0. Motivation

- Tunneling is such an interesting phenomenon. There are still many questions despite the age of this discovery.
- I picked this topic because I want to visualize the dynamics of a wave packet tunneling through a barrier.
- However, there are still leading questions about the tunneling time and such. The technique utilized in my project might not lead to the most accurate results of tunneling and its actual representation, but they show a general picture of the phenomenon.

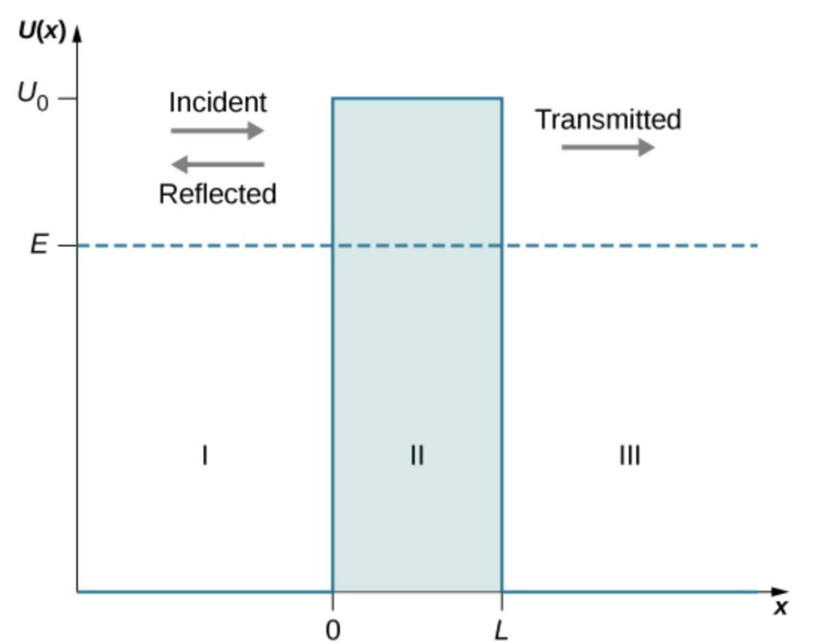
1. Description of the problem

An interesting question occurs when the energy of an incoming wave packet is less than the energy of a barrier.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x),$$

This situation exhibits the phenomenon of tunneling

General Model



$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I(x)}{dx^2} = E\psi_I(x),$$

in region I: $-\infty < x < 0$,

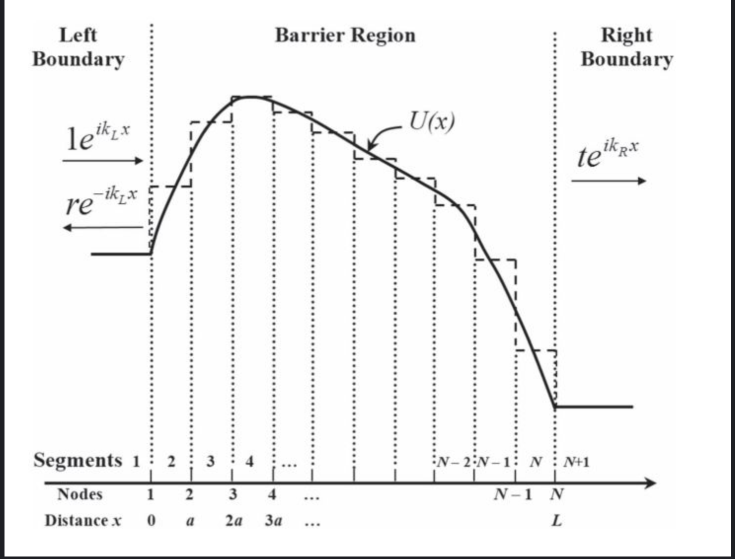
$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}(x)}{dx^2} + U_0\psi_{II}(x) = E\psi_{II}(x)$$

in region II: $0 < x < L$,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{III}(x)}{dx^2} = E\psi_{III}(x)$$

in region III: $L < x < +\infty$,

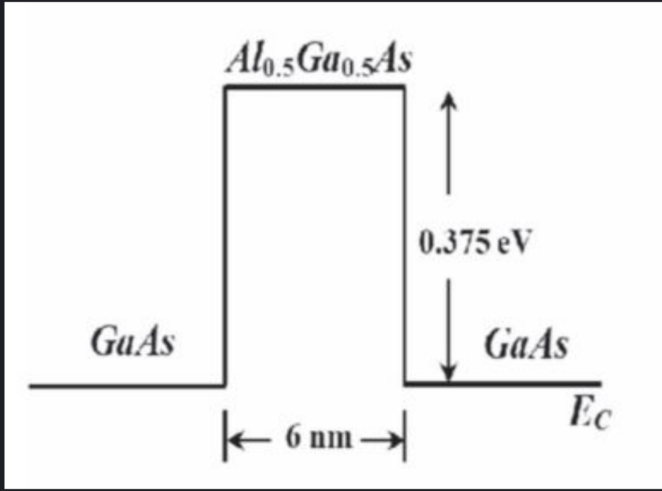
Certain barriers could be solved analytically with the application of PDE when we separate them into multiple equations. Analytically, solving some tunneling problems is impossible and needs the involvement of numerical methods. Therefore, I utilize split operator and fourier methods in this project.

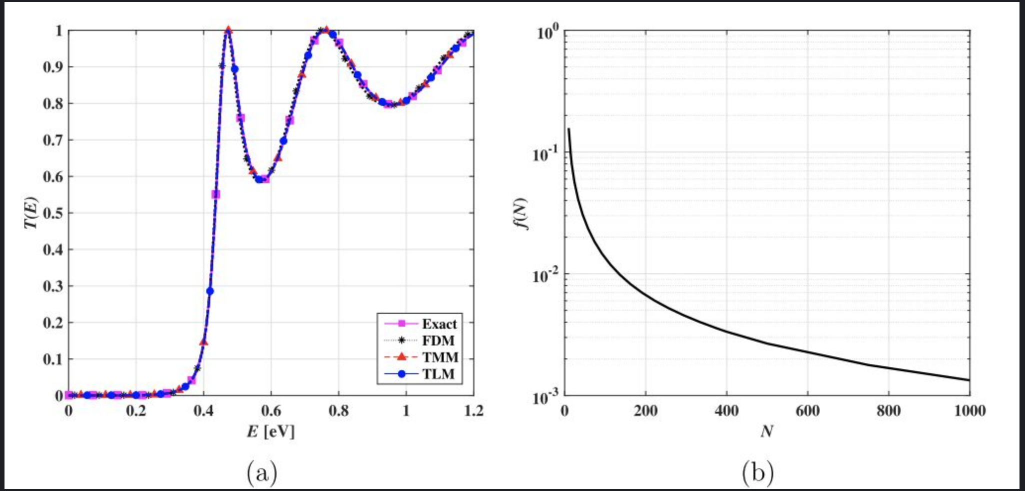


Finite Difference Method (FDM) separates the space into multiple discretizations.

$$\psi_{\mathrm{L}}(x) = \exp(ik_{\mathrm{L}}x) + r\exp(-ik_{\mathrm{L}}x);\ x < 0,$$

$$\psi_{\mathrm{R}}(x) = t\exp(ik_{\mathrm{R}}x);\ x > L,$$





Applying central derivative will give us this discretion of a wave packet.

$$f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) + \cdots,$$

$$f(x-\Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) - \cdots,$$

Taylor Series

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x},$$

$$f''(x) = \frac{\frac{f(x+\Delta x)-f(x)}{\Delta x} - \frac{f(x)-f(x-\Delta x)}{\Delta x}}{\Delta x} = \frac{f(x+\Delta x) - 2f(x) + f(x -}{(\Delta x)^2}$$

$$\frac{d}{dx}\left(\frac{\psi}{m^*}\right)\bigg|_i = \frac{\psi_{i+1} - \psi_i}{m_i^* a}, \quad \frac{d}{dx}\left(\frac{\psi}{m^*}\right)\bigg|_{i-1} = \frac{\psi_i - \psi_{i-1}}{m_{i-1}^* a},$$

$$\frac{d^2}{dx^2}\left(\frac{\psi}{m^*}\right)\bigg|_i = \frac{1}{a}\left(\frac{\psi_{i+1} - \psi_i}{m_i^* a} - \frac{\psi_i - \psi_{i-1}}{m_{i-1}^* a}\right),$$

Schrodinger in a discretized form

```
temp1  = (hbar)**2/(2*dx**2*mass(a-dx))
temp2 = (hbar)**2/(2*dx**2*mass(a))
Kl = sqrt(2*mass(a-dx)*(E-potential2(a-dx)))/hbar
psi(2) = (2*Im*temp1*sin(Kl*dx)-(temp2*exp(Im*Kl*dx)+E-potential2(x)-(temp1+temp2))*psi(1))/temp2
do i=2, N-2
    x=a+dx*float(i-1)
    temp1 = (hbar)**2/(2*dx**2*mass(x))
    temp2 = (hbar)**2/(2*dx**2*mass(x-dx))
    psi(i+1) = (temp2*psi(i-1)+(E-potential2(x)-(temp1+temp2))*psi(i))/temp1
enddo
!find psiN
temp1 = (hbar)**2/(2*dx**2*mass(b-dx))
temp2 = (hbar)**2/(2*dx**2*mass(b))
KR = sqrt(2*mass(b+dx)*(E-potential2(b+dx)))/hbar
psi(N)=-temp1*psi(N-1)/(E-potential2(b)-temp1-temp2+temp2*exp(Im*KR*dx))
```

Find node 1

$$[\eta_1 \exp(ik_L a) + E - U_1 - (\eta_1 + \eta_L)]\psi_1 + \eta_1\psi_2 = 2i\eta_L \sin(k_L a),$$

Find node between

$$\eta_{i-1}\psi_{i-1} + [E - U_i - (\eta_i + \eta_{i-1})]\psi_i + \eta_i\psi_{i+1} = 0$$

Find node N

$$\eta_{N-1}\psi_{N-1} + [E - U_N - (\eta_{N-1} + \eta_R) + \eta_R \exp(ik_R a)]\psi_N = 0$$

$$k_{L,R} = \sqrt{2m^*_{L,R}(E - U_{L,R})}/\hbar.$$

$$\tau(E) = |t|^2 k_R/k_L$$

We'll be able to find all the values of the wave in the barrier

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2. Main Numerical Methods Used

Fast Fourier Transform

$$\Delta x \Delta k = \frac{2\pi}{N}$$

$$\psi_n = \frac{\Delta k}{\sqrt{2\pi}} \sum_{m=0}^{N-1} \phi_m e^{ik_m x_n} \quad \Leftrightarrow \quad \phi_m = \frac{\Delta x}{\sqrt{2\pi}} \sum_{n=0}^{N-1} \psi_n e^{-ik_m x_n}.$$

I used fast fourier transform package to find the wave packet in momentum and space coordinates

```
call zfftf(N,psi,wsave) !forward Fourier transform
```

```fortran
!~~~~~~~~~~~~Momentum Space~~~~~~~~~~~~~~~!
!save momentum probability density space
if(mod(nt,n_save)==0)then !<-- save psi every n_save steps
    nt_tmp=nt_tmp+1
    do i=i_min,i_max
        psi_save_momentum(i,nt_tmp)=abs(psi(i)*Ns)**2!*sqrt(CMPLX(N,0.0d0)))**2
        psi_save_momentum_parts(i,nt_tmp)=psi(i)*Ns!*sqrt(CMPLX(N,0.0d0))
    enddo
endif
!--- calculate average p and deviation of p ---!
tmp1=0.0
tmp2=0.0
do i=1,N
    if(i<=(N/2))then !<-- momentum in Fourier space
        p=hbar*2.0*pi*(i-1)/(dx*N) !positive
    else
        p=-hbar*2.0*pi*(N+1-i)/(dx*N) !negative
    endif
    tmp1=tmp1+p*abs(psi(i)*Ns)**2
    tmp2=tmp2+(p**2)*abs(psi(i)*Ns)**2
enddo
av_p(nt)=tmp1*dp !average p
tmp2=tmp2*dp !average p**2
delta_p(nt)=sqrt(abs(tmp2)-av_p(nt)**2)

!psi=psi/Ns !1/sqrtN is needed due to fourth and back fft
call zfftb(N,psi,wsave) !backward Fourier transform
```

Saving the dynamics of momentum space

Calculate the momentum in Momentum Space

Record the average momentum and momentum uncertainty

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```fortran
call zfftb(N,psi,wsave) !backward Fourier transform
!save the coordinate space
if(mod(nt,n_save)==0)then !<-- save psi every n_save steps
    !nt_tmp=nt_tmp
    do i=i_min,i_max
        psi_save(i,nt_tmp)=abs(psi(i))**2
        psi_save_parts(i,nt_tmp)=psi(i)
    enddo
endif

!--- calculate average x and deviation of x ---!
tmp1=0.0
tmp2=0.0
do i=1,N
    x=a+dx*float(i)
    tmp1=tmp1+x*abs(psi(i))**2
    tmp2=tmp2+(x**2)*abs(psi(i))**2
enddo
av_x(nt)=tmp1*dx !average x
tmp2=tmp2*dx !average x**2
delta_x(nt)=sqrt(abs(tmp2)-av_x(nt)**2) !uncertainty
```

Saving the dynamics of coordinate space

Calculate the position in Coordinate Space

Record the average position and position uncertainty

Split technique for unitary operator

$$\psi(\mathbf{x}, \Delta t) = e^{-i\hat{H}\Delta t/\hbar}\psi(\mathbf{x}, 0)$$

$$\psi(\mathbf{x}, t + \Delta t) \approx \mathcal{F}^{-1}\left[e^{-i\mathbf{p}^2\Delta t/4m\hbar}\mathcal{F}\left[e^{-iV(\mathbf{x},t)\Delta t/\hbar}\mathcal{F}^{-1}\left[e^{-i\mathbf{p}^2\Delta t/4m\hbar}\mathcal{F}[\psi(\mathbf{x}, t)]\right]\right]\right]$$

```
psi(i)=exp_V*psi(i)  psi=exp_T*psi/float(N)
```

Starting with the wave packet from 0. I used split operator to propagate the wave packet moving through a potential barrier.

3. Tunneling/Results

There are a lot that we can play with tunneling. There are many things we can do such that:

- Interacting with an Arbitrary barrier
- Propagating with an Arbitrary Wave Packet
- Trapping a Wave Packet
- Changing the width/height of the barrier

In this project, I will go through the fourth one mainly to explore the physics of tunneling. Besides, I will add some interesting topics that I could further explore if I have more time.

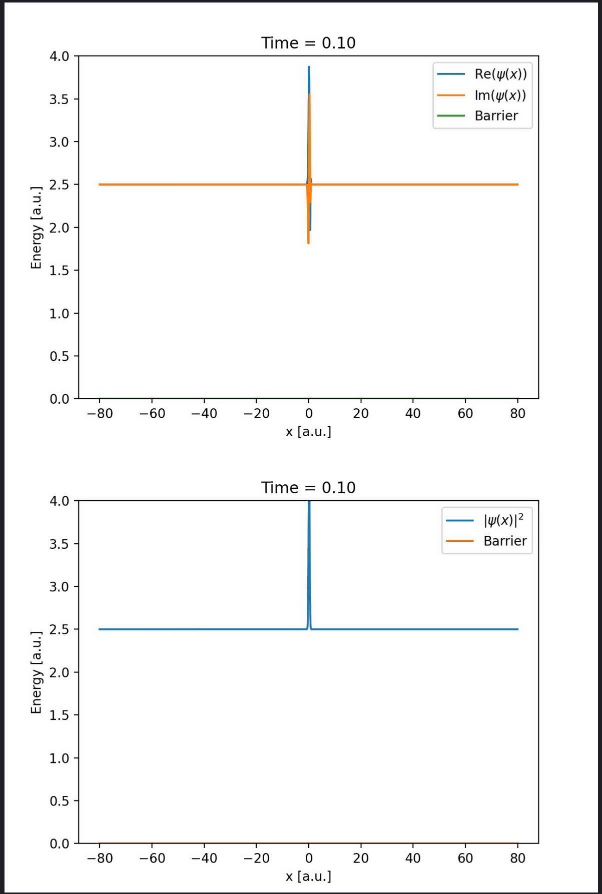
Simple Potential Barrier

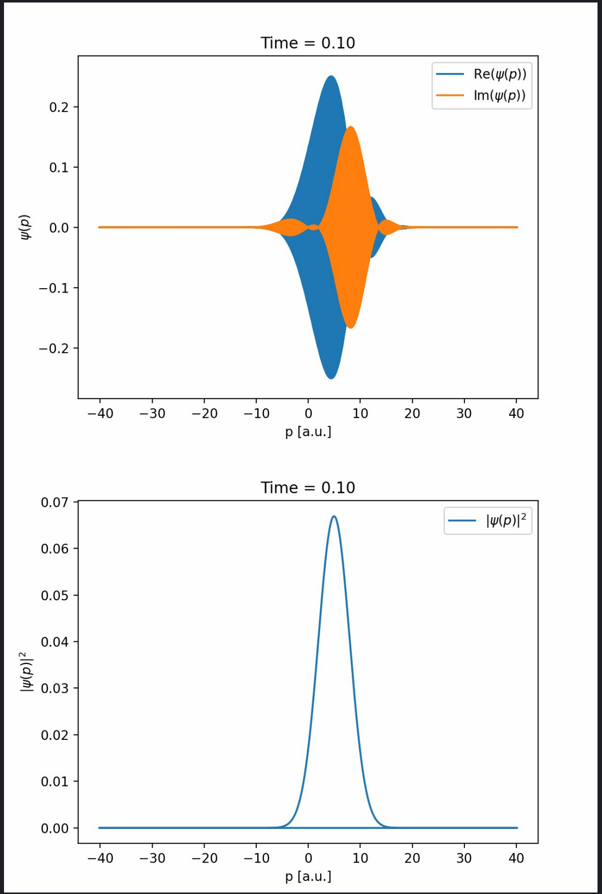
I want to discover what happen to the wave dynamic when I increase the barrier height and the barrier width for a simple potential barrier.

Fixing the width of the barrier at 5, I want to explore how the height affects the Wave Packet.

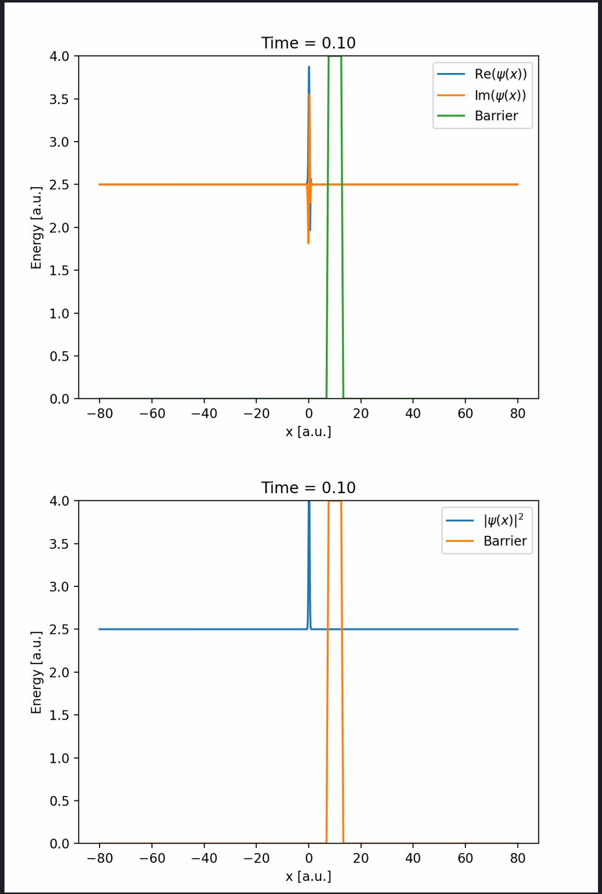
Width=5

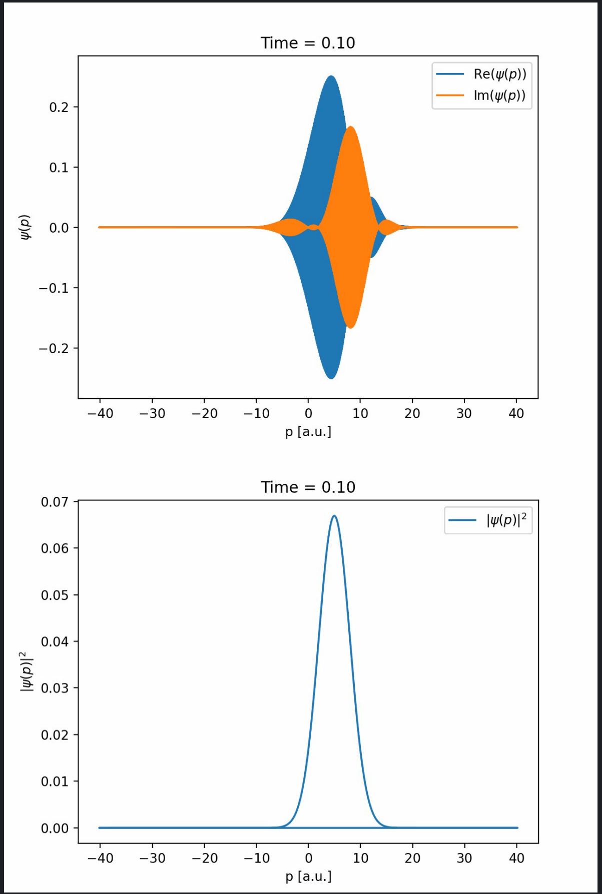
Height=0


Time = 0.10
Re($\psi(x)$)
Im($\psi(x)$)
Barrier
Energy [a.u.]
x [a.u.]
Time = 0.10
$|\psi(x)|^2$
Barrier
Energy [a.u.]
x [a.u.]


Time = 0.10
Re($\psi(p)$)
Im($\psi(p)$)
$\psi(p)$
p [a.u.]
Time = 0.10
$|\psi(p)|^2$
$|\psi(p)|^2$
p [a.u.]

Height=04





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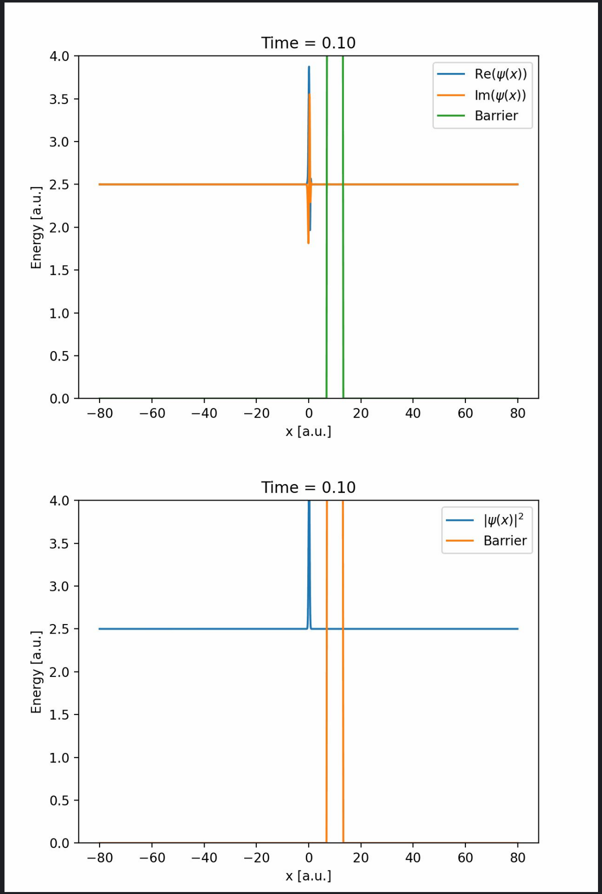
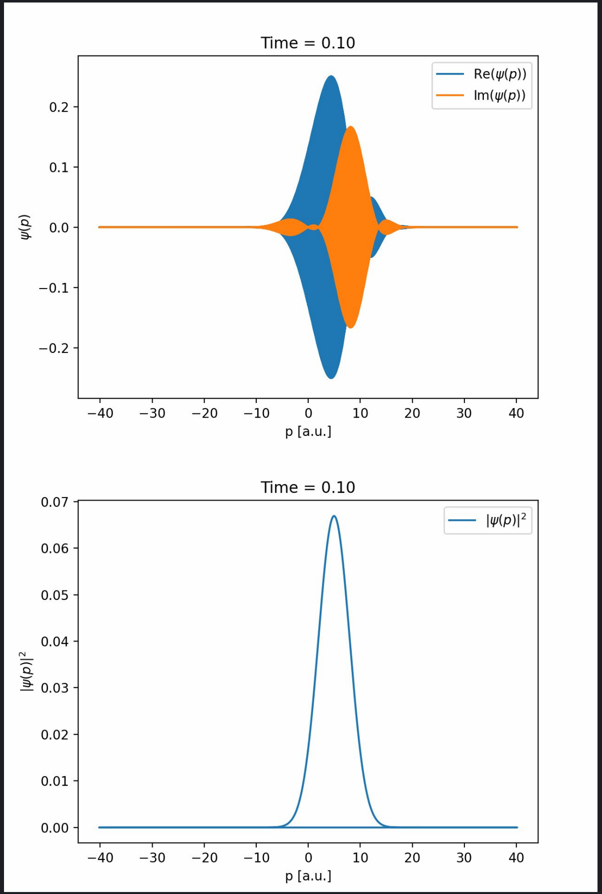
Height=20





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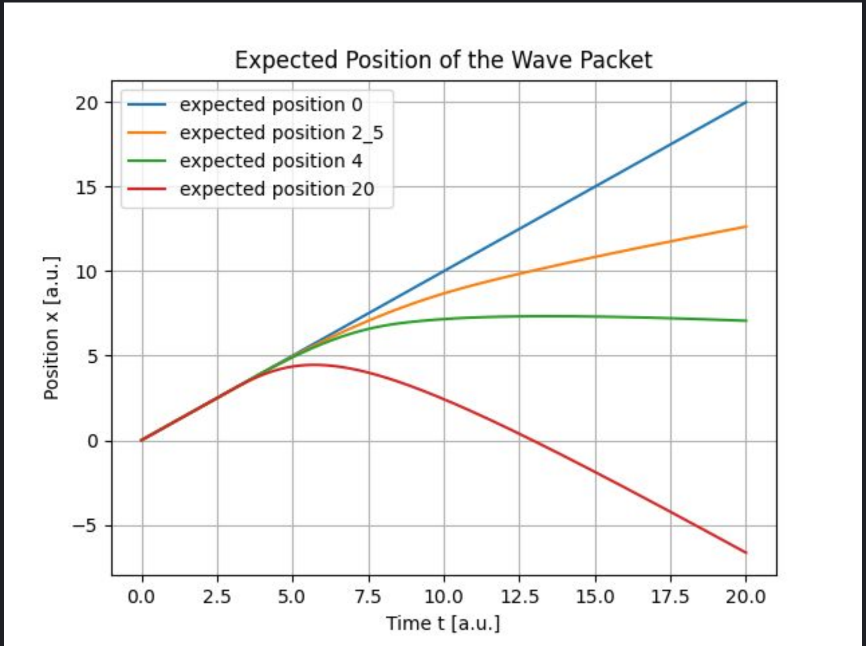
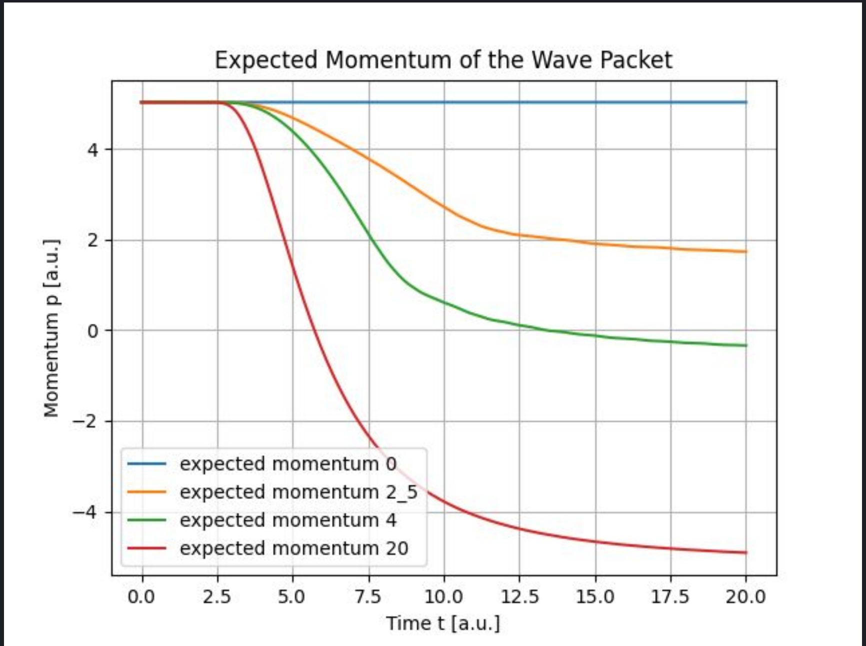
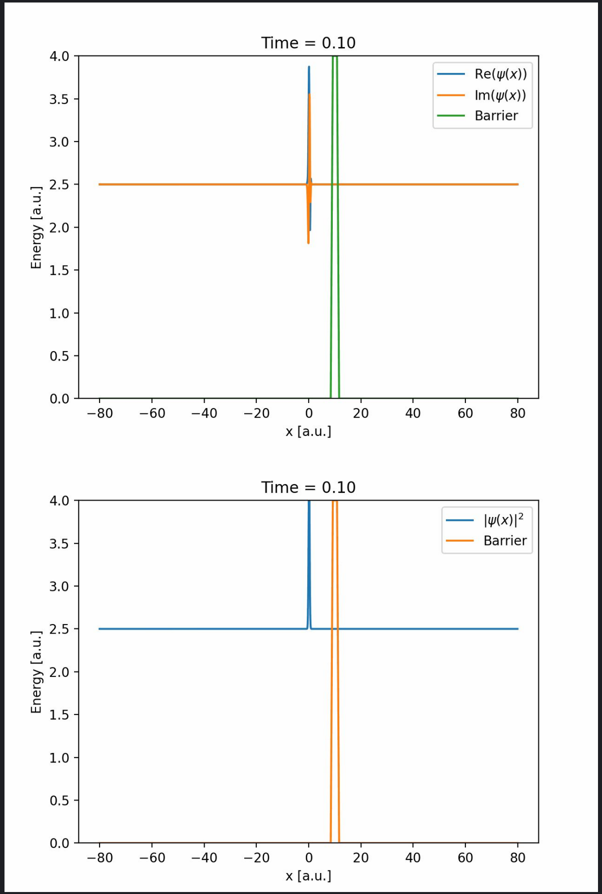

Expected Position of the Wave Packet
expected position 0
expected position 2_5
expected position 4
expected position 20
Position x [a.u.]
Time t [a.u.]

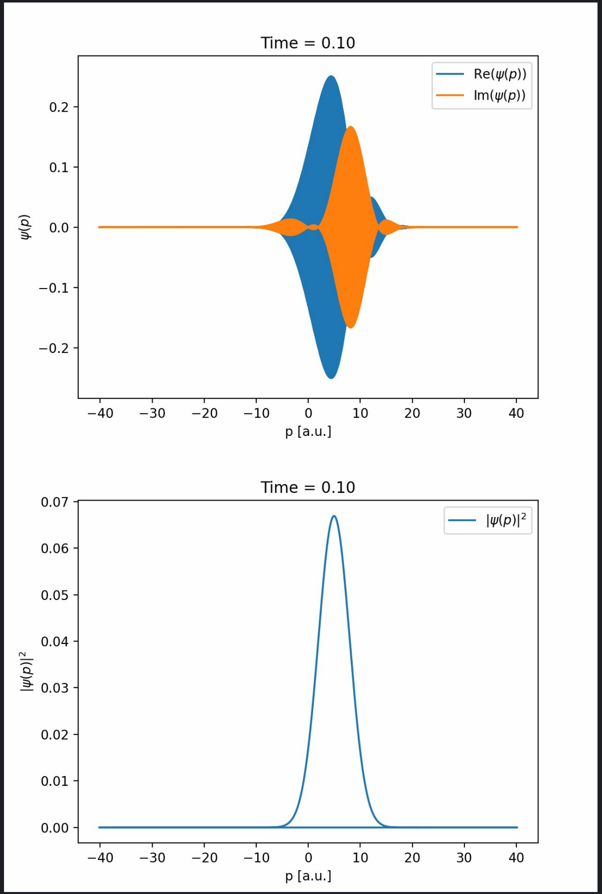

Expected Momentum of the Wave Packet
expected momentum 0
expected momentum 2_5
expected momentum 4
expected momentum 20
Momentum p [a.u.]
Time t [a.u.]

Now, we fix the height at 4 to investigate how the packet change with the width of the barrier

Height=4

Width=2.5





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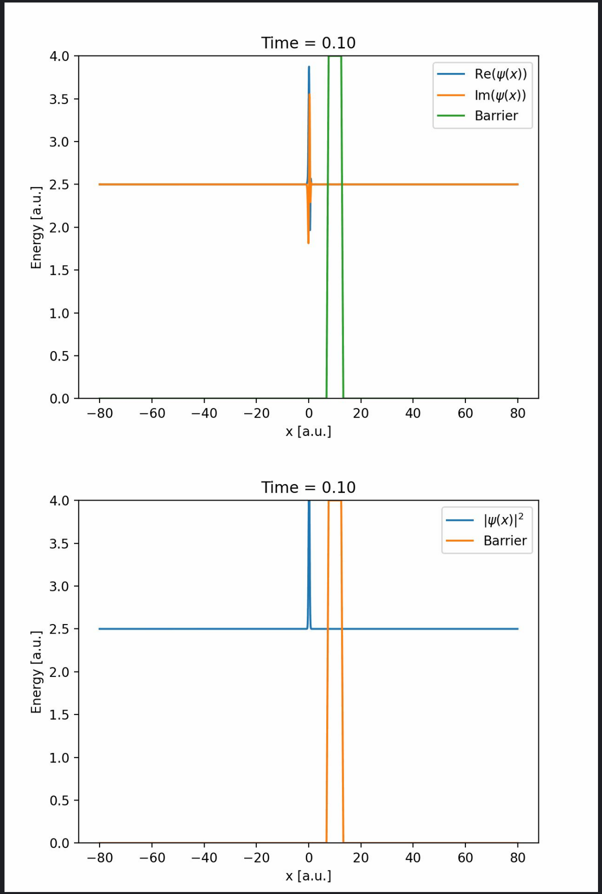
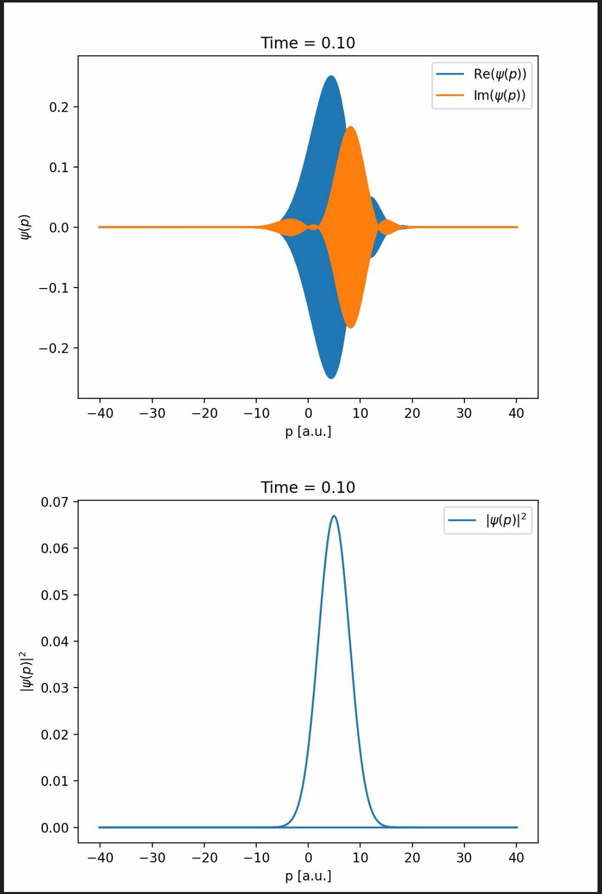
Width=5





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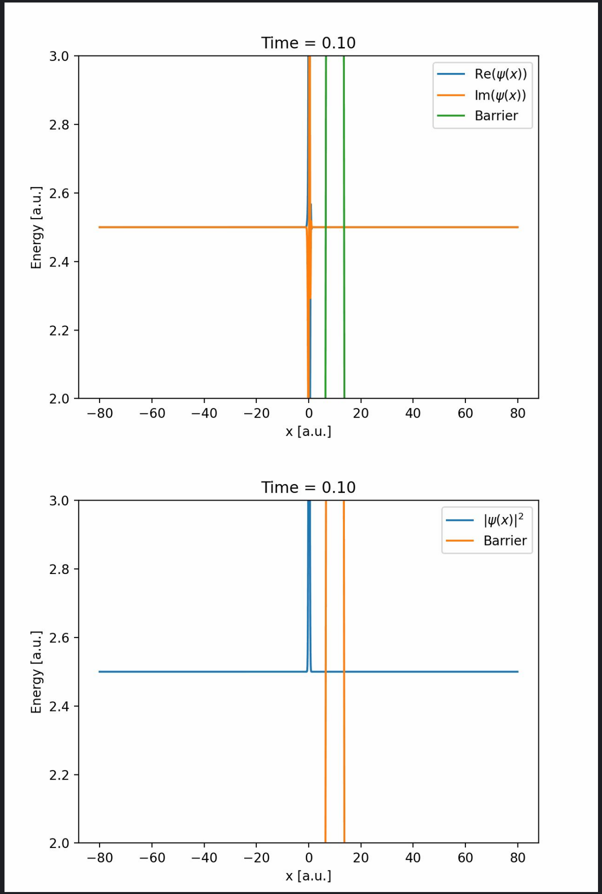
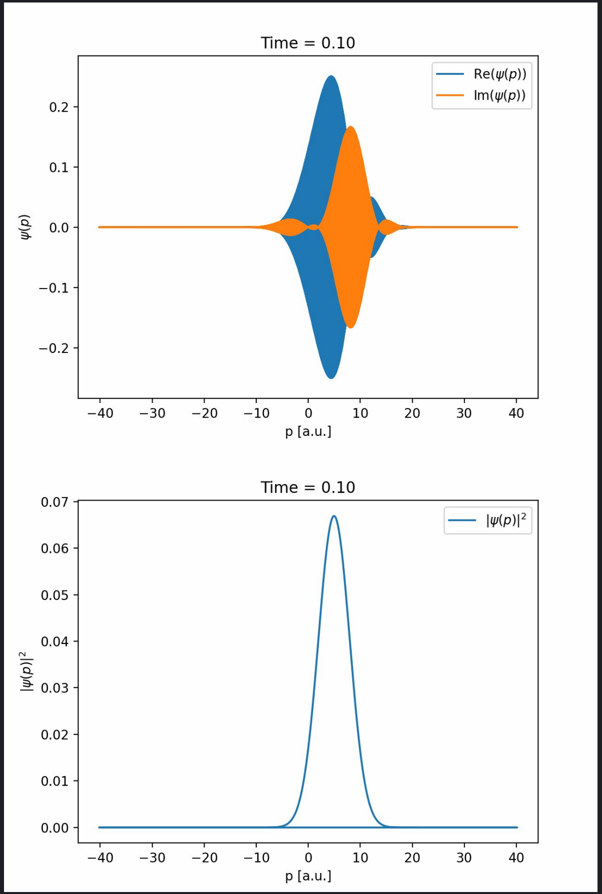
Width=7.5





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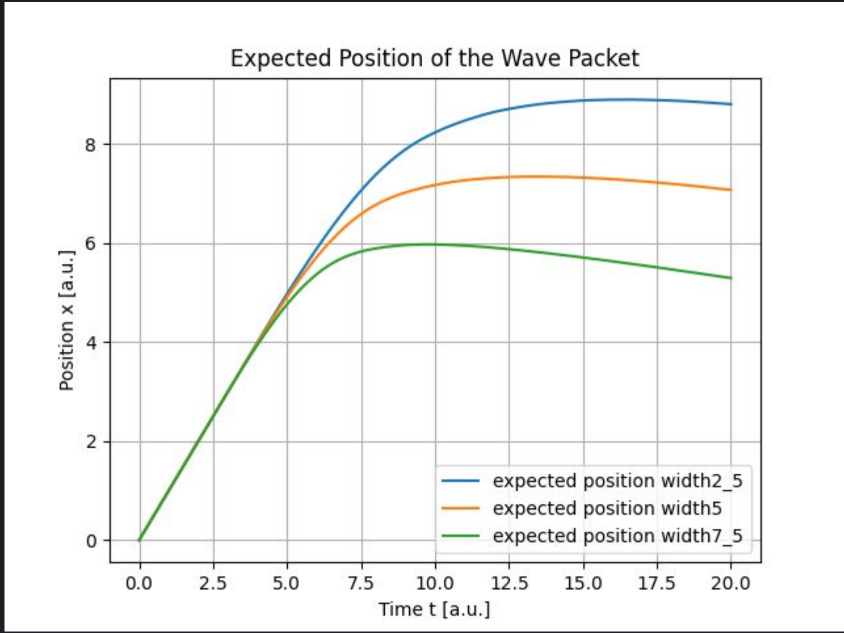
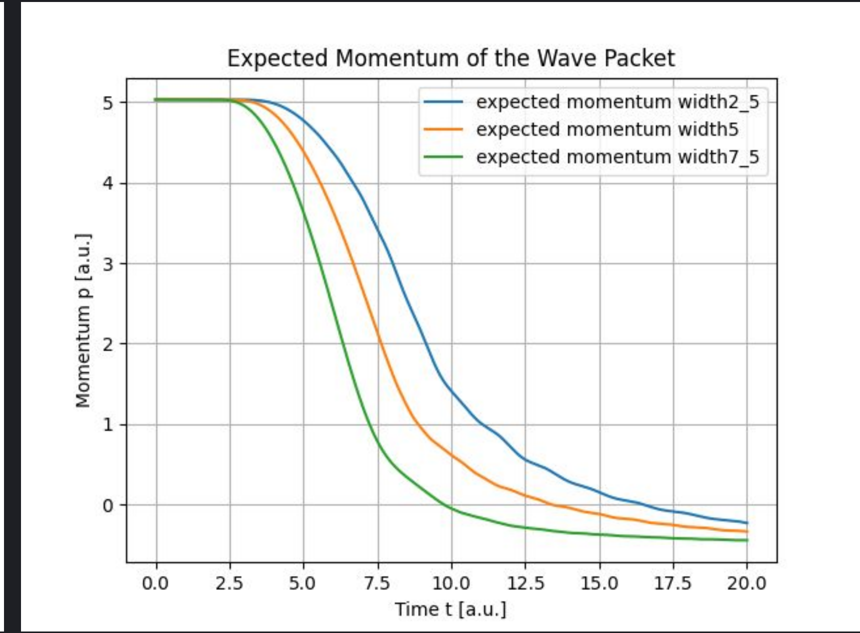

Expected Position of the Wave Packet
Position x [a.u.]
Time t [a.u.]
0
2
4
6
8
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
expected position width2_5
expected position width5
expected position width7_5

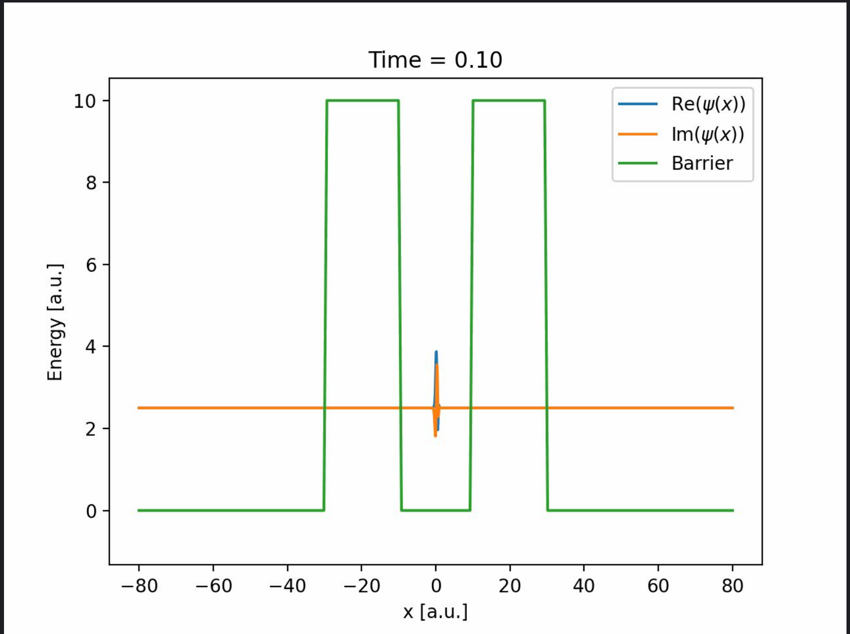

Expected Momentum of the Wave Packet
Momentum p [a.u.]
Time t [a.u.]
0
1
2
3
4
5
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
expected momentum width2_5
expected momentum width5
expected momentum width7_5

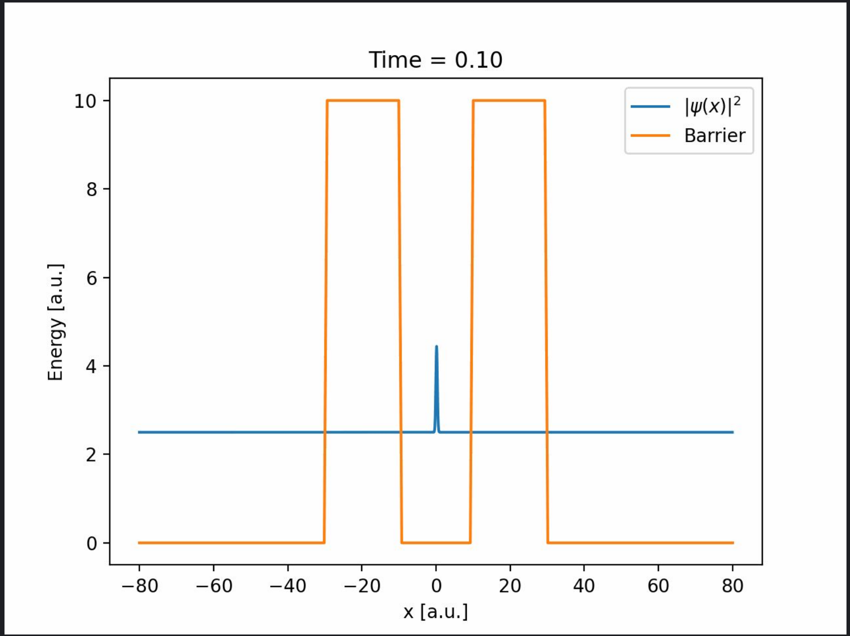
Conclusion:

- We have shown the effects that the width and height of a barrier to an incoming wave packet.
- Firstly, increasing the height of a barrier will limit more parts of the wave packet to tunnel through.
- Secondly, increasing the the width of a barrier will result in the wave packet taking a shorter time to ‘feel’ the barrier significantly.
- Note: These results are derived from the operator technique while these might not represent the actual physical phenomena.

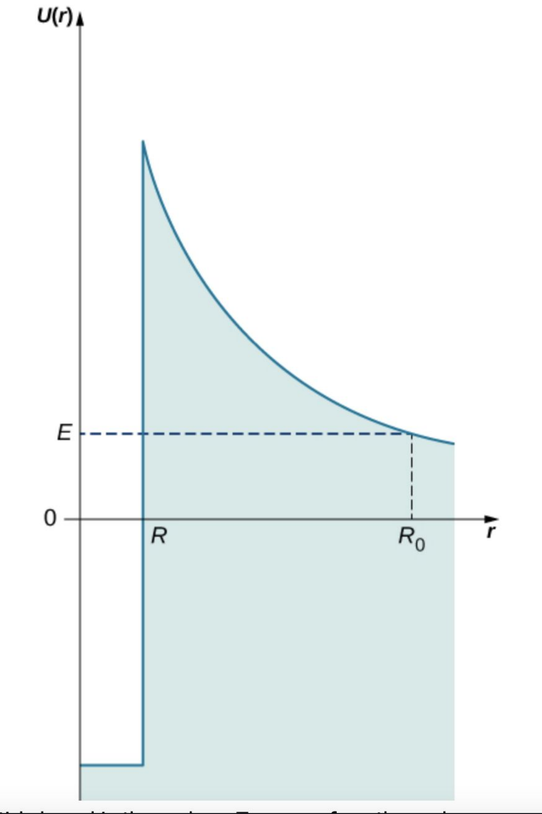
Ongoing/future projects

Trapped Wave Packet

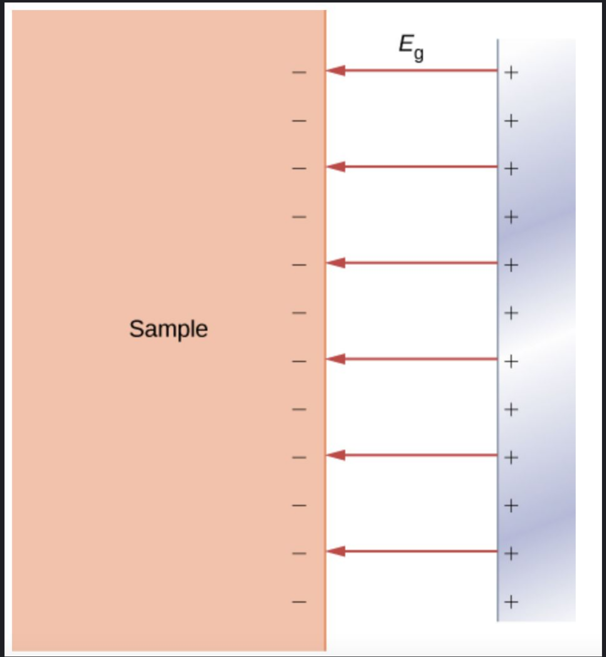




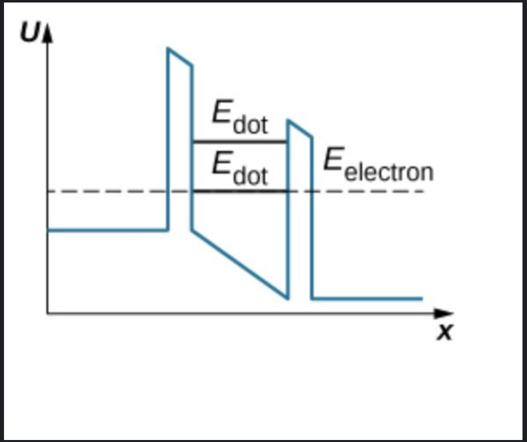
Radioactive Decay



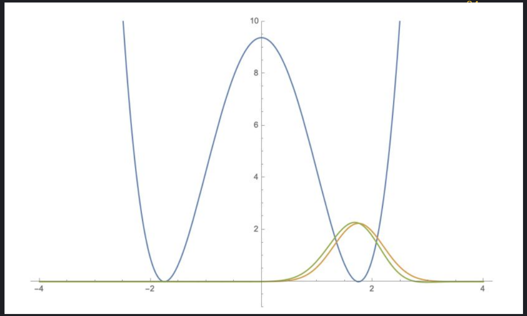
Field Emission



Explore Quantum Dot



Double Well



Resources:

- Numerical simulation of tunneling through arbitrary potential barriers applied on MIM and MIIM rectenna diodes
- Quantum Tunneling of Particles through Potential Barriers