DOING PHYSICS WITH PYTHON

QUANTUM MECHANICS

SCATTERING FROM A STEP POTENTIAL

Ian Cooper

matlabvisualphysics@gmail.com

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qm030.py

Numerical solution of the Schrodinger equation for an electron beam incident (electron energy E) upon a finite square potential.

qm031.py

Analytical solution of the Schrodinger equation for an electron beam incident (electron energy E) upon a finite square potential.

qm032.py

Animation of the electron beam scattering from a step potential

GitHub

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INTRODUCTION

In this article, we shall investigate the solutions of the time-independent Schrodinger wave equation for an electron beam where the potential energy $U(x)$ is represented by a step function

(1) $\quad x \le 0 \quad U(x) = 0 \qquad x > 0 \quad U(x) = U_0 \quad U_0 = \text{constant}$

This is an idealized potential which approximates many potentials that occur in real situations. The results we obtain using our idealized potential illustrate a number of characteristic quantum mechanical phenomena.

We may think of $U(x)$ as an approximate representation of the potential energy function for an electron moving along the X axis of a system of two electrodes, separated by a small gap which are held at two voltages. Also, a step potential is a good approximation for the motion a conduction electron moving near the surface of a metal.

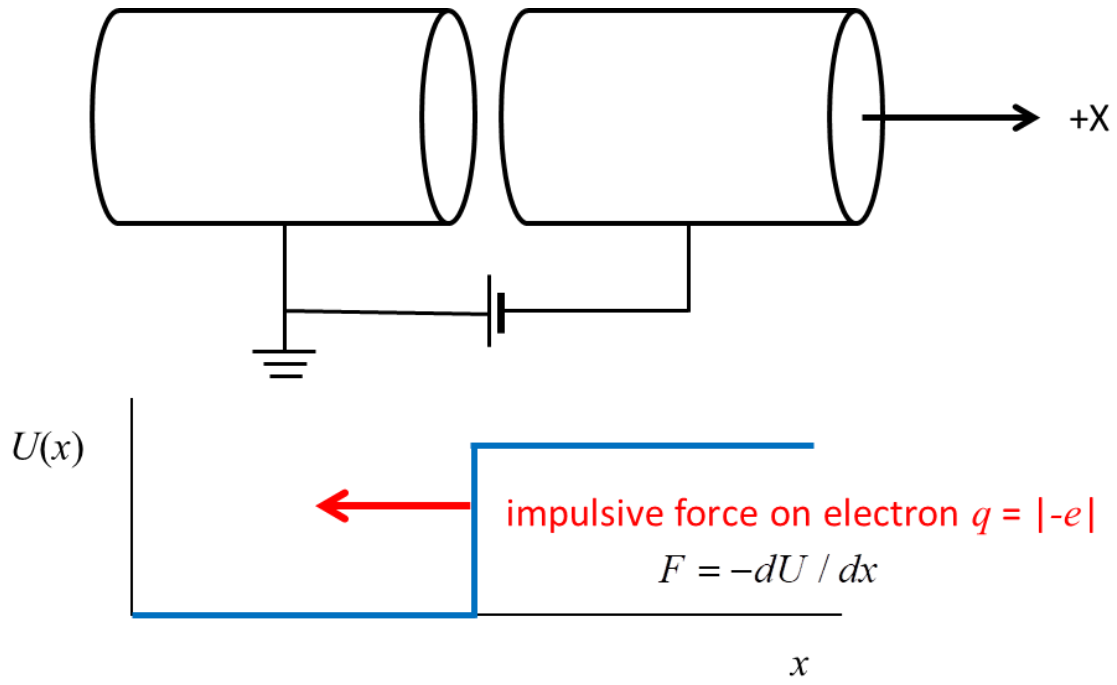

Fig. 1. Step potential function. The electron moves along the X axis of two cylindrical electrodes held at different voltages. The potential energy of the system is constant when an electron is inside either electrode, but changes rapidly when passing from one to the other.

For a classical particle, the subsequent motion when it impacts the step barrier depends on the kinetic energy of the classical particle and the height of the barrier as shown in figure 2.

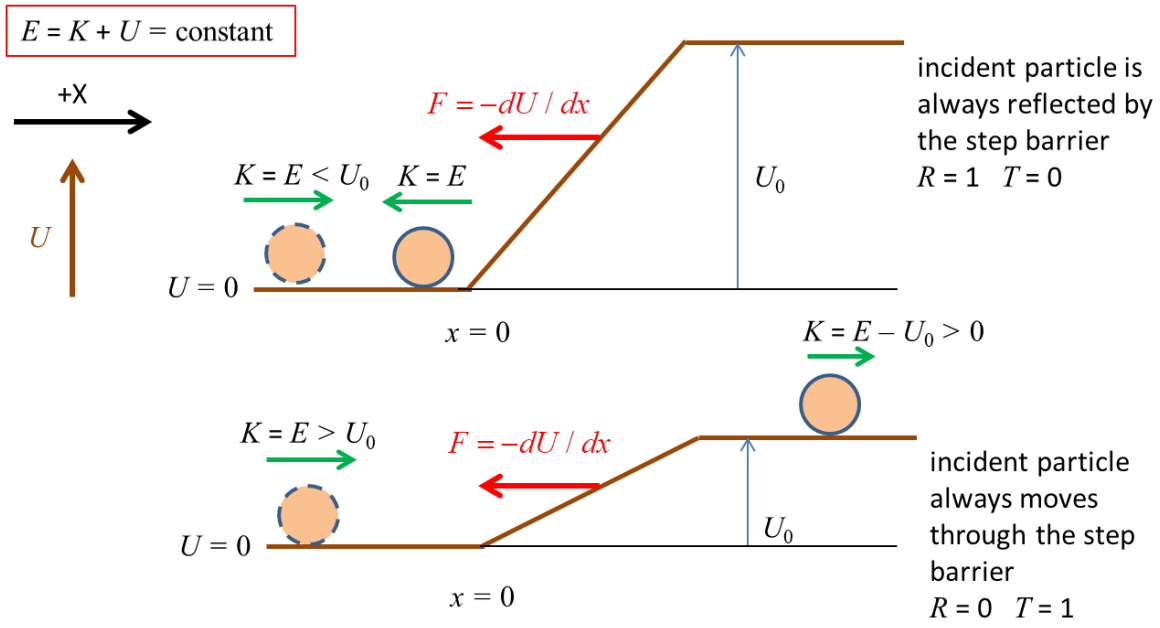

Fig. 2. The total energy of a classical particle is conserved, $E = K + U = \text{constant}$. If the incident particle has a total energy which is less than the height of the step potential $E < U_0$, then the particle will always be reflected (reflection coefficient $R = 1$, transmission coefficient $T = 0$). The particle cannot enter the region where $U = U_0$. If the incident particle has a total energy which is greater than the height of the step potential $E > U_0$, then the particle will always be transmitted pass the barrier ($R = 0$ and $T = 1$).

To determine the motion of an electron according to quantum mechanics, we must find a solution of the time independent Schrodinger equation, since the potential energy function is independent of time. We can solve the Schrodinger equation (equation 2) numerically using the Python ordinary differential equation solver

odeint. It is often much easier to solve the Schrodinger equation numerically, rather than doing lots of algebra to get an analytical solution. Also, for more realistic potential energy functions, there are no analytical solutions.

The time independent Schrodinger equation is

$$(2) \qquad -\frac{\hbar^2}{2m_E}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = E\,\psi(x)$$

where the solution is the **eigenfunction** $\psi(x)$ and the corresponding **wavefunction** $\Psi(x,t)$ which includes the time dependency is

$$(3) \qquad \Psi(x,t) = \psi(x)e^{-i\omega t} \qquad E = \hbar\omega$$

The Codes **qm030.py** (numerically) and **qm031.py** (analytically) solves the Schrodinger equation (equation 2) for the case where an electron beam is incident upon the step barrier

$$x \le 0 \quad U(x) = 0 \qquad x > 0 \quad U(x) = U_0$$

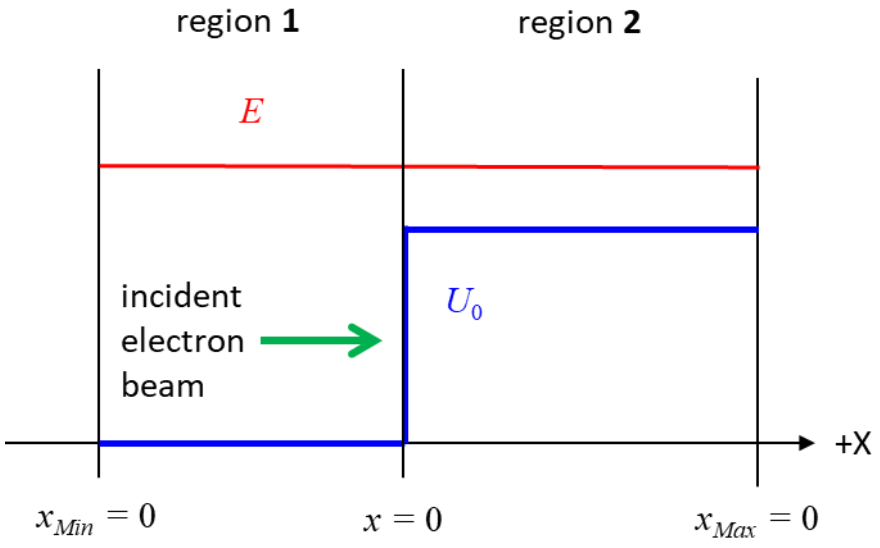

Fig. 3. Step potential $E > U_0$

For an electron beam travelling to the right (direction of increasing x) equation 3 can be expressed as

$$\Psi(x,t) = A\, e^{i\left(\frac{p}{\hbar}x - \frac{E}{\hbar}t\right)} = A\, e^{i(kx-\omega t)} = A\, e^{ikx}\, e^{-i\omega t}$$

$$\psi(x) = A\, e^{ikx}$$ $\psi(x)$ is called an **eigenfunction**

propagation constant (wave number) $k = \frac{p}{\hbar} = \frac{\sqrt{2mE}}{\hbar}$

angular frequency $\omega = \frac{E}{\hbar}$

de Broglie wavelength $\lambda = \frac{h}{p}$

momentum $p = \hbar k = h/\lambda$

velocity $v = p/m = h/m\lambda = \hbar k/m$

For a free particle the total energy can have any value greater than or equal to zero since the particle is not confined.

THE ANALYTICAL MODEL

An analytical solution of the Schrodinger equation for the step potential energy function is

(4A) $x < 0$ $\psi(x) = A\exp(i k_1 x) + B\exp(-i k_1 x)$

(4B) $x > 0$ $\psi(x) = C\exp(i k_2 x)$

where $p_1 = \hbar k_1 = \sqrt{2mE}$ $k_1 = \sqrt{2mE}/\hbar$

$$p_2 = \hbar k_2 = \sqrt{2m(E - U_0)} \quad k_2 = \sqrt{2m(E - U_0)}/\hbar$$

In equation 4A, the first term corresponds to a wave travelling to the right (incident beam: direction of increasing x) and the second term to a wave traveling to the left (reflected beam: direction of decreasing x).

- If $E > U_0$ (k_2 real) then equation 4B describes the motion of a free particle of momentum $p_2 = \hbar k_2$ moving to the right (wave only propagates in the direction of increasing x).
- If $E < U_0$ (k_2 imaginary) then equation 4B describes an exponential decreasing eigenfunction where

  $$\alpha = \sqrt{2m(U_0 - E)}/\hbar$$

  is called the **attenuation coefficient**.

The eigenfunction $\psi(x)$ is finite and continuous at the step $x = 0$. Therefore, at $x = 0$, its value and first derivative $d\psi(x)/dx$ must be single valued. Hence,

$$A + B = C \qquad i k_1 (A - B) = i k_2 C$$

Solving for *B* and *C* in terms of *A*

$$B = \frac{k_1 - k_2}{k_1 + k_2} A \qquad C = \frac{2k_1 k_2}{k_1 + k_2} A$$

Thus, the eigenfunctions for the incident, reflected and transmitted beams are

$$\psi_{inc} = A \exp(i k_1 x)$$

$$\psi_{refl} = B \exp(i k_1 x)$$

$$\psi_{trans} = C \exp(i k_2 x)$$

Number density *n* probability (beam intensity) *j*

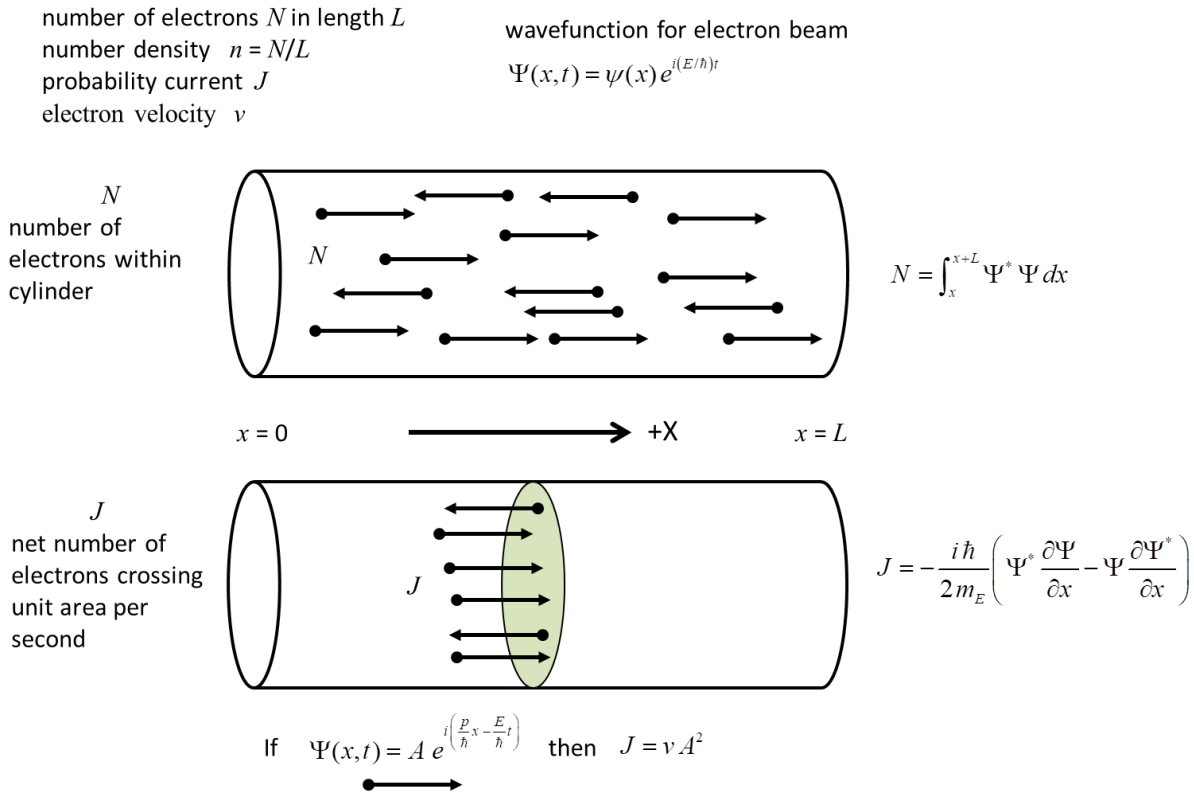

Fig. 4. Probability current.

For a free travelling beam with A being the amplitude of the eigenfunction, the number of particles N in a length L is

$$N = nL = \int_0^L \psi_A^{\,*}\, \psi_A\, dx = A^2$$

The number densities [number of particles per unit length] n are:

Incident beam $$n_{inc} = \frac{1}{L_1}\int_0^{L1} \psi_A^{\,*}\, \psi_A\, dx = A^2$$

Reflected beam $$n_{refl} = \frac{1}{L_1}\int_0^{L1} \psi_B^{\,*}\, \psi_B\, dx = B^2$$

Transmitted beam $$n_{trans} = \frac{1}{L_2}\int_0^{L2} \psi_C^{\,*}\, \psi_C\, dx = C^2$$

The beam intensities or probability fluxes [s^{-1}] J are:

Incident beam $J_{inc} = v_1 A^2$

Reflected beam $J_{refl} = -v_1 B^2$

Transmitted beam $J_{trans} = v_2 C^2$

The probability flux of our system is a constant, independent of both position and time. So, the probability flux in region 1 must be equal to the probability flux in region 2. We shall refer to this as the **net flux** J_{net}.

Region 1 $J_1 = J_{inc} + J_{refl} = J_{net}$

Region 2 $J_2 = J_{trans} = J_{net}$

A stream of electrons constitutes a flow of charged particles and hence an electric current. Such a current can be quantitatively described in terms of wavefunctions. We can define the quantity, J which is called the **probability current**.

(8) $$J = -\frac{i\hbar}{2m_E}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right) = \frac{\hbar k}{m} A^2$$

The reflection coefficient R and the transmission coefficients T are:

$$R = \frac{J_{refl}}{J_{inc}} = \frac{B^2}{A^2} = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 \qquad T = \frac{J_{trans}}{J_{inc}} = \frac{C^2}{A^2} = \left(\frac{2k_1}{k_1 + k_2} \right)^2$$

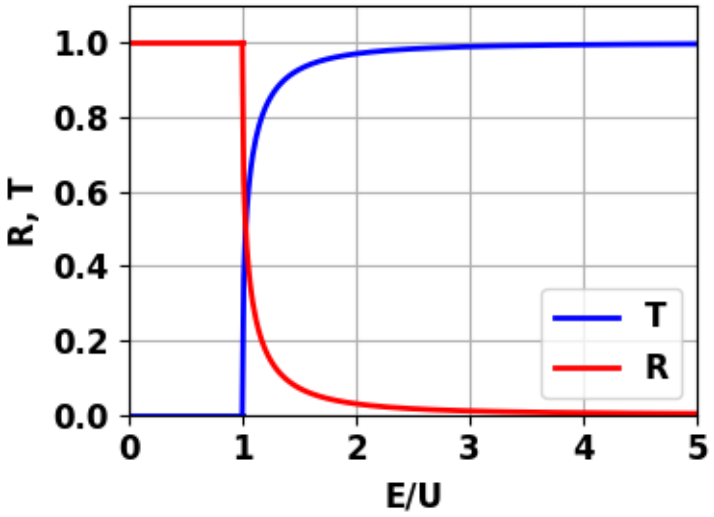

Fig. 5. Transmission T, and Reflection coefficients. **qm031.py**

SIMULATIONS qm031.py qm030.py qm032.py

The Code **qm031.py** gives the analytical solution of the Schrodinger equation for the step potential. The results of are displayed numerically in the Console Window and graphically.

$E > U_0$

```
E  = 80  eV
U0 = 50  eV
K1  = 80  eV
K2  = 30  eV
omega    = 1.215e+17  rad/s
period T  = 5.170e-17  s
deBroglie lambda1 = 0.137 nm
deBroglie lambda2 = 0.224 nm
Jinc    = 5.30e+06  1/s
Jref    = -3.07e+05 1/s
Jnet    = 5.00e+06  1/s
Jtrans  = 5.00e+06  1/s
Reflection coeff.   R = 0.06
Transmission coeff. T = 0.94
```

Note: The kinetic energy of the electrons in the beam in region 1 is greater than the kinetic energy in region 2. The beam slows down after entering region 2, hence the longer wavelength than in region 1. The probability current is constant and the same in both regions. Most of the electrons in the beam are transmitted and not reflected.

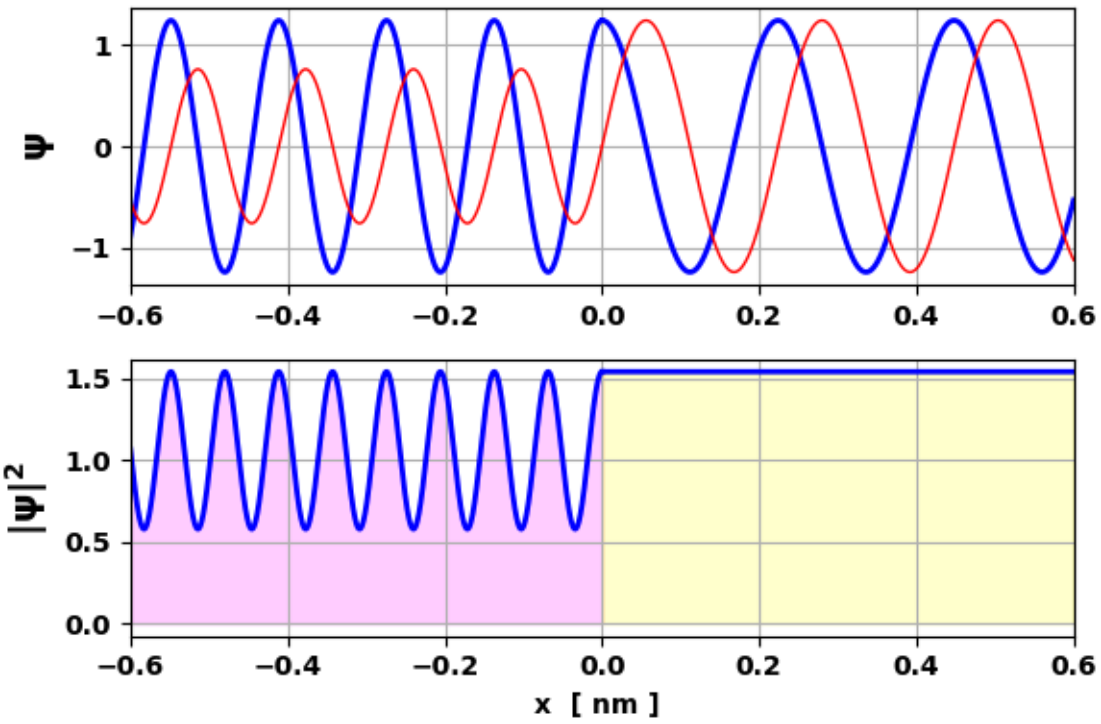

Fig. 6. **Real** and **imaginary** parts of the wavefunction and the probability density function for $E > U_0$ at time t.
E = 80 eV, U0 = 50 eV

In region 1 the incident wave travels to the right while the reflected wave travels to the left. The two waves interfere with each other and produce a partial standing wave (the positions of nodes and antinodes vary slightly with time as the amplitudes of the incident and reflected waves are not equal). In region 2, a travelling wave propagates to the right.

If the height of the step is increased then the reflection is increased and the transmission decreased as shown in figure 7.

E = 80 eV
U0 = 70 eV
K1 = 80 eV
K2 = 10 eV
omega = 1.215e+17 rad/s
period T = 5.170e-17 s
deBroglie lambda1 = 0.137 nm
deBroglie lambda2 = 0.388 nm
Jinc = 5.30e+06 1/s
Jref = -1.21e+06 1/s
Jnet = 4.09e+06 1/s
Jtrans = 4.09e+06 1/s
Reflection coeff. R = 0.23
Transmission coeff. T = 0.77

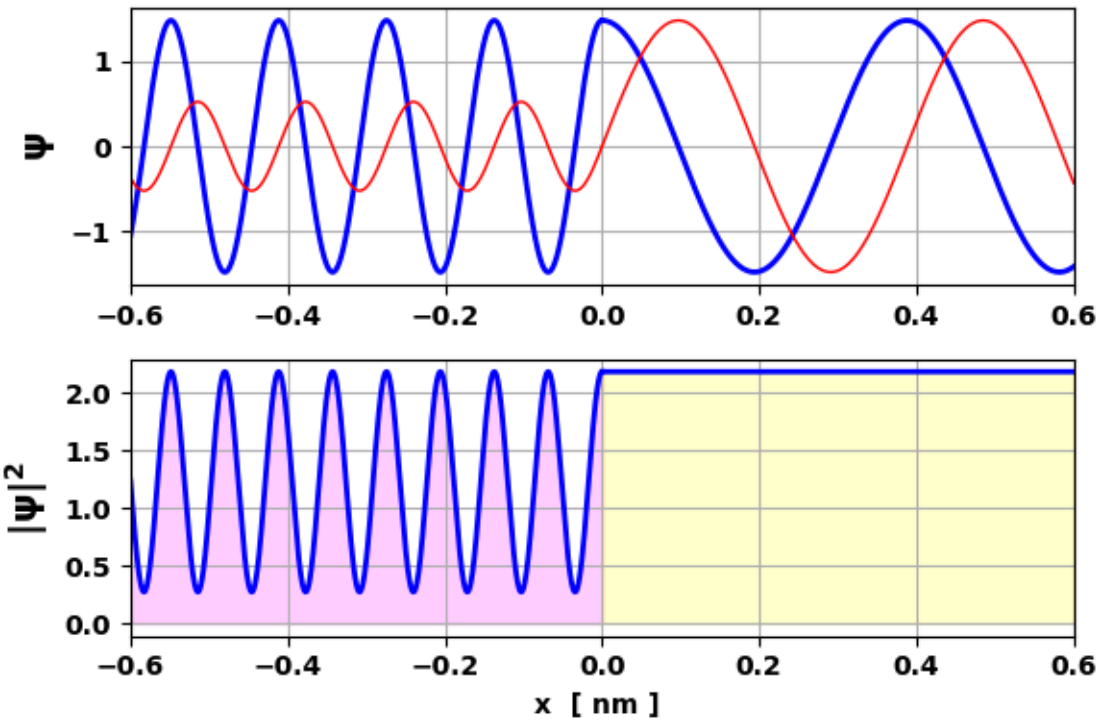

Fig. 7. Note the significant increase in the wavelength of the wavefunction in region 2. E = 80 eV, U0 = 70 eV

$E < U_0$

E = 80.0 eV
U0 = 80.5 eV
K1 = 80 eV
K2 = -0 eV
omega = 1.215e+17 rad/s
period T = 5.170e-17 s
deBroglie lambda1 = 0.137 nm
deBroglie lambda2 = 0.000 nm
Jinc = 5.30e+06 1/s
Jref = -5.04e+06 1/s
Jnet = 2.62e+05 1/s
Jtrans = 2.62e+05 1/s

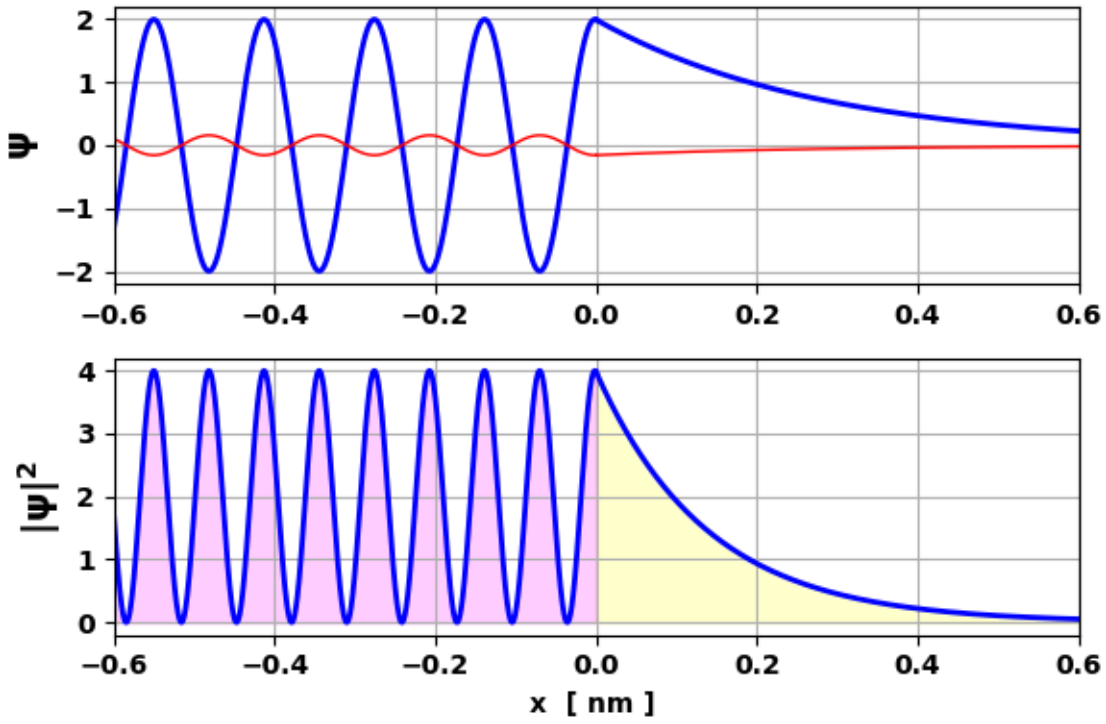

Fig. 8. For the finite square step potential in the case E < U0, there is a finite non-zero probability that the electron will penetrate the step, even though there is no possibility of tunnelling through it.
E = 80 eV, U0 = 80.5 eV

As the height of the step potential is increased further, the penetration into the classical forbidden region (region 2) results in rapid decline in the penetration distance (figure 9).

E = 80.0 eV
U0 = 100.0 eV
K1 = 80 eV
K2 = -20 eV
omega = 1.215e+17 rad/s
period T = 5.170e-17 s
deBroglie lambda1 = 0.137 nm
deBroglie lambda2 = 0.000 nm
Jinc = 5.30e+06 1/s
Jref = 1.49e+06 1/s
Jnet = 6.79e+06 1/s
Jtrans = 6.79e+06 1/s

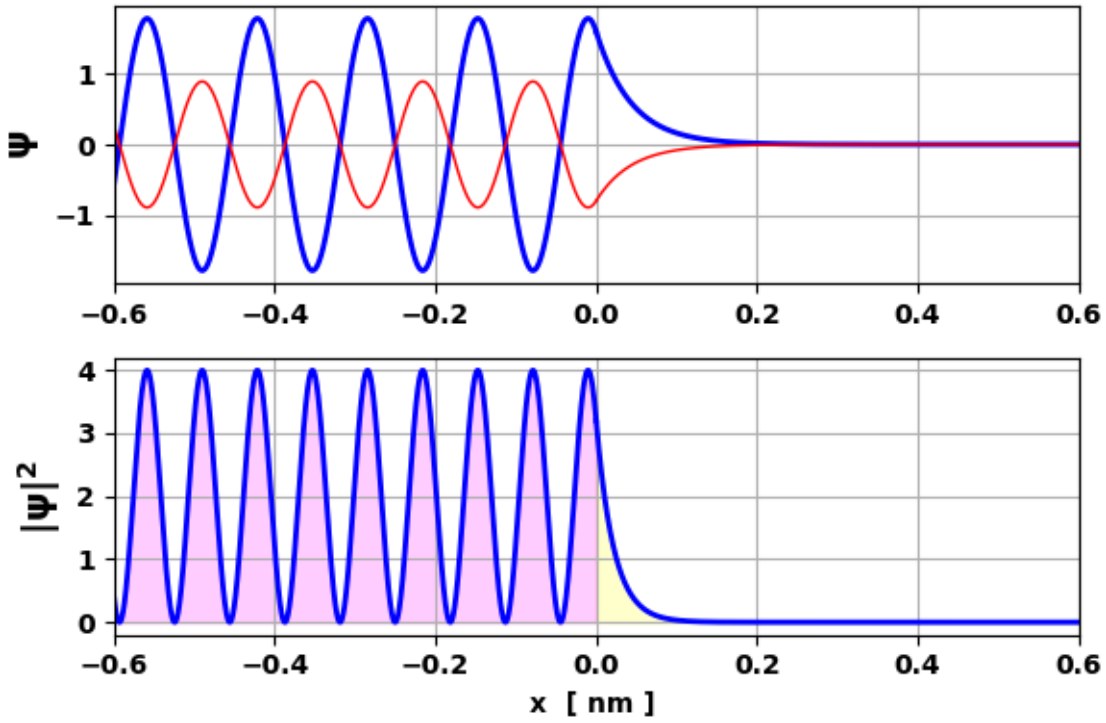

Fig. 9. E = 80 eV, U0 = 100 eV

NUMERICAL SOLUTION qm030.py

Surprisingly, it is not easy to solve the [1D] time independent Schrodinger equation for the step potential.

(1) $x \le 0 \quad U(x) = 0 \qquad x > 0 \quad U(x) = U_0 \quad U_0 = \text{constant}$

(2)
$$-\frac{\hbar^2}{2m_E}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\psi(x) = E\psi(x)$$
$$\frac{\partial^2\psi(x)}{\partial x^2} = -\frac{2m_E}{\hbar^2}\big(E - U(x)\big)\psi(x)$$

To use the Python function **odeint** to solve the Schrodinger equation, we need to write the Schrodinger equation as a set of first order ODE.

Let $C = -\dfrac{2m_E}{\hbar^2} \qquad u = \psi(x) \qquad v = du/dx$ then

$$v = \frac{du}{dx} \qquad \frac{dv}{dx} = C\big(E - U\big)u$$

The Python function in the code **qm030.py** used is

```
def lorenz(x, state):
    u, v = state
    P = E0
      if x > 0:
     P = E0 - U0
      du = v
    dv = C*P*u
    return [du, dv]
```

To call the function one has to be very careful in setting the correct initial conditions. The initial conditions are specified by the vector u with component u1 for the initial value of the wavefunction and u2 for the slope of the wavefunction. Also, the integration must be done from xMax to xMin and this is done using the **flip** command. The wavefunction is a complex quantity $\left(\psi = \psi_R + \psi_I\ j \quad j = \sqrt{-1}\right)$, so the Schrodinger equation must be solved for both the real and imaginary parts. Finally, the wavefunction must be flip because of the x span was reversed and its maximum value set to 1.

Figure 10 shows a sample output with the same parameters for E and U0 as in figure 6. The analytical (**qm031.py**) solution and numerical solution (**qm030.py**) produce the same wavefunctions but with different amplitudes and phases and the same probability density.

```
xSpan = np.flip(x)
u1 = 0; u2 = k1
u0 = [u1,u2]
sol = odeint(lorenz, u0, xSpan,  tfirst=True)
psiR = sol[:,0]
u1 = 1; u2 = 0
u0 = [u1,u2]
sol = odeint(lorenz, u0, xSpan, tfirst=True)
psiI = sol[:,0]
psiR = np.flip(psiR)/np.amax([psiI,psiR])
psiI = np.flip(psiI)/np.amax([psiI,psiR])
probD = psiR**2 + psiI**2
```

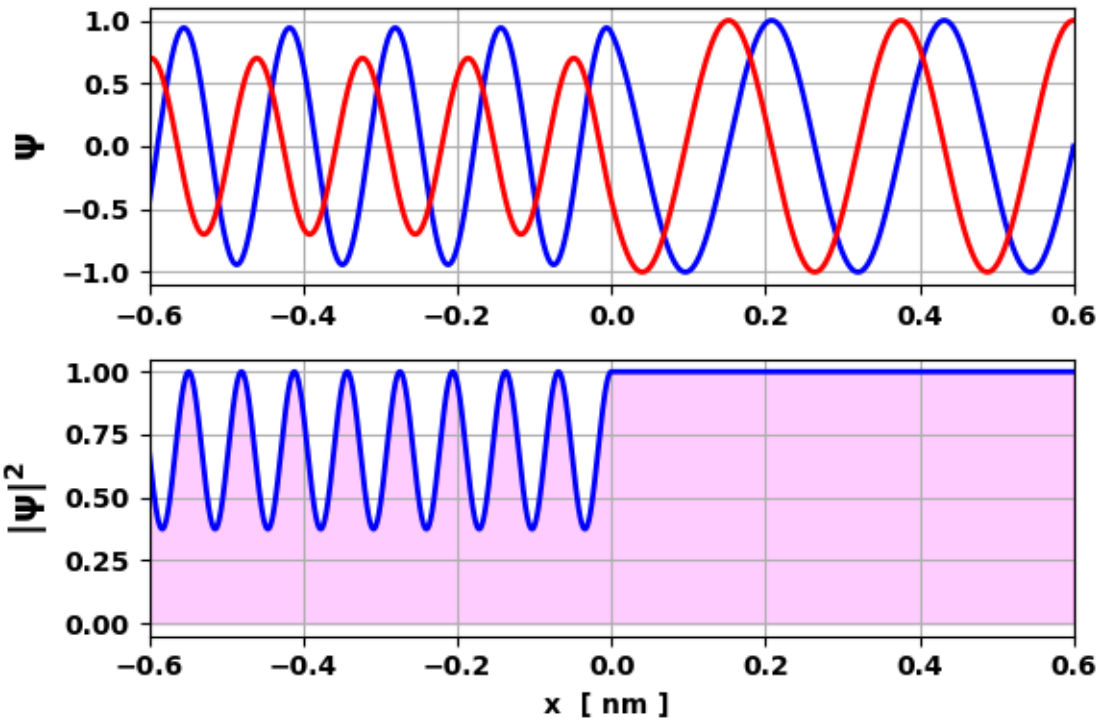

Fig.10. **Real** and **imaginary** parts of the wavefunction and the probability density function for $E > U_0$ at time t.

E = 80 eV, U0 = 50 eV

You can view animated images of the scattering of the electron beam from the finite step potential by viewing the following two links:

- E < U0
- E > U0