Folders

DiffEq\SeqnIn1d(3).docx

In the folders under 1-d the potential, V(x), is independent of time so that

$$\psi\left(x,t,E\right)=\phi\left(x\right)\exp\left(-i\frac{Et}{\hbar}\right) \quad (1)$$

For

$$\phi\left(x\right)=\begin{cases}\exp\left(p_p\left(x\right)\right)\\ \exp\left(-p_m\left(x\right)\right)\end{cases} \qquad (2)$$

$$\begin{aligned} z_p\left(x\right)&=\frac{dp_p\left(x\right)}{dx}\\ z_m\left(x\right)&=\frac{dp_m\left(x\right)}{dx}\end{aligned} \qquad (3)$$

The Schrodinger equation, ..\SchrodingerEqn.docx (3) in Hartree units is

$$-\frac{\nabla^2\phi\left(x\right)}{2}+V\left(x\right)\phi\left(x\right)=E_H\phi \qquad (4)$$

$$\nabla\phi\left(x\right)=\begin{cases}\dfrac{dp_p\left(x\right)}{dx}\exp\left(p_p\left(x\right)\right)\\ -\dfrac{dp_m\left(x\right)}{dx}\exp\left(-p_m\left(x\right)\right)\end{cases}$$

$$\nabla^2\phi\left(x\right)=\begin{cases}\left(\dfrac{d^2p_p\left(x\right)}{dx^2}+z_p^2\left(x\right)\right)\exp\left(p_p\left(x\right)\right)\\ \left(-\dfrac{d^2p_m\left(x\right)}{dx^2}+z_m^2\left(x\right)\right)\exp\left(-p_m\left(x\right)\right)\end{cases} \qquad (5)$$

$$\nabla^2\phi\left(x\right)=\begin{cases}\left(\dfrac{dz_p\left(x\right)}{dx}+z_p^2\left(x\right)\right)\exp\left(p_p\left(x\right)\right)\\ \left(-\dfrac{dz_m\left(x\right)}{dx}+z_m^2\left(x\right)\right)\exp\left(-p_m\left(x\right)\right)\end{cases}$$

So that (4) becomes

$$\begin{aligned} -\frac{1}{2}\left(\frac{dz_p\left(x\right)}{dx}+z_p^2\left(x\right)\right)\exp\left(p_p\left(x\right)\right)+V\left(x\right)\exp\left(p_p\left(x\right)\right)&=E_H\exp\left(p_p\left(x\right)\right)\\ -\frac{1}{2}\left(-\frac{dz_m\left(x\right)}{dx}+z_m^2\left(x\right)\right)\exp\left(p_m\left(x\right)\right)+V\left(x\right)\exp\left(p_m\left(x\right)\right)&=E_H\exp\left(p_m\left(x\right)\right)\end{aligned} \qquad (6)$$

Cancelling the common exponential factors

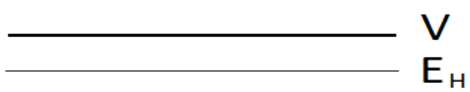
$$\frac{dz_p(x)}{dx} = -\left(2\left(E_H - V(x)\right) - z_p^2(x)\right)$$
$$\frac{dz_m(x)}{dx} = \left(2\left(E_H - V(x)\right) - z_m^2(x)\right) \quad (7)$$

Bob *** stop

For V and z independent of x, both lines in (7) are solved by

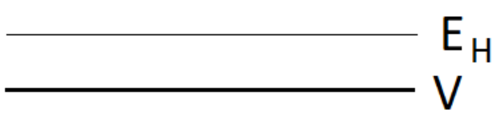
$$z^2(x) = 2\left(V(x) - E_H\right)$$
$$p(x) = \int z(x)dx \quad (1)$$

For $V>E_H$
The two solutions are



$$z = \sqrt{2(V-E_H)}$$
$$z = -\sqrt{2(V-E_H)}$$
$$\phi(x) = A_C \exp\left(x\sqrt{2(V-E_H)}\right) + B_C \exp\left(-x\sqrt{2(V-E_H)}\right) \quad (2)$$

For $E_H>V$
The two Solutions are



$$z = i\sqrt{2(V-E_H)}$$
$$z = -i\sqrt{2(V-E_H)}$$
$$\phi(x) = C_C \exp\left(x\sqrt{2(V-E_H)}\right) + D_C \exp\left(-x\sqrt{2(V-E_H)}\right)$$

The -iEt in (1) means that the positive exponents represent probability moving from left to right, and the negative exponents represent probability moving from right to left. The coefficients A_C,B_C,C_C, and D_C are arbitrary complex coefficients that can be used to make the wave function and its derivative continuous at the point where V_1 becomes V_2. The four potentials are given in
Potential .docx

The fourth potential is a visual fit of a harmonic oscillator potential to the barrier potential.
The potential near any minimum, $dV(x_{min})/dx = 0$ can be expanded as.

$$V(x) = V\left(x_{\min}\right) + \frac{1}{2}\left(x - x_{\min}\right)^2 \left.\frac{d^2V\left(x_{\min}\right)}{dx^2}\right)_{x_{\min}}$$

The Harmonic Oscillator states are derived from raising operators in HarmonicOscillator/Welcome.htm These are the same as the ones used in ../AngularMomentum.pdf The states in this potential are discussed in HarmonicOscillator .docx

Each of the four potentials is considered as a series of V_i values in
Flats .docx

The differential equation can be solved numerically, especially when the starting point is a potential minimum.
DiffEq .docx