region**
In this region

$$\left[E - V(x)\right]\frac{2m}{\hbar^2} = k^2(x) > 0 \tag{3}$$

This suggests that we can write the general solution for $\psi(x)$ in the following form

$$\psi(x) = R(x)e^{iu(x)} \tag{4}$$

Then

$$\frac{d\psi}{dx} = \left[\frac{dR}{dx} + iR(x)\frac{du}{dx}\right]e^{iu(x)} \tag{5}$$

$$\begin{aligned}
\frac{d^2\psi}{dx^2} &= \left[\frac{d^2R}{dx^2} + i\frac{dR}{dx}\frac{du}{dx} + iR(x)\frac{d^2u}{dx^2}\right] e^{iu(x)} \\
&+ \left[\frac{dR}{dx} + iR(x)\frac{du}{dx}\right] i\frac{du}{dx}e^{iu(x)} \\
&= \left[\frac{d^2R}{dx^2} + i2\frac{dR}{dx}\frac{du}{dx} + iR(x)\frac{d^2u}{dx^2} - R(x)\left(\frac{du}{dx}\right)^2\right] e^{iu(x)} \qquad (6)
\end{aligned}$$

Substituting the above result back into the 1D TISE, we get

$$\left[\frac{d^2R}{dx^2} + i2\frac{dR}{dx}\frac{du}{dx} + iR(x)\frac{d^2u}{dx^2} - R(x)\left(\frac{du}{dx}\right)^2 + k^2(x)R(x)\right] e^{iu(x)} = 0 \qquad (7)$$

i.e.,

$$\begin{cases} \dfrac{d^2R}{dx^2} - R(x)\left(\dfrac{du}{dx}\right)^2 + k^2(x)R(x) = 0 & \text{real term} \\ 2\dfrac{dR}{dx}\dfrac{du}{dx} + R(x)\dfrac{d^2u}{dx^2} = 0 & \text{imaginary part} \end{cases} \qquad (8)$$

• Let's consider the imaginary term first:

$$R(x)\frac{d}{dx}\left(\frac{du}{dx}\right) = -2\frac{dR}{dx}\frac{du}{dx} \qquad (9)$$

i.e.,

$$\frac{\frac{d}{dx}\left(\frac{du}{dx}\right)}{\frac{du}{dx}} = -2\frac{\frac{dR}{dx}}{R(x)} \qquad (10)$$

$$\Rightarrow \frac{d\,(du/dx)}{du/dx} = -2\frac{dR}{R} \qquad (11)$$

Integrating the last equation gives

$$\ln\left(\frac{du}{dx}\right) = \ln\left(\frac{C}{R^2(x)}\right) \qquad (12)$$

or

$$\boxed{\frac{du}{dx} = \frac{C}{R^2(x)}} \qquad (13)$$

We now use the result for $du/dx$ in the real term expression to get

$$\frac{d^2R}{dx^2} - R(x)\left[\frac{C}{R^2(x)}\right]^2 + k^2(x)R(x) = 0 \qquad (14)$$

i.e.,

$$\boxed{\frac{d^2R}{dx^2} = R(x)\left\{\left[\frac{C}{R^2(x)}\right]^2 - k^2(x)\right\}} \tag{15}$$

At this point we make the approximation that

$$\frac{d^2R}{dx^2} \approx 0 \tag{16}$$

which leads to

$$\left[\frac{C}{R^2(x)}\right]^2 - k^2(x) = 0 \tag{17}$$

$$\Rightarrow \frac{C}{R^2(x)} = k(x) \tag{18}$$

$$\Rightarrow \boxed{R(x) = \frac{\sqrt{C}}{\sqrt{k(x)}}} \tag{19}$$

Using this result into the expression for $(du/dx)$ gives

$$\frac{du}{dx} = \frac{C}{C/k(x)} \tag{20}$$

$$= k(x) \tag{21}$$

$$\Rightarrow \boxed{u(x) = \int k(x)dx} \tag{22}$$

• The general solution of the 1 D TISE is, thus, of the form

$$\boxed{\psi(x) = R(x)e^{iu(x)} \approx \frac{A}{\sqrt{k(x)}}e^{i\int k(x)dx}} \tag{23}$$

where $A$ is some arbitrary constant.

• The condition for the validity of the approximation $d^2R/dx^2 \approx 0$ is shown in the following way: If $V(x) = 0$ then $k^2(x) = k^2$ is spatially - independent, in which case we have:

$$\psi(x) \sim e^{ikx} \tag{24}$$

i.e.,

$$u(x) = k \cdot x \tag{25}$$

Then

$$\frac{du}{dx} = k \tag{26}$$

and

$$\frac{C}{R^2(x)} = \frac{du}{dx} = k \tag{27}$$

which gives

$$\frac{d^2R}{dx^2} = k^2 - k^2 \tag{28}$$

$$= 0 \tag{29}$$

We may thus conclude that the condition $d^2R/dx^2 = 0$ is satisfied only when $V(x)$ is SLOWLY - VARYING potential.

- The probability density function is

$$p(x) = |\psi(x)|^2 \tag{30}$$

$$\approx \frac{A^2}{k^2(x)} \tag{31}$$

The above probability density agrees with the classical results: $k(x)$ is proportional to the velocity of the particle and the probability of finding a particle in a range $dx$ is inversely proportional to its velocity in the interval $dx$.

**(B) Classically - forbidden region**

By similar argument, it is easy to show that in the classically - forbidden region

$$\psi(x) \approx \frac{A}{\sqrt{\gamma(x)}} e^{-\int \gamma(x)\, dx}; \qquad \gamma(x) = \sqrt{\frac{2m}{\hbar^2}\left[V(x) - E\right]} \tag{32}$$

**(C) Connection Formulas**

At the points where $E - V(x) = 0$, special treatment is required because $R(x)$ is singular. The way of handling the solution near the turning point is a little bit more technical, but the basic idea is that we have a solution to the left and to the right of the turning point, and one needs a formula that interpolates between them. In other words, in the vicinity of the turning point, one approximates

$$\sqrt{2m\left[E - V(x)\right]/\hbar^2} \tag{33}$$

by a straight line over a small interval and solves the TISE exactly. This leads to the following connection formulas:

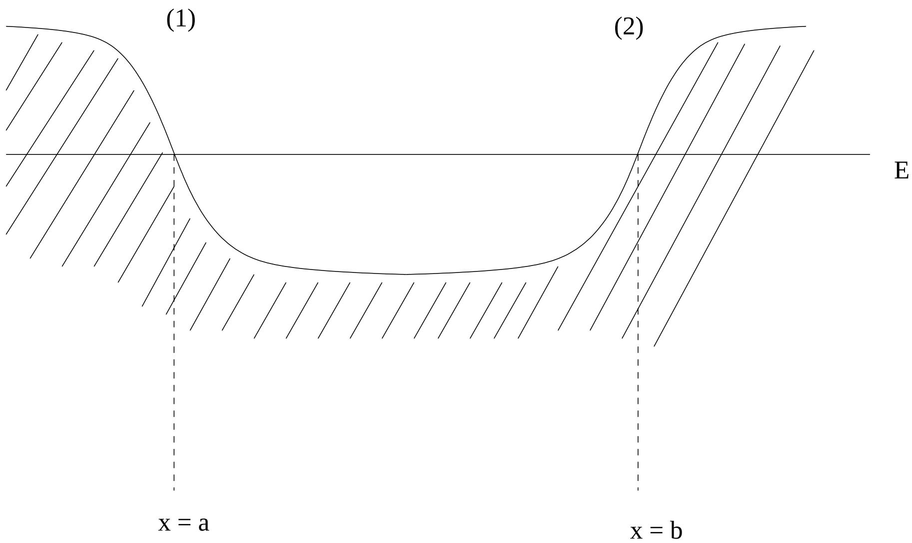


Figure 2: Potential energy profile used to describe the connection formulas.

(1) Barrier to the right

$$\frac{2}{\sqrt{k}}\cos\left[\int_x^b k(x)dx-\frac{\pi}{4}\right] \quad \begin{smallmatrix}\longleftarrow\\ \longrightarrow\end{smallmatrix} \quad \frac{1}{\gamma}e^{-\int_b^x \gamma(x)dx} \tag{34}$$

$$\frac{1}{\sqrt{k}}\sin\left[\int_x^b k(x)dx-\frac{\pi}{4}\right] \quad \begin{smallmatrix}\longleftarrow\\ \longrightarrow\end{smallmatrix} \quad \frac{1}{\gamma}e^{\int_b^x \gamma(x)dx} \tag{35}$$

(2) Barrier to the left

$$\frac{2}{\sqrt{k}}\cos\left[\int_a^x k(x)dx-\frac{\pi}{4}\right] \quad \begin{smallmatrix}\longleftarrow\\ \longrightarrow\end{smallmatrix} \quad \frac{1}{\gamma}e^{-\int_x^a \gamma(x)dx} \tag{36}$$

$$-\frac{1}{\sqrt{k}}\sin\left[\int_a^x k(x)dx-\frac{\pi}{4}\right] \quad \begin{smallmatrix}\longleftarrow\\ \longrightarrow\end{smallmatrix} \quad \frac{1}{\gamma}e^{\int_x^a \gamma(x)dx} \tag{37}$$

The connection formulas enable us to obtain relationship between the solutions in a region at some distance to the right of the turning point with those in a region at some distance to the left.

**(C) Application of the connection formulas to calculating the tunneling coefficient**

• One of the most important problems to which the connection formulas apply is that of a penetration of a potential barrier. The barrier is shown in the figure below, and the energy is such that the turning points are at $x = a$ and $x = b$.

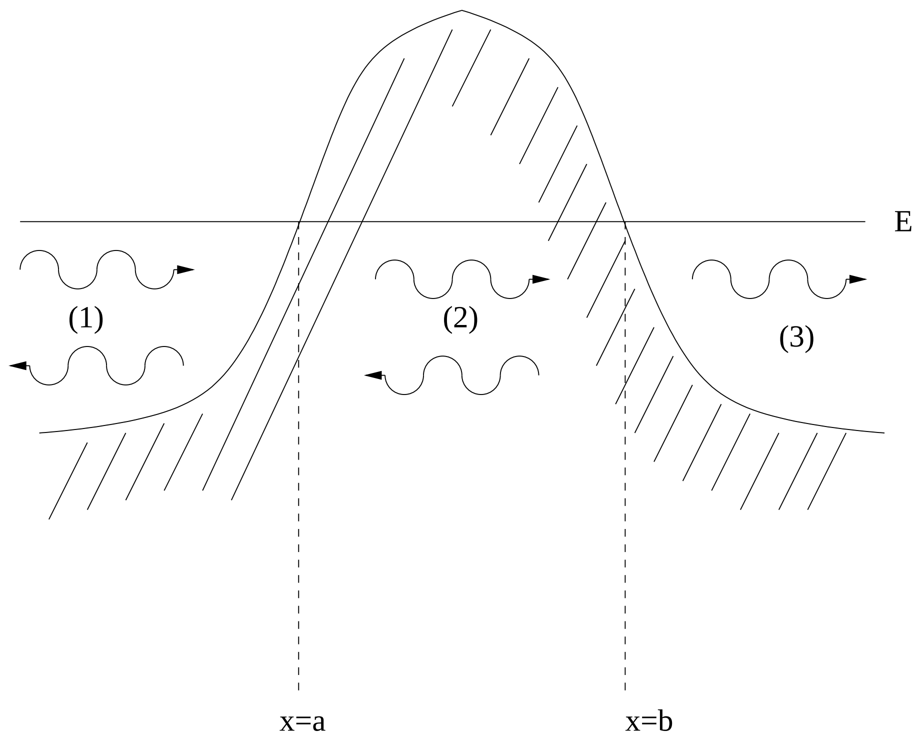


Figure 3: Tunneling potential barrier.

• Suppose that the particles are incident from the left. Some will be reflected and some transmitted, so that in region (3) we will have

$$\begin{aligned} \psi_3(x) &= \frac{1}{\sqrt{k}} e^{i \int_b^x k(x)dx - i\pi/4} \\ &= \frac{1}{\sqrt{k}} \cos\left[\int_b^x k(x)dx - \frac{\pi}{4}\right] + i\frac{1}{\sqrt{k}} \sin\left[\int_b^x k(x)dx - \frac{\pi}{4}\right] \qquad (38) \end{aligned}$$

The phase factor is included for convenience of applying the connection formulas:

• In region (2) we have

$$
\begin{array}{ccc}
\frac{1}{\sqrt{k}} \cos\left[\int_b^x k(x)dx - \frac{\pi}{4}\right] & & +i\frac{1}{\sqrt{k}} \sin\left[\int_b^x k(x)dx - \frac{\pi}{4}\right] \\
\downarrow & & \downarrow \\
\frac{1}{2}\frac{1}{\sqrt{\gamma}} \exp\left[-\int_x^b \gamma(x)dx\right] & & -i\frac{1}{\sqrt{\gamma}} \exp\left[\int_x^b \gamma(x)dx\right]
\end{array} \tag{39}
$$

i.e.,

$$
\psi_2(x) = \frac{1}{2}\frac{1}{\sqrt{\gamma}} e^{-\int_x^b \gamma(x)dx} - i\frac{1}{\sqrt{\gamma}} e^{\int_x^b \gamma(x)dx} \tag{40}
$$

Now using

$$
\int_x^b \gamma(x)dx = \int_x^a \gamma(x)dx + \int_a^b \gamma(x)dx \tag{41}
$$

$$
= -\int_a^x \gamma(x)dx + \alpha \tag{42}
$$

we can write $\psi_2(x)$ as

$$
\psi_2(x) = \frac{1}{2}\frac{1}{\sqrt{\gamma}} e^{\int_a^x \gamma(x)dx - \alpha} - i\frac{1}{\sqrt{\gamma}} e^{-\int_a^x \gamma(x)dx + \alpha} \tag{43}
$$

$$
= \underbrace{\frac{1}{2}\frac{1}{\sqrt{\gamma}} e^{\int_a^x \gamma(x)dx}}_{\downarrow} e^{-\alpha} \quad \underbrace{-i\frac{1}{\sqrt{\gamma}} e^{-\int_a^x \gamma(x)dx}}_{\downarrow} e^{\alpha} \tag{44}
$$

• Again, using the connection formulas for the case where the barrier to the right, we get

$$
\psi_3(x) = \overbrace{\frac{1}{2} e^{-\alpha} \frac{1}{\sqrt{k}} \sin\left[\int_x^a k(x)dx - \frac{\pi}{4}\right]}^{\downarrow} \quad \overbrace{-i\frac{2}{\sqrt{k}} \cos\left[\int_x^a k(x)dx - \frac{\pi}{4}\right] e^{\alpha}}^{\downarrow} \tag{45}
$$

$$
= \frac{1}{2}\frac{1}{\sqrt{k}} e^{-\alpha} \sin(u) - i\frac{2}{\sqrt{k}} e^{\alpha} \cos(u) \tag{46}
$$

$$
= \frac{1}{\sqrt{k}} \left[\frac{1}{2} e^{-\alpha} \frac{e^{iu} - e^{-iu}}{i2} - i\not{2} e^{\alpha} \frac{e^{iu} + e^{-iu}}{\not{2}}\right] \tag{47}
$$

$$
= \frac{1}{\sqrt{k}} \left[-i\frac{1}{4} e^{-\alpha} \left(e^{iu} - e^{-iu}\right) - i e^{\alpha} \left(e^{iu} + e^{-iu}\right)\right] \tag{48}
$$

$$
\begin{aligned}
&= -\frac{i}{\sqrt{k}}\left[\frac{1}{4}e^{-\alpha}\left(e^{iu}-e^{-iu}\right)+e^{\alpha}\left(e^{iu}+e^{-iu}\right)\right] && (49)\\
&= -\frac{i}{\sqrt{k}}\left[\underset{\substack{\uparrow\\ \text{forward propagating}\\ \text{wave}}}{e^{iu}}\left(e^{\alpha}+\frac{1}{4}e^{-\alpha}\right)+\underset{\substack{\uparrow\\ \text{backward propagating}\\ \text{wave}}}{e^{-iu}}\left(e^{\alpha}-\frac{1}{4}e^{-\alpha}\right)\right] && (50)
\end{aligned}
$$

Hence

$$
\begin{cases}
\psi_1^{\text{inc}}(x) = -\dfrac{i}{\sqrt{k}}\left(e^{\alpha}+\dfrac{1}{4}e^{-\alpha}\right)e^{i\int_x^a k(x)dx - i\pi/4}\\
\psi_1^{\text{ref}}(x) = -\dfrac{i}{\sqrt{k}}\left(e^{\alpha}-\dfrac{1}{4}e^{-\alpha}\right)e^{-i\int_x^a k(x)dx - i\pi/4}
\end{cases}
\tag{51}
$$

• Having obtained the expression for $\psi_1^{\text{inc}}(x)$ and $\psi_1^{\text{ref}}(x)$, we are now in a position to calculate the transmission coefficient using

$$
\begin{aligned}
T &\sim \frac{k}{k}\left|\frac{\psi_3(x)}{\psi_1^{\text{inc}}(x)}\right|^2 && (52)\\
&= \left|\frac{\psi_3(x)}{\psi_1^{\text{inc}}(x)}\right|^2 && (53)\\
&= \frac{1}{\left(e^{\alpha}+\frac{1}{4}e^{-\alpha}\right)^2} && (54)
\end{aligned}
$$

$$
T \cong \frac{e^{-2\alpha}}{\Big(1+\frac{1}{4}\underset{\substack{\downarrow\\ \text{0 for large}\\ \text{attenuation of the barrier}}}{\boxed{e^{-2\alpha}}}\Big)^2}
\tag{55}
$$

To summarize, for a barrier with large attenuation, the tunneling probability equals to

$$
\boxed{T = \frac{e^{-2\alpha}}{\left(1+\frac{1}{4}e^{-2\alpha}\right)^2} \approx e^{-2\alpha} = e^{-2\int_a^b \gamma(x)dx}}
\tag{56}
$$

• The reflection coefficient is

$$
R = \left|\frac{\psi_1^{\text{ref}}(x)}{\psi_1^{\text{inc}}(x)}\right|^2
\tag{57}
$$

$$= \left| \frac{e^{\alpha} - \frac{1}{4}e^{-\alpha}}{e^{\alpha} + \frac{1}{4}e^{-\alpha}} \right|^2 \quad (58)$$

The sum of the reflection and transmission coefficients is

$$T + R = \frac{1}{\left(e^{\alpha} + \frac{1}{4}e^{-\alpha}\right)^2} + \frac{\left(e^{\alpha} - \frac{1}{4}e^{-\alpha}\right)^2}{\left(e^{\alpha} + \frac{1}{4}e^{-\alpha}\right)^2} \quad (59)$$

$$= \frac{1 + e^{2\alpha} - \frac{1}{2} + \frac{1}{16}e^{-2\alpha}}{\left(e^{\alpha} + \frac{1}{4}e^{-\alpha}\right)^2} \quad (60)$$

$$= \frac{e^{2\alpha} + \frac{1}{2} + \frac{1}{16}e^{-2\alpha}}{e^{2\alpha} + \frac{1}{2} + \frac{1}{16}e^{-2\alpha}} \quad (61)$$

$$= 1 \quad (62)$$

$$\Rightarrow \boxed{T + R = 1} \quad (63)$$

**(E) Bound States**

Let us now consider the problem of a potential well in the WKB approximation:

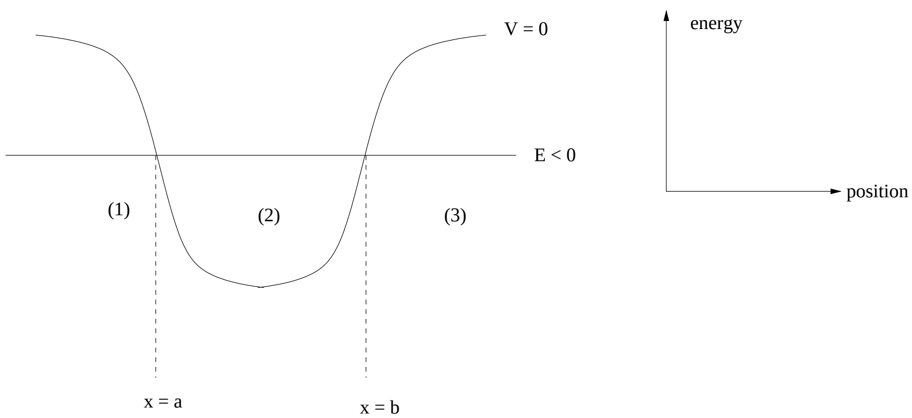


Figure 4: Bound state problem

• For $E < 0$ the particle will, according to classical theory, oscillate back and forth between the limit $x = a$ and the limit $x = b$, where the kinetic energy vanishes. According to quantum theory, the wavefunction penetrates into the region where $V > E$. In this region, according to the WKB approximation:

$$\psi_1(x) = \frac{1}{\sqrt{\gamma}} e^{-\int_x^a \gamma(x) dx} \quad (64)$$

• The application of the connection formula for region (2) gives

$$\psi_2(x) = \frac{2}{\sqrt{k}} \cos\left[\int_a^x k(x)dx - \frac{\pi}{4}\right] \tag{65}$$

where

$$\int_a^x k(x)dx = \int_a^b k(x)dx + \int_b^x k(x)dx \tag{66}$$

$$= \underbrace{\int_a^b k(x)dx}_{\alpha} - \underbrace{\int_x^b k(x)dx}_{u} \tag{67}$$

Substituting the above result into the expression for $\psi_2(x)$ we get

$$\cos\left[\int_a^x k(x)dx - \frac{\pi}{4}\right] = \cos\left[\alpha - u - \frac{\pi}{4}\right] \tag{68}$$

$$= \cos\left[u + \frac{\pi}{4} - \alpha\right] \tag{69}$$

$$= \sin\left[\frac{\pi}{2} - u - \frac{\pi}{4} + \alpha\right] \tag{70}$$

$$= \sin\left[\frac{\pi}{4} - u + \alpha\right] \tag{71}$$

$$= \sin\left[\frac{\pi}{4} - u\right]\cos(\alpha) + \cos\left[\frac{\pi}{4} - u\right]\sin(\alpha) \tag{72}$$

$$= \underbrace{\sin(\alpha)\cos\left[u - \frac{\pi}{4}\right]}_{\substack{\text{connects to}\\ \text{exponentially}\\ \text{decaying}\\ \text{solution}\\ \text{(acceptable)}}} - \underbrace{\cos(\alpha)\sin\left[u - \frac{\pi}{4}\right]}_{\substack{\text{connects to}\\ \text{exponentially}\\ \text{growing}\\ \text{solution}\\ \text{(not acceptable)}}} \tag{73}$$

To eliminate the physically unadmissible solution, we must have

$$\alpha = \int_a^b k(x)dx = (2n-1)\frac{\pi}{2} \tag{74}$$

$$= \left(n - \frac{1}{2}\right)\pi \tag{75}$$

For $n = 1$ and $V(x) = 0$ for $a < x < b$, we have

$$k \cdot (b - a) = \left(1 - \frac{1}{2}\right) \tag{76}$$

$$= \frac{1}{2}\pi \tag{77}$$

$$b - a = \frac{\pi}{2k}, \qquad k = \frac{2\pi}{\lambda} \tag{78}$$

$$b - a = \frac{\pi}{2\frac{2\pi}{\lambda}} \tag{79}$$

$$= \underbrace{\frac{\lambda}{4}}_{\substack{\text{only quarter wavelengths need to be} \\ \text{fitted into the classically allowed} \\ \text{region instead of half-wavelengths} \\ \text{for infinite barriers}}} \tag{80}$$