Chapter 1

Appendix

1.1 Quantum Harmonic Oscillator

For a free particle with a mass m, the time independent Schrödinger equation in one spacial dimension takes the form of:

$$\hat{H}\psi = E\psi \tag{1.1}$$

where:

$$\hat{H} = \frac{\hat{p}}{2m} + V(x) \tag{1.2}$$

With the potential [**?**]:

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{1.3}$$

the Schrödinger equation can be expressed as:

$$\left[-\frac{\partial^2}{\partial x^2} + \alpha^2 x^2\right]\psi = \frac{2m}{\hbar^2}E\psi \tag{1.4}$$

where $\alpha = m\omega/\hbar$. This equation has the solution:

$$\psi_n = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\alpha}x\right) e^{-\frac{\alpha}{2}x^2} \tag{1.5}$$

Where $H_n(x)$ is the Hermite polynomial:

$$H_n(x) = (-1)^n e^{x^n} \frac{d^n}{dx^n} e^{-x^n} \tag{1.6}$$

The Hermite polynomials for the first three values of n are:

$$H_0(x) = 1 \tag{1.7}$$

$$H_1(x) = 2x \tag{1.8}$$

$$H_2(x) = 4x^2 - 2 \tag{1.9}$$

Therefore the wave-functions for the first three energy levels become:

$$\psi_0 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha}{2}x^2} \tag{1.10}$$

$$\psi_1 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} \sqrt{2\alpha} x e^{-\frac{\alpha}{2}x^2} \tag{1.11}$$

$$\psi_2 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}} \left(2\alpha x^2 - 1\right) e^{-\frac{\alpha}{2}x^2} \tag{1.12}$$

Using these wave-functions in Equation (1.4) produces the first three energy levels:

$$E_0 = \frac{\hbar\omega}{2} \tag{1.13}$$

$$E_1 = \frac{3}{2}\hbar\omega \tag{1.14}$$

$$E_2 = \frac{5}{2}\hbar\omega \tag{1.15}$$

With these energy levels the expression for energy can be generalised to:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{1.16}$$

1.2 Evaluating p_z

To evaluate the expression:

$$\frac{1}{1-\hat{p}_z} e^{ik_z z} \tag{1.17}$$

use the Taylor expansion:

$$\begin{aligned} \frac{1}{1-\hat{p}_z} e^{ik_z z} &= \left(1 + \hat{p}_z + \hat{p}_z^2 + ...\right) e^{ik_z z} && (1.18) \\ &= \left(1 - i\hbar\frac{\partial}{\partial z} - \hbar^2\frac{\partial^2}{\partial z^2} + ...\right) e^{ik_z z} && (1.19) \\ &= \left(1 + \hbar k_z + \hbar^2 k_z^2 + ...\right) e^{ik_z z} && (1.20) \end{aligned}$$

From this the relation:

$$\hat{p}_z = \hbar k_z \tag{1.21}$$

can be made, which results in:

$$\frac{1}{1-\hat{p}_z} e^{ik_z z} = \frac{1}{1-\hbar k_z} e^{ik_z z} \tag{1.22}$$

1.3 Schrödinger WKB Barrier

The scattering properties of the Schrödinger smooth potential will derived in this section. This will be used as a comparison for the graphene case.

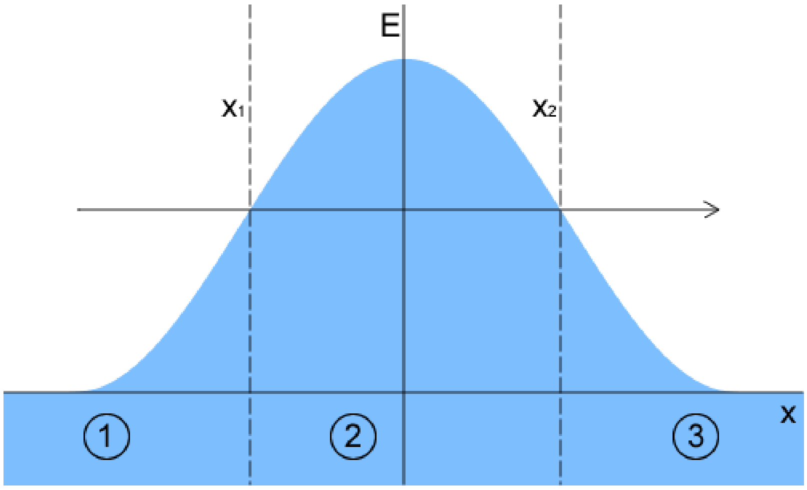

Figure 1.1: Diagram showing a smooth potential barrier for an arbitrary potential $V(x)$. The two turning points $x_{1,2}$ and the three independent barrier regions have been labelled.

1.3.1 Defining the Schrödinger System

Starting with the Schrödinger equation:

$$\hat{H}y(x) = Ey(x) \tag{1.23}$$

with the Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m_e} + V(x) \tag{1.24}$$

and the substitutions:

$$h = \frac{\hbar}{\sqrt{2m_e}} \qquad q(x) = E - V(x) \tag{1.25}$$

the Schrödinger equation can take the form:

$$h^2 y''(x) + q(x)\,y(x) = 0 \tag{1.26}$$

where h is the small parameter and prime denotes differentiation with respect to x. Here we will introduce the variables, and remove the function notations for convenience:

$$z = z(x) \qquad \varphi(z) = \sqrt{z'}\,y(x) \tag{1.27}$$

With the Schrödinger equation in this form and the definitions of z and φ, the equation:

$$h^2\varphi'' + \varphi(\Delta - R(z)) = 0 \tag{1.28}$$

will now be considered with Δ as a constant and $R(x)$ as an arbitrary function to be defined properly later. This equation can be expressed in terms of y:

$$h^2 z'^2 y'' + h^2 z' z'' y' + h^2 m y + z'^2 y(\Delta - R(z)) = 0 \tag{1.29}$$

with:

$$m = \frac{1}{2}z'z''' - \frac{1}{4}z''^2 \tag{1.30}$$

The terms containing h^2 shall be considered as too small, therefore $h^2 \to 0$ and the two equations in terms of y can be used to find z in terms of $q(x)$:

$$h^2 z'^2 y'' + h^2 z' z'' y' + h^2 m y + z'^2 y \left(\Delta - R\left(z\right)\right) = h^2 y'' + q\left(x\right) y \tag{1.31}$$

$$z'^2 \left(\Delta - R\left(z\right)\right) = q\left(x\right) \tag{1.32}$$

For the case where $\Delta = 1$ and $R\left(z\right) = 0$ these equations show that:

$$z'^2 = q\left(x\right) \tag{1.33}$$

$$z = \int \sqrt{\pm q}\, dx \tag{1.34}$$

1.3.2 Wave-functions Far From the Turning Points

Far from the turning points Equation (1.28) may be used with $\Delta = 1$ and $R\left(z\right) = 0$. The general solution of $h^2 \varphi'' + \varphi = 0$:

$$\varphi = e^{\frac{i}{h}z} \tag{1.35}$$

can be expressed in terms of y with a reflected component:

$$y = \frac{1}{\sqrt{z'}}\left(c_1 e^{\frac{i}{h}z} + c_2 e^{-\frac{i}{h}z}\right) \tag{1.36}$$

with a substitution of values for z the wave-functions far from the turning points are of the form:

$$y_1 = q^{-\frac{1}{4}}\left(a_1 e^{\frac{i}{h}\int_{x_1}^{x}\sqrt{q}dx} + a_2 e^{-\frac{i}{h}\int_{x_1}^{x}\sqrt{q}dx}\right) \tag{1.37}$$

$$y_2 = \left(-q\right)^{-\frac{1}{4}}\left(c_1 e^{\frac{1}{h}\int_{x_1}^{x}\sqrt{-q}dx} + c_2 e^{-\frac{1}{h}\int_{x_1}^{x}\sqrt{-q}dx}\right) \tag{1.38}$$

$$y_3 = q^{-\frac{1}{4}}\left(d_1 e^{\frac{i}{h}\int_{x_2}^{x}\sqrt{q}dx} + d_2 e^{-\frac{i}{h}\int_{x_2}^{x}\sqrt{q}dx}\right) \tag{1.39}$$

1.3.3 Wave-functions Close to the Turning Points

For wave-functions close to the turning points Equation (1.28) can be used with $\Delta = 0$ and $R\left(z\right) = z$, the general solution becomes:

$$y = \frac{h^{\frac{1}{6}}}{\sqrt{z'}}\left(k_3 A_i\left(\frac{z}{h^{\frac{2}{3}}}\right) + k_4 B_i\left(\frac{z}{h^{\frac{2}{3}}}\right)\right) \tag{1.40}$$

where $A_i\left(x\right), B_i\left(x\right)$ are the Airy functions, which are defined as:

$$A_i\left(x\right) = x^{-\frac{1}{4}}\sin\left(\frac{2}{3}x^{\frac{3}{2}} + \frac{\pi}{4}\right) \tag{1.41}$$

$$B_i\left(x\right) = x^{-\frac{1}{4}}\cos\left(\frac{2}{3}x^{\frac{3}{2}} + \frac{\pi}{4}\right) \tag{1.42}$$

for $x < 0$ and:

$$A_i\left(x\right) = 2x^{-\frac{1}{4}}e^{-\frac{2}{3}x^{\frac{3}{2}}} \tag{1.43}$$

$$B_i\left(x\right) = x^{-\frac{1}{4}}e^{\frac{2}{3}x^{\frac{3}{2}}} \tag{1.44}$$

when $x > 0$. The wave-functions near each turning point can then be derived in terms of the Airy functions. When $x < x_1$, $q > 0$ and $z < 0$ the action can be found from the relation $z'^2\left(\Delta - R\left(z\right)\right) = q\left(x\right)$:

$$-zz'^2 = q\left(x\right) \tag{1.45}$$

$$\int_{z(x)}^{z(x_1)} \sqrt{-z}\frac{dz}{dx}dx = \int_{x}^{x_1} \sqrt{q}dx \tag{1.46}$$

$$z = -\left(\frac{3}{2}\int_{x}^{x_1} \sqrt{q}dx\right)^{\frac{2}{3}} \tag{1.47}$$

This results in the wave-function in exponential form:

$$y_4 = q^{-\frac{1}{4}}\left(\frac{b_1}{2i}\left(e^{-\frac{i}{h}\int_x^{x_1}\sqrt{q}dx-\frac{i\pi}{4}} - e^{\frac{i}{h}\int_x^{x_1}\sqrt{q}dx+\frac{i\pi}{4}}\right) + \frac{b_2}{2}\left(e^{\frac{i}{h}\int_x^{x_1}\sqrt{q}dx+\frac{i\pi}{4}} + e^{-\frac{i}{h}\int_x^{x_1}\sqrt{q}dx-\frac{i\pi}{4}}\right)\right) \tag{1.48}$$

and when $x > x_1$, $q < 0$ and $z > 0$ the action becomes:

$$\sqrt{z}z' = \sqrt{-q} \tag{1.49}$$

$$\int_{z(x_1)}^{z(x)} \sqrt{z}\frac{dz}{dx}dx = \int_{x_1}^{x} \sqrt{-q}dx \tag{1.50}$$

$$z = \left(\frac{3}{2}\int_{x_1}^{x} \sqrt{-q}dx\right)^{\frac{2}{3}} \tag{1.51}$$

Resulting in the wave-function:

$$y_5 = \left(-q\right)^{-\frac{1}{4}}\left(\frac{b_1}{2}e^{-\frac{1}{h}\int_{x_1}^{x}\sqrt{-q}dx} + b_2e^{\frac{1}{h}\int_{x_1}^{x}\sqrt{-q}dx}\right) \tag{1.52}$$

Then at the second turning point the conditions $x < x_2$, $q < 0$ and $z > 0$ produce:

$$z = \left(\frac{3}{2}\int_{x}^{x_2} \sqrt{-q}dx\right)^{\frac{2}{3}} \tag{1.53}$$

With the wave-function:

$$y_6 = \left(-q\right)^{-\frac{1}{4}}\left(\frac{b_3}{2}e^{-\frac{1}{h}\int_{x_1}^{x_2}\sqrt{-q}dx+\frac{1}{h}\int_{x_1}^{x}\sqrt{-q}dx} + b_4e^{\frac{1}{h}\int_{x_1}^{x_2}\sqrt{-q}dx-\frac{1}{h}\int_{x_1}^{x}\sqrt{-q}dx}\right) \tag{1.54}$$

When $x > x_2$, $q > 0$, $z < 0$ the action becomes:

$$z = -\left(\frac{3}{2}\int_{x_2}^{x} \sqrt{q}dx\right)^{\frac{2}{3}} \tag{1.55}$$

With the wave-function:

$$y_7 = q^{-\frac{1}{4}}\left(\frac{b_3}{2i}\left(e^{-\frac{i}{h}\int_{x_2}^{x}\sqrt{q}dx-\frac{i\pi}{4}} - e^{\frac{i}{h}\int_{x_2}^{x}\sqrt{q}dx+\frac{i\pi}{4}}\right) + \frac{b_4}{2}\left(e^{\frac{i}{h}\int_{x_2}^{x}\sqrt{q}dx+\frac{i\pi}{4}} + e^{-\frac{i}{h}\int_{x_2}^{x}\sqrt{q}dx-\frac{i\pi}{4}}\right)\right) \tag{1.56}$$

1.3.4 Matching and Transfer Matrix

By matching the Airy function solutions to the WKB solutions in each region the constants a and d can be found and a transfer matrix can be made. In the region before the first turning point $x < x_1$, therefore $y_1 = y_4$. By comparison the constants become:

$$a_1 = \frac{1}{2}\left(b_1 e^{i\frac{\pi}{4}} + b_2 e^{-i\frac{\pi}{4}}\right) \tag{1.57}$$

$$a_2 = \frac{1}{2}\left(b_1 e^{-i\frac{\pi}{4}} + b_2 e^{i\frac{\pi}{4}}\right) \tag{1.58}$$

After the first turning point, $x > x_1$ and $y_5 = y_2$. Again by comparison:

$$c_1 = \frac{1}{2} b_1 \tag{1.59}$$

$$c_2 = b_2 \tag{1.60}$$

Before the second turning point $x < x_2$, $y_2 = y_6$ and the constants are related by:

$$c_1 = b_4 e^{\frac{1}{h}Q} \tag{1.61}$$

$$c_2 = \frac{1}{2} b_3 e^{-\frac{1}{h}Q} \tag{1.62}$$

Where:

$$Q = \int_{x_1}^{x_2} \sqrt{-q}\,dx \tag{1.63}$$

Finally, after the second turning point $x > x_2$ and $y_7 = y_3$ resulting in the relation:

$$d_1 = \frac{1}{2}\left(b_3 e^{-i\frac{\pi}{4}} + b_4 e^{i\frac{\pi}{4}}\right) \tag{1.64}$$

$$d_2 = \frac{1}{2}\left(b_3 e^{i\frac{\pi}{4}} + b_4 e^{-i\frac{\pi}{4}}\right) \tag{1.65}$$

The constants can now be expressed in matrix form and $b_{1,2,3,4}$ can be eliminated producing:

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} e^{i\frac{\pi}{4}} & \frac{1}{2}e^{-i\frac{\pi}{4}} \\ e^{-i\frac{\pi}{4}} & \frac{1}{2}e^{i\frac{\pi}{4}} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{1.66}$$

$$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} e^{-\frac{1}{h}Q+i\frac{\pi}{4}} & \frac{1}{2}e^{\frac{1}{h}Q-i\frac{\pi}{4}} \\ e^{-\frac{1}{h}Q-i\frac{\pi}{4}} & \frac{1}{2}e^{\frac{1}{h}Q+i\frac{\pi}{4}} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{1.67}$$

The relations between the constants a and d can now be found by eliminating c_1 and c_2. With the definition of the transfer matrix T as $d = Ta$ the resulting transfer matrix becomes:

$$T = \begin{bmatrix} e^{\frac{1}{h}Q} + \frac{1}{4}e^{-\frac{1}{h}Q} & -ie^{\frac{1}{h}Q} + \frac{1}{4}ie^{-\frac{1}{h}Q} \\ ie^{\frac{1}{h}Q} - \frac{1}{4}ie^{-\frac{1}{h}Q} & e^{\frac{1}{h}Q} + \frac{1}{4}e^{-\frac{1}{h}Q} \end{bmatrix} \tag{1.68}$$

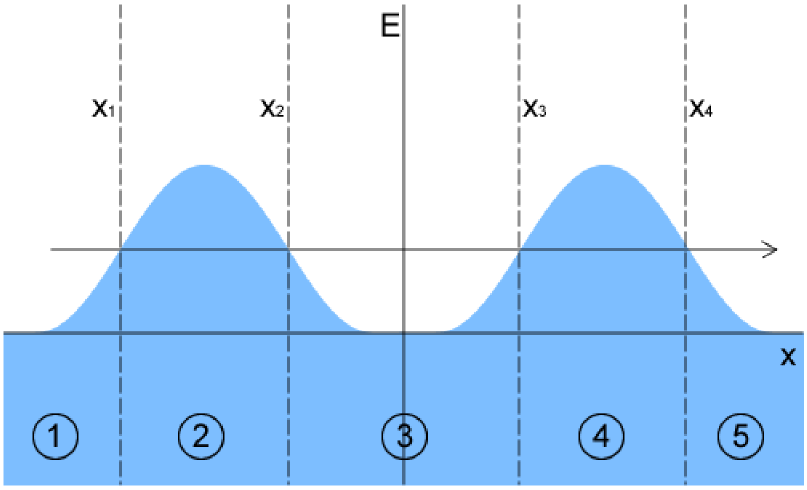

Figure 1.2: Diagram showing a double smooth potential barrier for an arbitrary potentials $V_1(x)$ and $V_2(x)$. The four turning points $x_{1,2,3,4}$ and the five independent barrier regions have been labelled.

1.3.5 The Double Potential Barrier

For a double potential barrier the transmitted wave-function from the first barrier must equal the incoming wave for the second barrier, however the distance between the barriers will create a phase shift. The phase shift can be obtained by matching the incoming and transmitted coefficients. The transmitted wave-function as defined previously:

$$y_t = q^{-\frac{1}{4}} \left(d_1 e^{\frac{i}{h}\int_{x_2}^{x} \sqrt{q}dx} + d_2 e^{-\frac{i}{h}\int_{x_2}^{x} \sqrt{q}dx} \right) \tag{1.69}$$

must be equal to the incoming wave at the second potential barrier:

$$y_i = q^{-\frac{1}{4}} \left(a_3 e^{\frac{i}{h}\int_{x_3}^{x} \sqrt{q}dx} + a_4 e^{-\frac{i}{h}\int_{x_3}^{x} \sqrt{q}dx} \right) \tag{1.70}$$

$$y_i = q^{-\frac{1}{4}} \left(a_3 e^{-\frac{i}{h}\int_{x_2}^{x_3} \sqrt{q}dx + \frac{i}{h}\int_{x_2}^{x} \sqrt{q}dx} + a_4 e^{\frac{i}{h}\int_{x_2}^{x_3} \sqrt{q}dx - \frac{i}{h}\int_{x_2}^{x} \sqrt{q}dx} \right) \tag{1.71}$$

Then the transfer matrix between the two barriers can then be defined as:

$$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} e^{-\frac{i}{h}P} & 0 \\ 0 & e^{\frac{i}{h}P} \end{bmatrix} \begin{bmatrix} a_3 \\ a_4 \end{bmatrix} \tag{1.72}$$

Where the potentials between the turning points are represented by:

$$P = \int_{x_2}^{x_3} \sqrt{q}dx \tag{1.73}$$

With the phase shift between barriers, the total transfer matrix becomes:

$$T = T_2 \begin{bmatrix} e^{-\frac{i}{h}P} & 0 \\ 0 & e^{\frac{i}{h}P} \end{bmatrix}^{-1} T_1 \tag{1.74}$$

Evaluating this with the transfer matrices for each barrier:

$$T_{11} = 2\cos\left(\frac{P}{h}\right)\left(e^{\frac{Q_2}{h}+\frac{Q_1}{h}} + \frac{1}{16}e^{-\frac{Q_2}{h}-\frac{Q_1}{h}}\right) + i\sin\left(\frac{P}{h}\right)\cosh\left(\frac{Q_2}{h}-\frac{Q_1}{h}\right) \tag{1.75}$$

$$T_{12} = 2i\cos\left(\frac{P}{h}\right)\left(-e^{\frac{Q_2}{h}+\frac{Q_1}{h}} + \frac{1}{16}e^{-\frac{Q_2}{h}-\frac{Q_1}{h}}\right) - \sin\left(\frac{P}{h}\right)\sinh\left(\frac{Q_2}{h}-\frac{Q_1}{h}\right) \tag{1.76}$$

$$T_{21} = 2i\cos\left(\frac{P}{h}\right)\left(e^{\frac{Q_2}{h}+\frac{Q_1}{h}} - \frac{1}{16}e^{-\frac{Q_2}{h}-\frac{Q_1}{h}}\right) - \sin\left(\frac{P}{h}\right)\sinh\left(\frac{Q_2}{h}-\frac{Q_1}{h}\right) \tag{1.77}$$

$$T_{22} = 2\cos\left(\frac{P}{h}\right)\left(e^{\frac{Q_2}{h}+\frac{Q_1}{h}} + \frac{1}{16}e^{-\frac{Q_2}{h}-\frac{Q_1}{h}}\right) - i\sin\left(\frac{P}{h}\right)\cosh\left(\frac{Q_2}{h}-\frac{Q_1}{h}\right) \tag{1.78}$$

Where each potential is represented by:

$$Q_1 = \int_{x_1}^{x_2} \sqrt{-q}dx \qquad Q_2 = \int_{x_3}^{x_4} \sqrt{-q}dx \tag{1.79}$$

There is a special case when using the Bohr-Sommerfeld quantisation rule and symmetrical barriers:

$$P = \pi\left(n + \frac{1}{2}\right) \qquad Q_1 = Q_2 \tag{1.80}$$

which will result in perfect transmission:

$$T = \frac{1}{|T_{22}|^2} = 1 \tag{1.81}$$

1.4 Mathematical Appendix for the WKB Potential Barrier

In this section some additional stages in derivations are presented. These stages may be required to fully replicate the results shown, but are too long to include in the main text.

1.4.1 Solutions to Equation (??)

The solutions to the equation:

$$h^2\omega'' + \omega\left(\frac{\epsilon^2 - p_y^2}{\alpha^2} + \frac{ih}{\alpha}\right) = 0 \tag{1.82}$$

are required in the forms:

$$\omega_{1,3} = \omega^+ e^{\frac{i}{h}s} + \omega^- e^{-\frac{i}{h}s} \tag{1.83}$$

$$\omega_2 = \omega^+ e^{\frac{1}{h}s} + \omega^- e^{-\frac{1}{h}s} \tag{1.84}$$

For simplicity each term will be evaluated individually, so for $\omega = \omega^+ e^{\frac{i}{h}s}$ the derivitives:

$$\omega' = \frac{i}{h}s'\omega^+ e^{\frac{i}{h}s} + \omega'^+ e^{\frac{i}{h}s} \tag{1.85}$$

$$\omega'' = \frac{i}{h}s''\omega^+ e^{\frac{i}{h}s} - \frac{1}{h}s'^2\omega^+ e^{\frac{i}{h}s} + \frac{2i}{h}s'\omega'^+ e^{\frac{i}{h}s} + \omega''^+ e^{\frac{i}{h}s} \tag{1.86}$$

can be substituted into Equation (??):

$$his''\omega^+ - s'^2\omega^+ + 2ihs'\omega'^+ + h^2\omega''^+ + \frac{\epsilon^2 - p_y^2}{\alpha^2}\omega^+ + \frac{ih}{\alpha}\omega^+ = 0 \tag{1.87}$$

Takeing only h^0 terms the expression for s' becomes:

$$s' = \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} \tag{1.88}$$

Then with only h order terms:

$$\frac{2}{\omega^+}\omega'^+ = -\frac{s''}{s'} - \frac{1}{\alpha s'} \tag{1.89}$$

With the value of s':

$$s'' = \frac{\alpha\epsilon - \left(\epsilon^2 - p_y^2\right)\alpha'}{\alpha^2\sqrt{\epsilon^2 - p_y^2}} \tag{1.90}$$

Substituting values of s' and s'' results in:

$$2\frac{\partial}{\partial\epsilon}\ln(\omega^+) = -\frac{\epsilon}{\epsilon^2 - p_y^2} + \frac{\partial}{\partial\epsilon}\ln(\alpha) - \frac{1}{\sqrt{\epsilon^2 - p_y^2}} \tag{1.91}$$

and integrating:

$$2\int_{-p_y}^{\epsilon}\frac{\partial}{\partial\epsilon}\ln(\omega^+)d\epsilon = -\int_{-p_y}^{\epsilon}\frac{\epsilon}{\epsilon^2 - p_y^2}d\epsilon + \int_{-p_y}^{\epsilon}\frac{\partial}{\partial\epsilon}\ln(\alpha)d\epsilon - \int_{-p_y}^{\epsilon}\frac{1}{\sqrt{\epsilon^2 - p_y^2}}d\epsilon \tag{1.92}$$

results in:

$$\omega^+ = \frac{\sqrt{\alpha}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}}\frac{1}{D^-} \tag{1.93}$$

where:

$$D^\pm = \sqrt{\frac{\epsilon + \left(\epsilon^2 - p_y^2\right)^{\frac{1}{2}}}{\pm p_y}} \tag{1.94}$$

The same calculation must then be done for $\omega = \omega^- e^{-\frac{i}{h}s}$. With this definition of ω, Equation (??) can be evaluated to:

$$his''\omega^- - s'^2\omega^- + 2ihs'\omega'^- + h^2\omega''^- + \frac{\epsilon^2 - p_y^2}{\alpha^2}\omega^- - \frac{ih}{\alpha}\omega^- = 0 \tag{1.95}$$

Using only the terms of order h^0 produces the same result for s' as in the previous case. To find the value of ω^-, take only the terms of order h:

$$2\frac{\partial}{\partial\epsilon}\ln(\omega^-) = -\frac{s''}{s'} + \frac{1}{\alpha s'} \tag{1.96}$$

With the values of s' and s'' this relation can be integrated to produce:

$$\omega^- = \frac{\sqrt{\alpha}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}}D^- \tag{1.97}$$

With $\omega = \omega^{+} e^{\frac{1}{h}s}$ in Equation (**??**) requires the derivities:

$$\omega' = \frac{1}{h}s'\omega^{+}e^{\frac{1}{h}s} + \omega'^{+}e^{\frac{1}{h}s} \tag{1.98}$$

$$\omega'' = \frac{1}{h}s''\omega^{+}e^{\frac{1}{h}s} + \frac{1}{h^2}s'^2\omega^{+}e^{\frac{1}{h}s} + \frac{1}{h}2s'\omega'^{+}e^{\frac{1}{h}s} + \omega''^{+}e^{\frac{1}{h}s} \tag{1.99}$$

Equation (**??**) can now be written as:

$$s''h\omega^{+} + s'^2\omega^{+} + 2s'h\omega'^{+} + h^2\omega''^{+} + \frac{\epsilon^2 - p_y^2}{\alpha^2}\omega^{+} + \frac{ih}{\alpha}\omega^{+} = 0 \tag{1.100}$$

With only h^0 terms, s' becomes:

$$s' = \frac{\sqrt{p_y^2 - \epsilon^2}}{\alpha} \tag{1.101}$$

With only terms of order h:

$$2\frac{\partial}{\partial\epsilon}\ln(\omega^{+}) = -\frac{\partial}{\partial\epsilon}\ln(s') - \frac{i}{\sqrt{p_y^2 - \epsilon^2}} \tag{1.102}$$

Integrating then results in:

$$\omega^{+} = \frac{\sqrt{\alpha}}{\left(p_y^2 - \epsilon^2\right)^{\frac{1}{4}}} e^{-\frac{1}{2}i\arcsin\left(\frac{\epsilon}{p_y}\right) - \frac{i\pi}{4}} \tag{1.103}$$

Finally using $\omega = \omega^{-} e^{-\frac{1}{h}s}$ with Equation (**??**) produces:

$$-s''h\omega^{-} + s'^2\omega^{-} - 2s'h\omega'^{-} + h^2\omega''^{-} + \frac{\epsilon^2 - p_y^2}{\alpha^2}\omega^{-} + \frac{ih}{\alpha}\omega^{-} = 0 \tag{1.104}$$

The expression produced for s' is identical to that of ω^{+}. Taking only h terms gives the equation:

$$2\frac{\omega'^{-}}{\omega^{-}} = -\frac{s''}{s'} + \frac{i}{s'\alpha} \tag{1.105}$$

Which when integrated produces:

$$\omega^{-} = \frac{\sqrt{\alpha}}{\left(p_y^2 - \epsilon^2\right)^{\frac{1}{4}}} e^{\frac{1}{2}i\arcsin\left(\frac{\epsilon}{p_y}\right) + \frac{i\pi}{4}} \tag{1.106}$$

1.4.2 Matching Change of Variables to Solutions of Equation (??)

The wave-functions produced from the change in variables:

$$\omega = \sqrt{\alpha}\left(\frac{u+v}{2}\right) \tag{1.107}$$

must match those from the direct solutions from Equation (**??**). With the trigonometric equations:

$$\cos^2(x) = \frac{1}{1+\tan^2(x)} \qquad \cos(x) = \frac{1-\tan^2\left(\frac{x}{2}\right)}{1+\tan^2\left(\frac{x}{2}\right)} \qquad \sin(x) = \frac{\tan(x)}{\sqrt{1+\tan^2(x)}} \tag{1.108}$$

The grouped terms from the change in variables before and after the barrier can be expressed in the form:

$$\frac{A^+}{P^+} = \frac{1 - e^{i\theta}}{\sqrt{1 + e^{2i\theta}}} = -\frac{i\sqrt{2}\sin\left(\frac{\theta}{2}\right)}{\sqrt{\cos(\theta)}} = -\sqrt{\frac{2}{1 - \cot^2\left(\frac{\theta}{2}\right)}} \tag{1.109}$$

$$\frac{A^-}{P^-} = \frac{1 + e^{-i\theta}}{\sqrt{1 + e^{-2i\theta}}} = \frac{\sqrt{2}\cos\left(\frac{\theta}{2}\right)}{\sqrt{\cos(\theta)}} = \sqrt{\frac{2}{1 - \tan^2\left(\frac{\theta}{2}\right)}} \tag{1.110}$$

Then with the additional identities:

$$\frac{q + p_y}{-\epsilon} = \tan(\alpha) \qquad \frac{-q + p_y}{-\epsilon} = \tan(-\alpha) \qquad \tan^2(x) - 1 = -\frac{\cos(2x)}{\cos^2(x)} \tag{1.111}$$

The terms for use inside the barrier can be converted to:

$$\frac{B^+}{Q^+} = \frac{1 + i\tan(\alpha)}{\sqrt{-\frac{\cos(2\alpha)}{\cos^2(\alpha)}}} = \frac{\cos(\alpha) + i\sin(\alpha)}{\sqrt{-\cos(2\alpha)}} = \frac{e^{i\alpha}}{\sqrt{-\cos(2\alpha)}} \tag{1.112}$$

$$\frac{B^-}{Q^-} = \frac{1 + i\tan(-\alpha)}{\sqrt{-\frac{\cos(2\alpha)}{\cos^2(\alpha)}}} = \frac{\cos(-\alpha) + i\sin(-\alpha)}{\sqrt{-\cos(2\alpha)}} = \frac{e^{-i\alpha}}{\sqrt{-\cos(2\alpha)}} \tag{1.113}$$

The grouped terms in the direct solutions to Equation (**??**) must now be shown in the same form. With the additional equations:

$$\tan(\theta) = \frac{p_y}{p_x} = \frac{p_y}{\sqrt{\epsilon^2 - p_y^2}} \qquad \frac{1}{\tan^2(\theta)} = \frac{\epsilon}{p_y^2} - 1 = \frac{1}{\sin^2(\theta)} - 1 \qquad \frac{1}{\sin(\theta)} = \frac{\epsilon}{p_y} \tag{1.114}$$

$$\sin(x) = \frac{2\tan\left(\frac{x}{2}\right)}{\tan^2\left(\frac{x}{2}\right) + 1} \qquad \cos(x) = \frac{1 - \tan^2\left(\frac{x}{2}\right)}{1 + \tan^2\left(\frac{x}{2}\right)} \qquad \cot(x) = \frac{1 - \tan^2\left(\frac{x}{2}\right)}{2\tan\left(\frac{x}{2}\right)} \tag{1.115}$$

$$D^{\pm} = \sqrt{\frac{\epsilon + \sqrt{\epsilon^2 - p_y^2}}{-p_y}} \tag{1.116}$$

The grouped terms from the solutions of Equation (**??**) can be expressed as:

$$\frac{\sqrt{p_y}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}}\frac{1}{D^-} = \sqrt{-\frac{\tan(\theta)}{\frac{1}{\sin(\theta)} + \cot(\theta)}} = \sqrt{\frac{2}{1 - \cot^2\left(\frac{\theta}{2}\right)}} \tag{1.117}$$

$$\frac{\sqrt{p_y}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}}D^- = \sqrt{-\tan(\theta)\left(\frac{1}{\sin(\theta)} + \cot(\theta)\right)} = \sqrt{-\frac{2}{1 - \tan^2\left(\frac{\theta}{2}\right)}} \tag{1.118}$$

$$\frac{\sqrt{p_y}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}}\frac{1}{D^+} = \sqrt{-\frac{\tan(\theta)}{\frac{1}{\sin(\theta)} + \cot(\theta)}} = \sqrt{-\frac{2}{1 - \cot^2\left(\frac{\theta}{2}\right)}} \tag{1.119}$$

$$\frac{\sqrt{p_y}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}}D^+ = \sqrt{-\tan(\theta)\left(\frac{1}{\sin(\theta)} + \cot(\theta)\right)} = \sqrt{\frac{2}{1 - \tan^2\left(\frac{\theta}{2}\right)}} \tag{1.120}$$

Then the solutions inside the barrier can be converted with the definition:

$$\frac{\epsilon}{p_y} = \sin(2\alpha) \qquad \sin^2(x) = 1 - \cos^2(x) \qquad \sqrt{\frac{p_y^2 - \epsilon^2}{p_y^2}} = \cos(2\alpha) \tag{1.121}$$

$$\frac{\sqrt{p_y}}{\left(p_y^2 - \epsilon^2\right)^{\frac{1}{4}}} e^{\frac{i}{2}\arcsin\left(\frac{\epsilon}{p_y}\right)} = \frac{e^{i\alpha}}{\sqrt{\cos(2\alpha)}} \tag{1.122}$$

$$\frac{\sqrt{p_y}}{\left(p_y^2 - \epsilon^2\right)^{\frac{1}{4}}} e^{-\frac{i}{2}\arcsin\left(\frac{\epsilon}{p_y}\right)} = \frac{e^{-i\alpha}}{\sqrt{\cos(2\alpha)}} \tag{1.123}$$

1.4.3 Matching Solutions of Equation (??) to Schrödinger Solutions

Here it will be shown how the solutions to Equation (??) are comparable to the WKB solutions for the Schrödinger equation. The integral from Equation (??) shall be defined as:

$$I = \int_{-p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon \tag{1.124}$$

The change in variable:

$$y^2 = \epsilon^2 + mh\alpha \tag{1.125}$$

will now be introduced, this change in variable includes a small variation. To convert the integral I to terms of y, an expression for $d\epsilon/dy$ is required.

$$ydy = \left(2\epsilon + mh\alpha'\right) d\epsilon \tag{1.126}$$

With a further substitution of $\epsilon = \sqrt{y^2 - mh\alpha}$ this can take the form:

$$2\frac{d\epsilon}{dy} = \frac{1}{\sqrt{1 - \frac{mh\alpha}{y^2}} + \frac{mh\alpha'}{2y}} \tag{1.127}$$

A Taylor expansion of $\sqrt{1 - \frac{mh\alpha}{y^2}}$ at $\frac{mh\alpha}{y^2} = 0$ produces:

$$2\frac{d\epsilon}{dy} = \frac{1}{1 - \frac{mh\alpha}{2y^2} + \frac{mh\alpha'}{2y}} \tag{1.128}$$

A further Taylor expansion results in:

$$2\frac{d\epsilon}{dy} = 1 + \frac{mh\alpha}{2y^2} - \frac{mh\alpha'}{2y} \tag{1.129}$$

Next the function $\alpha(\epsilon)$ must be converted to be a function of y:

$$\alpha(\epsilon) = \alpha(\epsilon(y)) = \alpha\left(\sqrt{y^2 - mh\alpha}\right) \tag{1.130}$$

The Laurent series of $\sqrt{y^2 - mh\alpha}$ at $y = \infty$ results in:

$$\alpha(\epsilon) = \alpha\left(y - \frac{mh\alpha}{2y}\right) \tag{1.131}$$

Then the Taylor expansion at $mh\alpha/2y = 0$ shows:

$$\alpha(\epsilon) = \alpha(y) - \frac{mh\alpha}{2y}\alpha' \tag{1.132}$$

A final Taylor expansion around $mh\alpha'/2y = 0$ shows that:

$$\frac{1}{\alpha(\epsilon)} = \frac{1}{\alpha(y)}\left(1 + \frac{mh\alpha'}{2y}\right) \tag{1.133}$$

With these definitions the integral I can be expressed as:

$$I = \int_{-p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha(\epsilon)} d\epsilon = \int_{-p_y}^{y} \frac{\sqrt{y^2 - p_y^2}}{\alpha(y)}\left(1 + \frac{hm\alpha'}{2y}\right)\left(1 + \frac{mh\alpha}{2y^2} - \frac{mh\alpha'}{2y}\right) dy \tag{1.134}$$

Evaluating the brackets, and removing terms of order h^2:

$$I = \int_{-p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha(\epsilon)} d\epsilon = \int_{-p_y}^{y} \frac{\sqrt{y^2 - p_y^2}}{\alpha} dy + \frac{mh}{2}\int_{-p_y}^{y} \frac{\sqrt{y^2 - p_y^2}}{y^2} dy \tag{1.135}$$

Introducing a small pertubation to y changes the function $f(y) = f(y + \Delta y)$, this is required in a manor that $\Delta \gg h$. An expansion of this produces $f(y + \Delta y) = f(y) + \Delta y f'(y)$. This allows the integral:

$$\frac{mh}{2}\int_{-p_y}^{y} \frac{\sqrt{y^2 - p_y^2}}{y^2} dy = \frac{mh}{2}\int_{-p_y}^{y} \frac{\sqrt{y^2 - p_y^2}}{y^2} dy + \frac{mh}{2}\frac{\sqrt{y^2 - p_y^2}}{y} \tag{1.136}$$

To the leading order, $y = \epsilon$, therefore the integral can be evaluated to:

$$\int_{-p_y}^{\epsilon} \frac{\sqrt{y^2 - p_y^2}}{y^2} dy = \ln\left(\frac{\sqrt{\epsilon^2 + p_y^2} + \epsilon}{-p_y}\right) - \frac{\sqrt{\epsilon^2 + p_y^2}}{\epsilon} \tag{1.137}$$

These pertubations result in:

$$\int_{-p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon = \int_{-p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon + \frac{h}{2}\ln\left(\frac{\sqrt{\epsilon^2 + p_y^2} + \epsilon}{-p_y}\right) \tag{1.138}$$

For the wave-function before the barrier, $-p_y$ is larger then ϵ, therefore:

$$\int_{\epsilon}^{-p_y} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon = -\int_{-p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon - \frac{h}{2}\ln\left(\frac{\sqrt{\epsilon^2 + p_y^2} + \epsilon}{-p_y}\right) \tag{1.139}$$

and the wave-function component before the first turning point becomes:

$$\frac{\sqrt{\alpha}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}} a_1 \frac{1}{D^-} e^{\frac{i}{h}\int_{\epsilon}^{-p_y} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon} = \frac{1}{q^{\frac{1}{4}}} \bar{a}_1 e^{\frac{i}{h}\int_{x}^{x_1} \sqrt{q} dx} \tag{1.140}$$

with:

$$q = \sqrt{\frac{\epsilon^2 - p_y^2}{\alpha^2}} \qquad D^{\pm} = \sqrt{\frac{\epsilon + \sqrt{\epsilon^2 - p_y^2}}{\pm p_y}} \tag{1.141}$$

Similarly with the wave-function components:

$$\frac{\sqrt{\alpha}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}} a_2 D^- e^{-\frac{i}{\hbar}\int_{\epsilon}^{-p_y} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon} = \frac{1}{q^{\frac{1}{4}}} \bar{a}_2 e^{-\frac{i}{\hbar}\int_x^{x_1} \sqrt{q} dx} \tag{1.142}$$

$$\frac{\sqrt{\alpha}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}} d_1 \frac{1}{D^+} e^{\frac{i}{\hbar}\int_{p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon} = \frac{1}{q^{\frac{1}{4}}} \bar{d}_2 e^{\frac{i}{\hbar}\int_{x_2}^{x} \sqrt{q} dx} \tag{1.143}$$

$$\frac{\sqrt{\alpha}}{\left(\epsilon^2 - p_y^2\right)^{\frac{1}{4}}} d_2 D^+ e^{-\frac{i}{\hbar}\int_{p_y}^{\epsilon} \frac{\sqrt{\epsilon^2 - p_y^2}}{\alpha} d\epsilon} = \frac{1}{q^{\frac{1}{4}}} \bar{d}_1 e^{-\frac{i}{\hbar}\int_{x_2}^{x} \sqrt{q} dx} \tag{1.144}$$

For the case inside the barriers the additional terms included in the ω functions may be absorbed into the constants.