DOING PHYSICS WITH PYTHON

QUANTUM MECHANICS

SCATTERING FROM A POTENTIAL BARRIER

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qm033.py

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

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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 square potential barrier

$$
\begin{array}{lll}
 & x \le 0 \quad U(x) = 0 & \text{(region 1)} \\
(1) & 0 < x < a \quad U(x) = U_0 > 0 \quad U_0 = \text{constant} & \text{(region 2)} \\
 & x \ge a \quad U(x) = 0 & \text{(region 3)}
\end{array}
$$

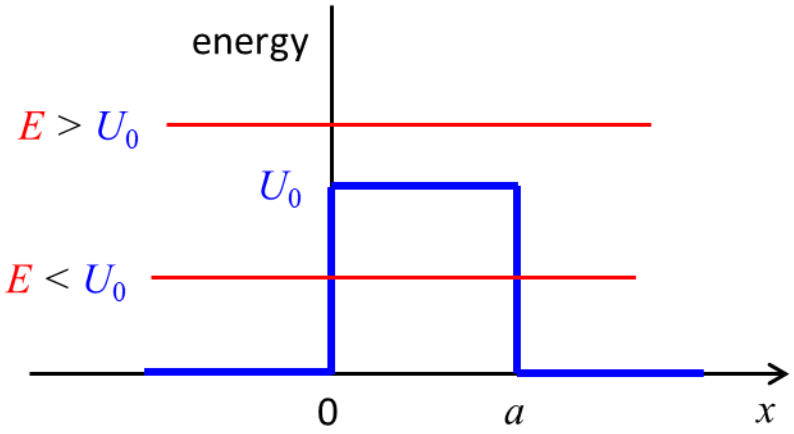
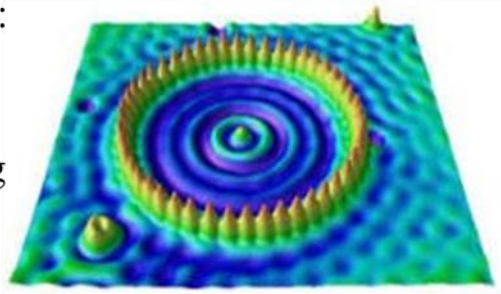


Fig. 1. Hill potential barrier.

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 such as tunnelling. Examples of tunnelling phenomena include alpha decay, fusion reactions, and the scanning tunnelling microscope.

Fig. 2 Tunnelling currents of electrons: iron atoms on a copper surface (ring – quantum corral). Surface electrons trapped inside the corral form standing waves.



For a classical particle of kinetic energy K, the subsequent motion after it impacts a potential hill barrier of heigh U_0 depends on whether $K > U_0$ or $K < U_0$

Classical particle:

$K > U_0$ the classical particle will penetrate the barrier

$K < U_0$ the classical particle will be reflected by the barrier

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

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

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

The Code **qm033.py** solves the Schrodinger equation (equation 2) numerically for a hill potential barrier (equation 1).

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

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

Total energy E, potential energy U, kinetic energy $K = E - U$

Propagation constant (wave number)

$$k_1=k_3=\frac{\sqrt{2mE}}{\hbar} \qquad k_2=\frac{\sqrt{2m(E-U_0)}}{\hbar}$$

de Broglie wavelength

$$\lambda_1=\lambda_2=\frac{2\pi}{k_1} \qquad \lambda_3=\frac{2\pi}{k_3}$$

Angular frequency $\omega = E/\hbar$

Momentum $p=\hbar k=h/\lambda=\sqrt{2mK}$

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

In regions 1 and 3, the propagation constants k_1 and k_3 are real numbers, so the eigenfunctions ψ_1 and ψ_3 are sinusoidal functions. If $E > U_0$ then k_2 is real and the eigenfunction is sinusoidal, but if $E < U_0$ then k_2 is an imaginary number, thus ψ_2 is an exponentially decreasing function.

The reflection coefficient R and the transmission coefficients T are:

$$R + T = 1 \qquad R = 1 - T$$

$$E > U_0$$

$$k\,a = \sqrt{\frac{2\,m\,U_0\,a^2}{\hbar^2}\left(\frac{E}{U_0} - 1\right)}$$

$$T = \left[1 + \frac{\sin^2(k\,a)}{4\left(\frac{E}{U_0}\right)\left(\frac{E}{U_0} - 1\right)}\right]^{-1}$$

$$E < U_0$$

$$k\,a = \sqrt{\frac{2\,m\,U_0\,a^2}{\hbar^2}\left(1 - \frac{E}{U_0}\right)}$$

$$T = \left[1 + \frac{\sinh^2(k\,a)}{4\left(\frac{E}{U_0}\right)\left(1 - \frac{E}{U_0}\right)}\right]^{-1}$$

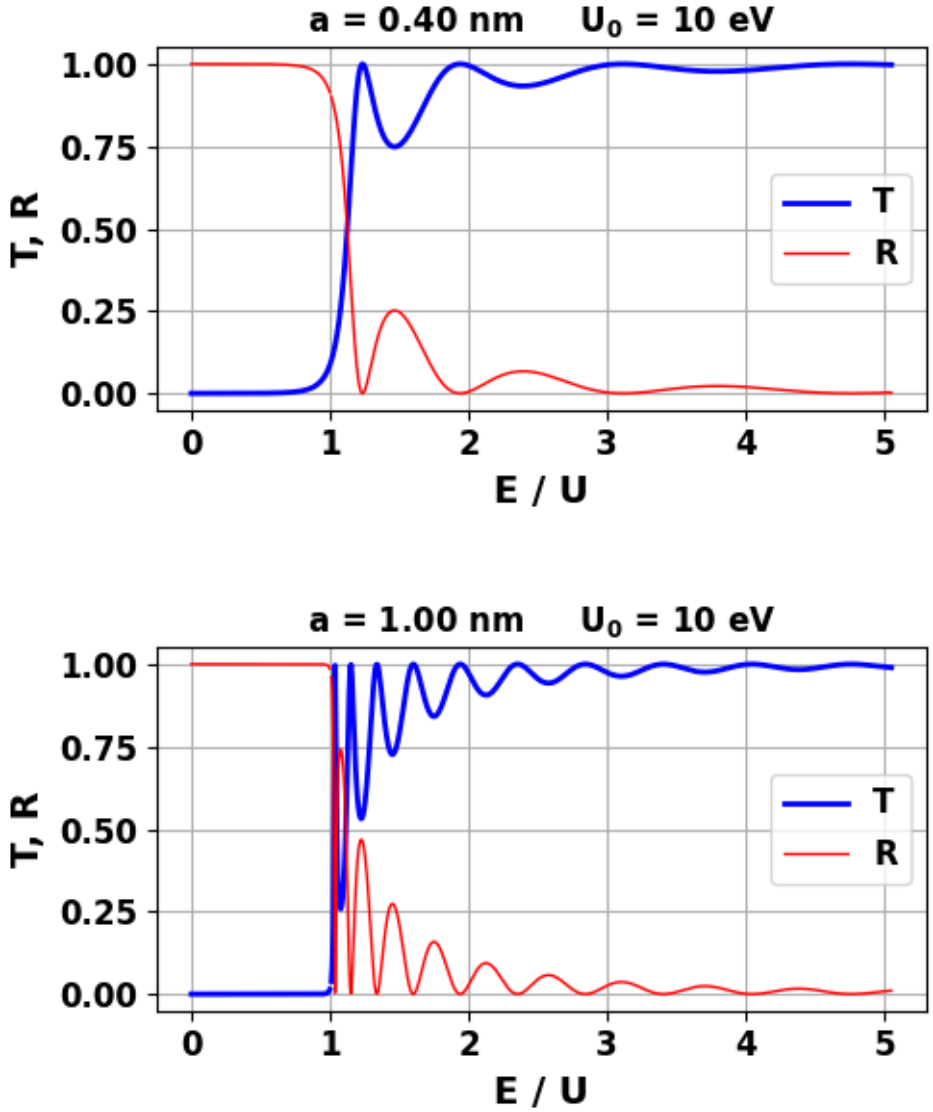


Fig. 3. Transmission *T*, and Reflection *R* coefficients for an electron incident upon a potential hill barrier of width *a* and height U_0. The oscillations in *T* at higher values of *E/U* are due to the interference of the reflections at the discontinuities of the potential energy function *U*.

Quantum mechanics predicts that there maybe some reflection when $E > U_0$ and that there is a certain probability that the electron will be transmitted through the barrier into the region $x > a$ when $E < U_0$. A particle in tunnelling through a barrier whose height exceeds its total energy is behaving purely like a wave. But, in the region beyond the barrier it can be detected as a localized particle.

For $E > U_0$, the transmission coefficient in general is somewhat less than one owing to reflections in the discontinuities of the potential. However, $T = 1$ when for region ,2 the width of the barrier a is equal to the distance of an integral number of de Broglie half-wavelengths and so the particles pass into region 3 without any reflection

$$E > U_0 \quad ka = n\pi \quad n\lambda = 2a \quad a = n(\lambda / 2) \quad n = 1, 2, 3, \ldots \quad T = 1$$

This occurs as a result of the interference between reflections at the edges of the barrier $x = 0$ and $x = a$ (figure 4).

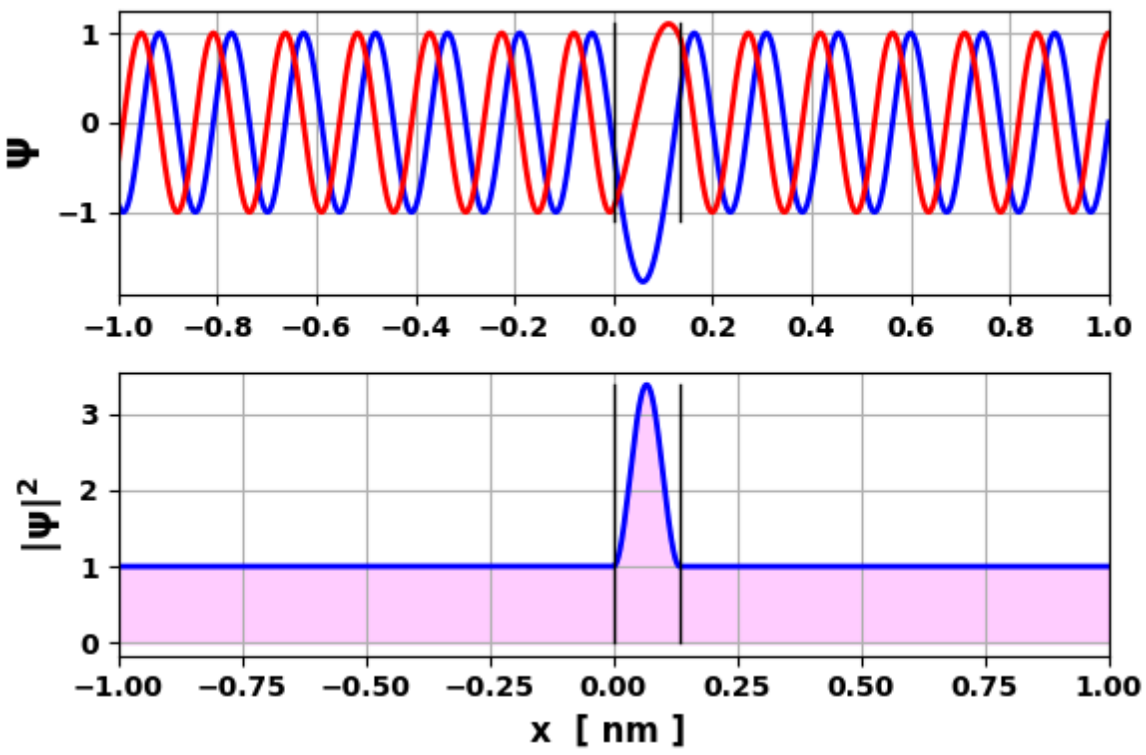


Fig. 4. Plots of the wavefunction and probabilty density $E_0 > U_0$.

E0 = 71 eV U0 = 50 eV a = 0.134 nm

wavelength: regions 1 & 3 wL = 0.146 nm

wavelength: region 2 wL2 = 0.268 nm

a/wL2 = 0.500

Transmission probability percentage T = 100

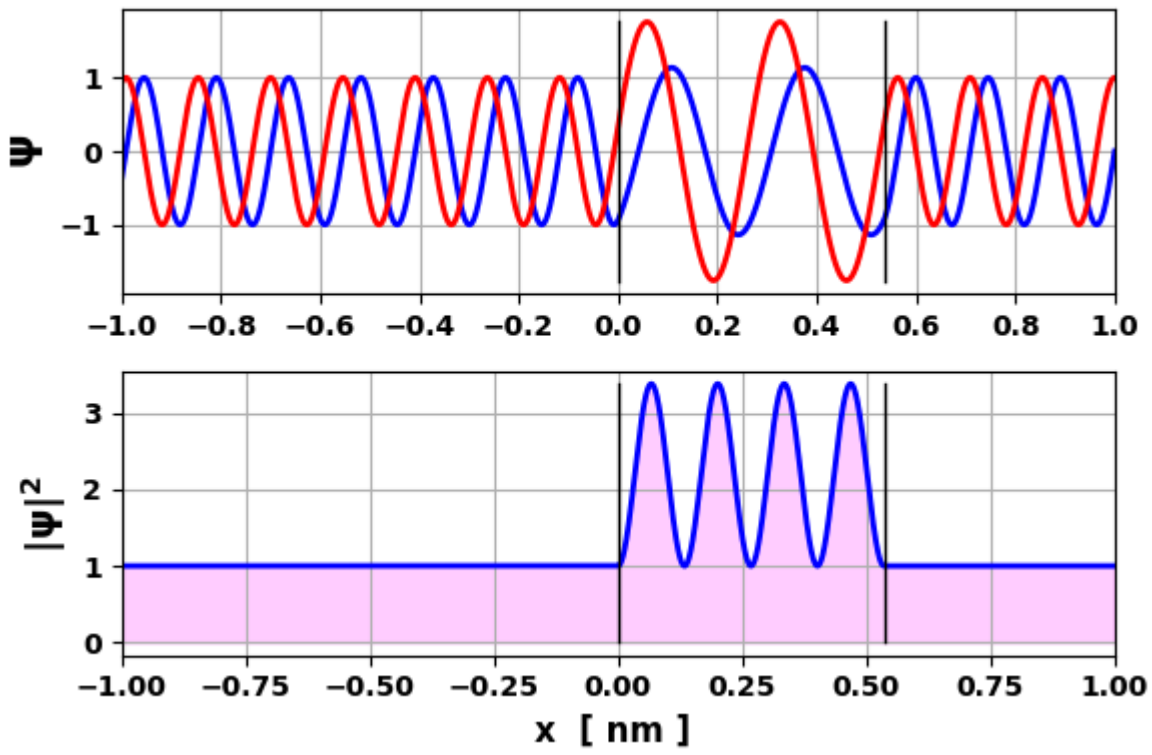


Fig. 5. Plots of the wavefunction and probabilty density $E_0 > U_0$.

E0 = 71 eV U0 = 50 eV a = 0.535 nm

wavelength: regions 1 & 3 wL = 0.146 nm

wavelength: region 2 wL2 = 0.268 nm

a/wL2 = 2.000

Transmission probability percentage T = 100

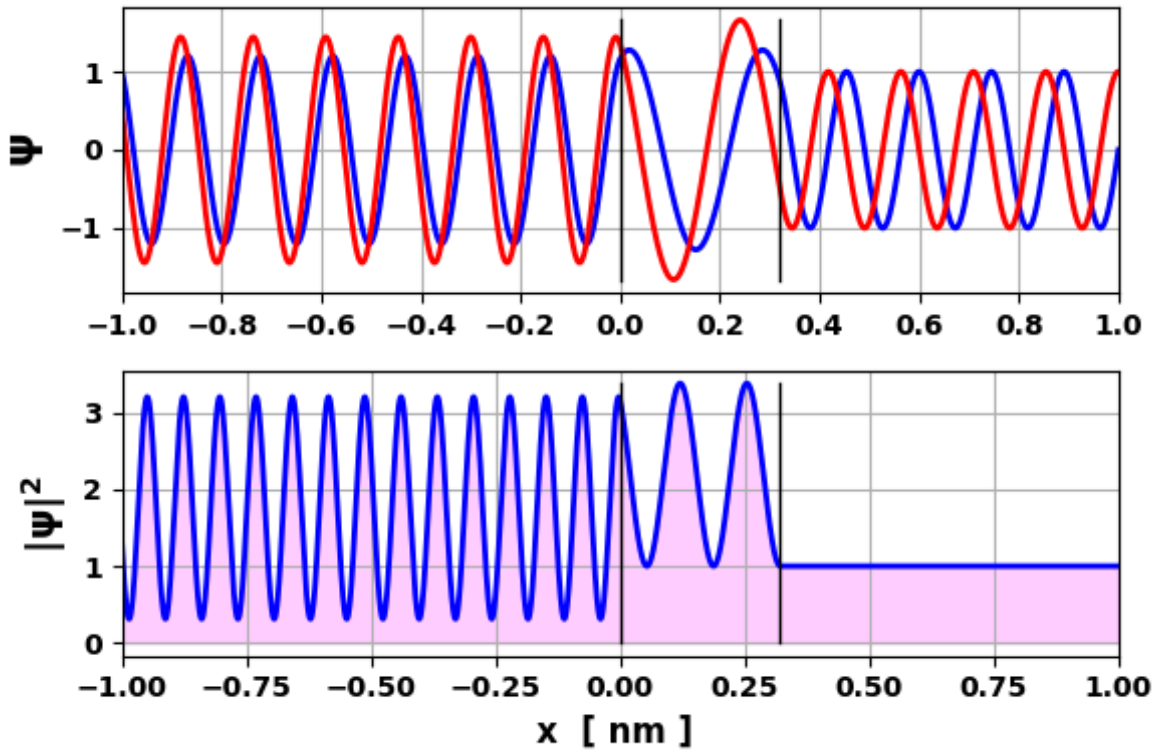


Fig. 6. Plots of the wavefunction and probabilty density $E_0 > U_0$.

E0 = 71 eV U0 = 50 eV a = 0.321 nm

wavelength: regions 1 & 3 wL = 0.146 nm

wavelength: region 2 wL2 = 0.268 nm

a/wL2 = 1.200

Transmission probability percentage T = 57

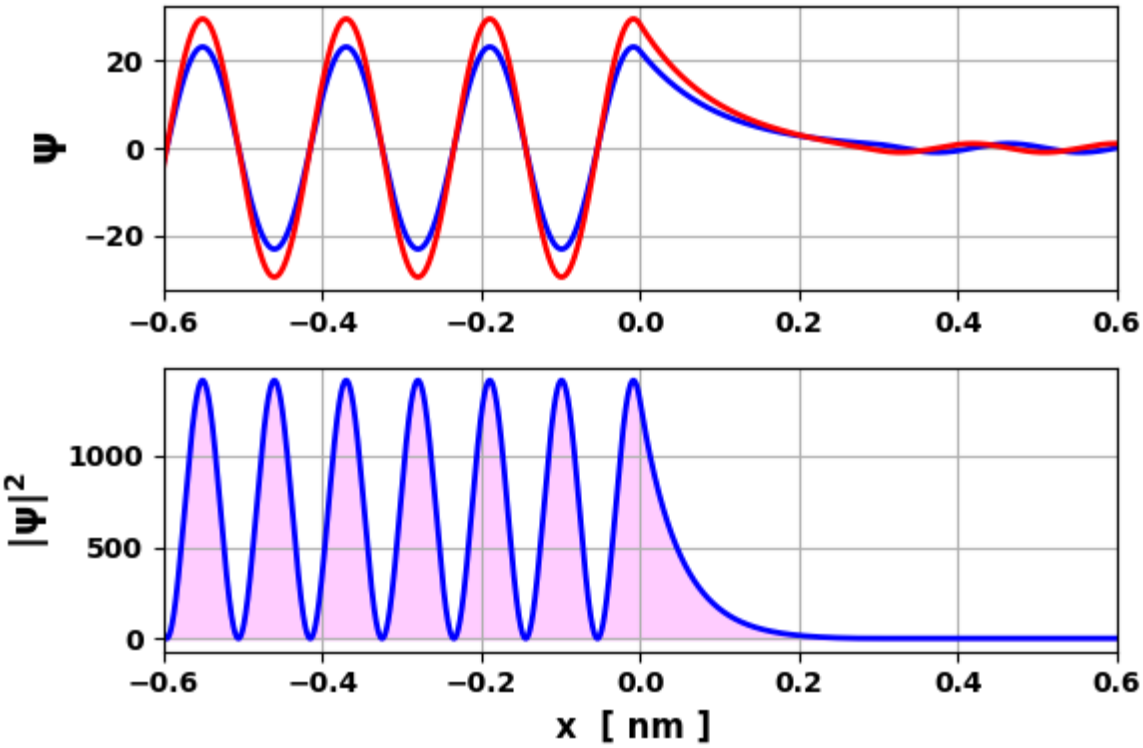


Fig. 7. Plots of the wavefunction and probabilty density $E_0 < U_0$. The decreasing curve in region 2 is not a simple exponential decline, but has both decreasing and increasing exponential contributions.

E0 = 46 eV U0 = 50 eV a = 0.321 nm

wavelength: regions 1 & 3 wL = 0.181 nm

Transmission probability percentage T = 0

The probability transmission percentage T21 is calculated in the Code **qm033.py** by finding the areas under the probability density function in regions 1 and 3 divided by the width of regions 1 and 3.

```
# Probability per unit length
fn = probD[x<0]
z = x[x<0]
prob1 = simps(fn,z)
fn = probD[x>aB]
z = x[x>aB]
prob2 = simps(fn,z)
  #   % Transmission probability
T21 = 100*(prob2/prob1)*(-xMin/(xMax-aB))
```

We can also investigate a potential well barrier. A sample simulation is shown in figure 8.

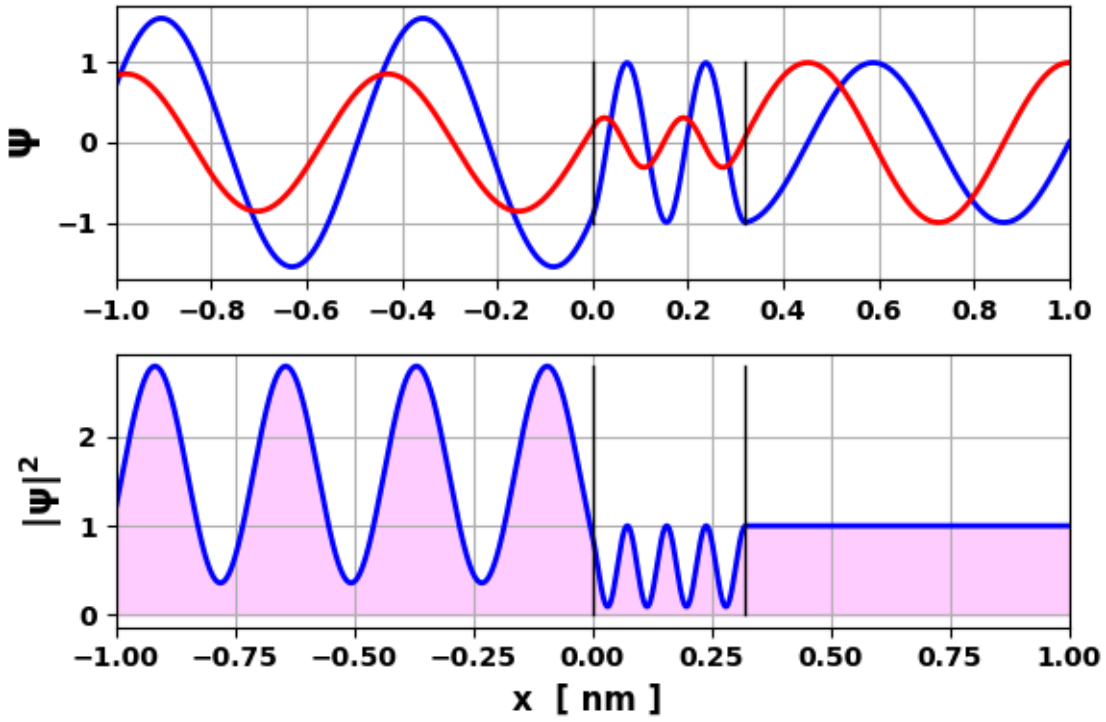


Fig. 8. A well potential barrier U_0 = -50.

E0 = 5 eV **U0 = -50 eV** a = 0.321 nm

wavelength: regions 1 & 3 wL = 0.548 nm

wavelength: region 2 wL2 = 0.165 nm

a/wL2 = 1.942

Transmission probability percentage T = 60

It is a very easy task to change the Code for a variety of different potential energy functions by simply changing the function for the integration

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