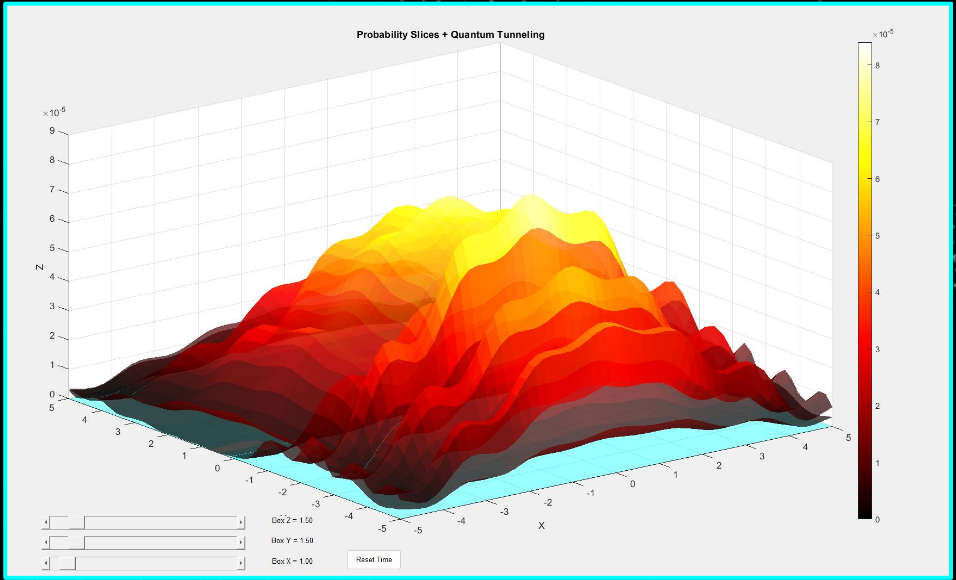
Quantum Tunneling:
Visualizing 3D Wave Packets & Evanescence



Fall 2025

PHYS 2213 - P. N. First

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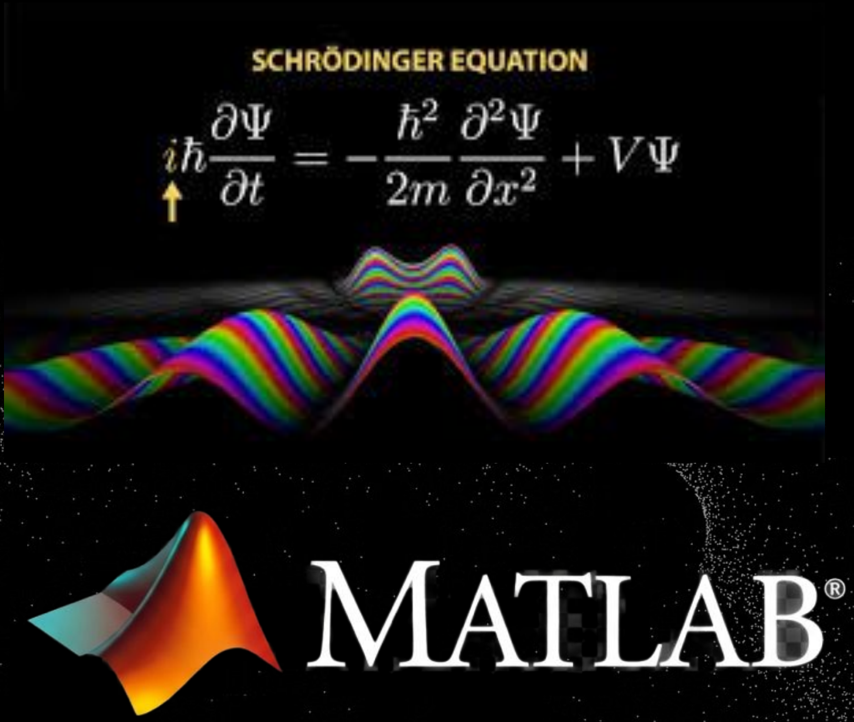


Proposal Topic

Quantum Tunneling and Evanescence Waves for Wave Packets: 3D Matlab Simulation

Questions:

1. **Transmission Input Variability:** How does T depend on inputs such as particle Energy, barrier geometry, and incidence angles?

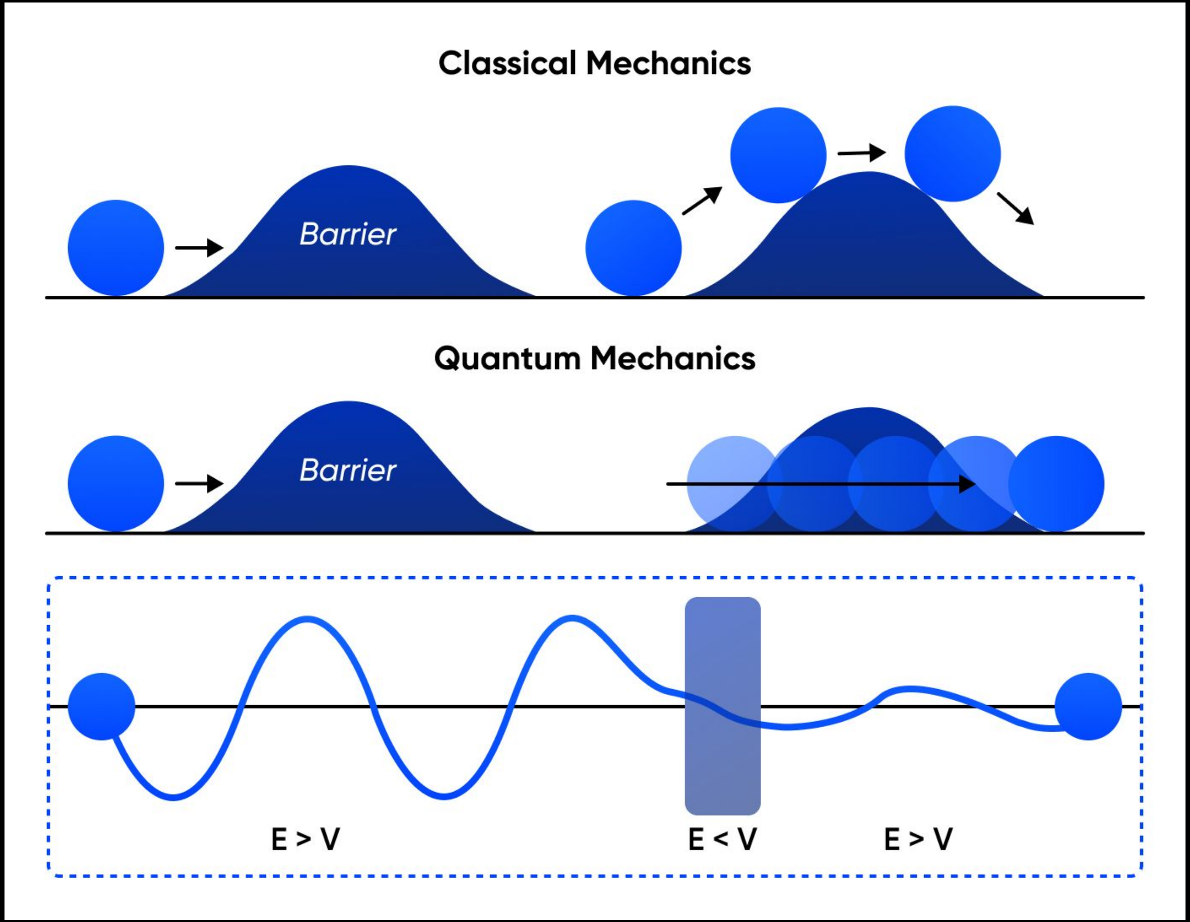
2. **Evanescent Wave Depiction:** Using Schrodinger's Wave Function, can we visualize a simulated 3D particle wave decaying?

3. **Quantum Transmission:** How can classically forbidden properties of quantum particles lead to macro-level structures (superlattice and circuits)

Relevance

1. **Biological Processes**: energy barriers
2. **'The Holy Grail of Energy'** : Nuclear Fusion
3. **MOSFETs:** storing energy via tunneling electrons

Proposal / Background



Assumptions & Calculations

1. **Single-Particle Approximation**

2. **Static Potential Barrier V (x,y,z)**
   [V(x,y,z) vs Ψ(t)]

3. **Double Absorbing Boundary Conditions**

4. **Time Discretion**
   [dt = 0.01 for rendering feasibility]

Calculations

TDSE in 3D: use gradient operator to expand

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]\Psi(\mathbf{r},t),\qquad \mathbf{r}=(x,y,z).$$

$$\begin{cases} C_x * C_y * C_Z * e^(ik_{x1}+ik_{y1}+ik_{z1}) * e^(-i\omega/t)) & x,y,z<-L/2 \\ ((A_x sin(k_{x2}x)+B_x cos(k_{x2}x)) * (A_y sin(k_{y2}y)+B_y cos(k_{y2}y) * (A_z sin(k_{z2}z)+B_z cos(k_{z2}z)) * e^(-i\omega/t) \\ C_x * C_y * C_Z * e^(-(ik_{x1}+ik_{y1}+ik_{z1})) * e^(-i\omega/t) & x,y,z>L/2 \end{cases}$$

$$-L/2\leq x,y,z\leq L/2$$

$$k_2=\sqrt{2mE}/(h/2\pi)$$

$$k_1=i\sqrt{2m(E-U)}/(h/2\pi)$$

$$\omega=E/(h/2\pi)$$

Model Demo & Explanation

Code

```
% Slider for X width
sliderX = uicontrol('Style','slider','Min',0.5,'Max',10,'Value',wellX,...
    'Position',[150 20 300 20],'Callback',@updateWellX);
txtX = uicontrol('Style','text','Position',[460 20 120 20],...
    'String',['Box X = ', num2str(wellX,'%.2f')]);

% Slider for Y width
sliderY = uicontrol('Style','slider','Min',0.5,'Max',10,'Value',wellY,...
    'Position',[150 50 300 20],'Callback',@updateWellY);
txtY = uicontrol('Style','text','Position',[460 50 120 20],...
    'String',['Box Y = ', num2str(wellY,'%.2f')]);

% Slider for Z width
sliderZ = uicontrol('Style','slider','Min',0.5,'Max',10,'Value',wellZ,...
    'Position',[150 80 300 20],'Callback',@updateWellZ);
txtZ = uicontrol('Style','text','Position',[460 80 120 20],...
    'String',['Box Z = ', num2str(wellZ,'%.2f')]);
```

Live Feedback
Barrier Input Control

$$e^{-i\frac{\hbar k^2}{2m}dt}$$

$$\hat{K} = \frac{p_x^2}{2m} = \frac{1}{2m}(-i\hbar)\frac{\partial}{\partial x}(-i\hbar)\frac{\partial}{\partial x} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\hat{K} = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$$

```
%% ------------------- Precompute k-space grids -----
kx = (2*pi/Lx)*(-floor(Nx/2) : ceil(Nx/2)-1);
ky = (2*pi/Ly)*(-floor(Ny/2) : ceil(Ny/2)-1);
kz = (2*pi/Lz)*(-floor(Nz/2) : ceil(Nz/2)-1);
[Kx,Ky,Kz] = ndgrid(kx,ky,kz);
Tprop = exp(-1i * dt * (hbar * (Kx.^2 + Ky.^2 + Kz.^2) / (2*m)));
```

Wave Numbers in 3D

Wave Packet Code Calculation

Code

```
% Wavepacket centered at origin
x0 = -max(X(:))/4; y0 = 0; z0 = 0; sigma = 0.8;
kx0 = 2; ky0 = 0; kz0 = 0;
psi = exp(-((X-x0).^2 + (Y-y0).^2 + (Z-z0).^2)/(2*sigma^2)) ...
      .* exp(1i*(kx0*X + ky0*Y + kz0*Z));
psi = psi / sqrt(sum(abs(psi(:)).^2));

% Potential barrier and well
V0 = 5; wellDepth = 10;
V = zeros(size(X));
V((X >= 0) & (X <= wX)) = V0; % barrier
xMax = max(X(:));
xMin = min(X(:));
yMin = min(Y(:)); zMin = min(Z(:));
V((X >= xMax-wX) & (X <= xMax) & ...
  (Y >= yMin) & (Y <= yMin+wY) & ...
  (Z >= zMin) & (Z <= zMin+wZ)) = -wellDepth; % small well

% Absorbing boundaries
absorbWidth = 3; sigma_absorb = 0.05;
absorbX = ones(Nx,1); absorbY = ones(Ny,1); absorbZ = ones(Nz,1);
for i=1:absorbWidth
    coeff = exp(-((absorbWidth - i)/absorbWidth)^2 * sigma_absorb);
    absorbX(i) = coeff; absorbX(end-i+1) = coeff;
    absorbY(i) = coeff; absorbY(end-i+1) = coeff;
    absorbZ(i) = coeff; absorbZ(end-i+1) = coeff;
end
```

3D Wave Packet &
3D Probability Density

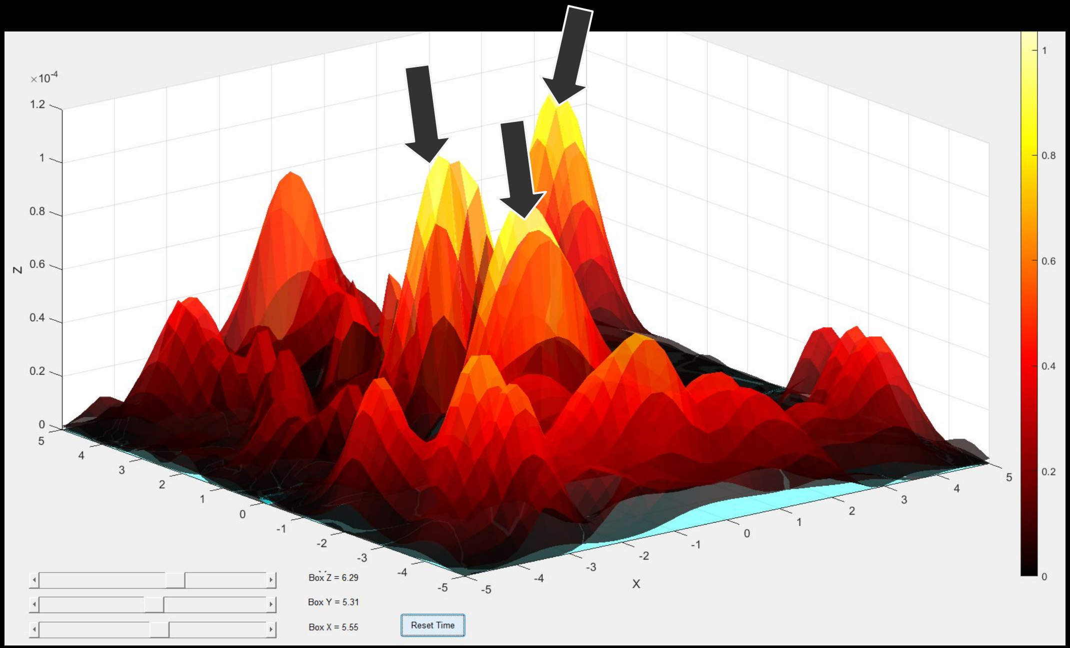
Potential Barrier
Input Control

Evanescent Wave
Decay Depiction

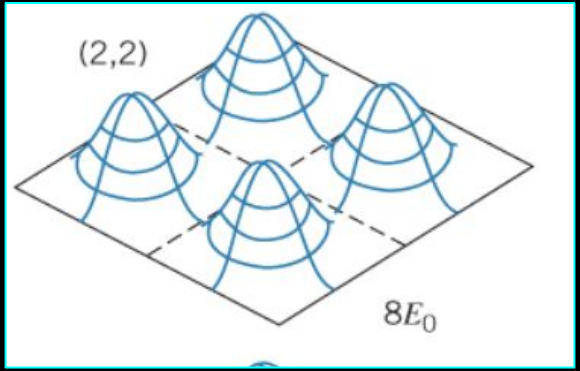
Findings / Principles

Findings / Principles

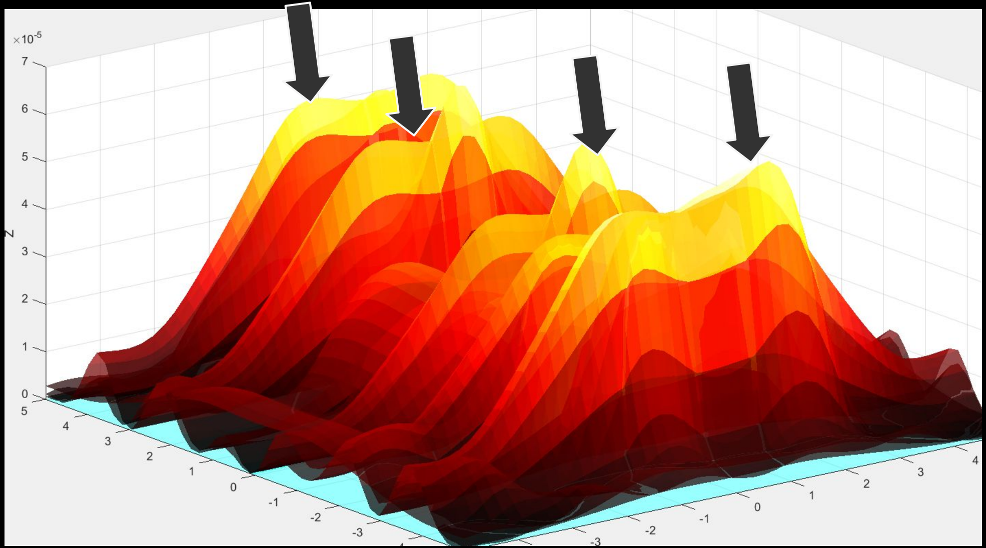
Barrier Input Data:
(x,y,z) = (6.3,5.3,5.5)



Quantum Degeneracy



Barrier Input Data:
(x,y,z) = (1.5,10,1.5)

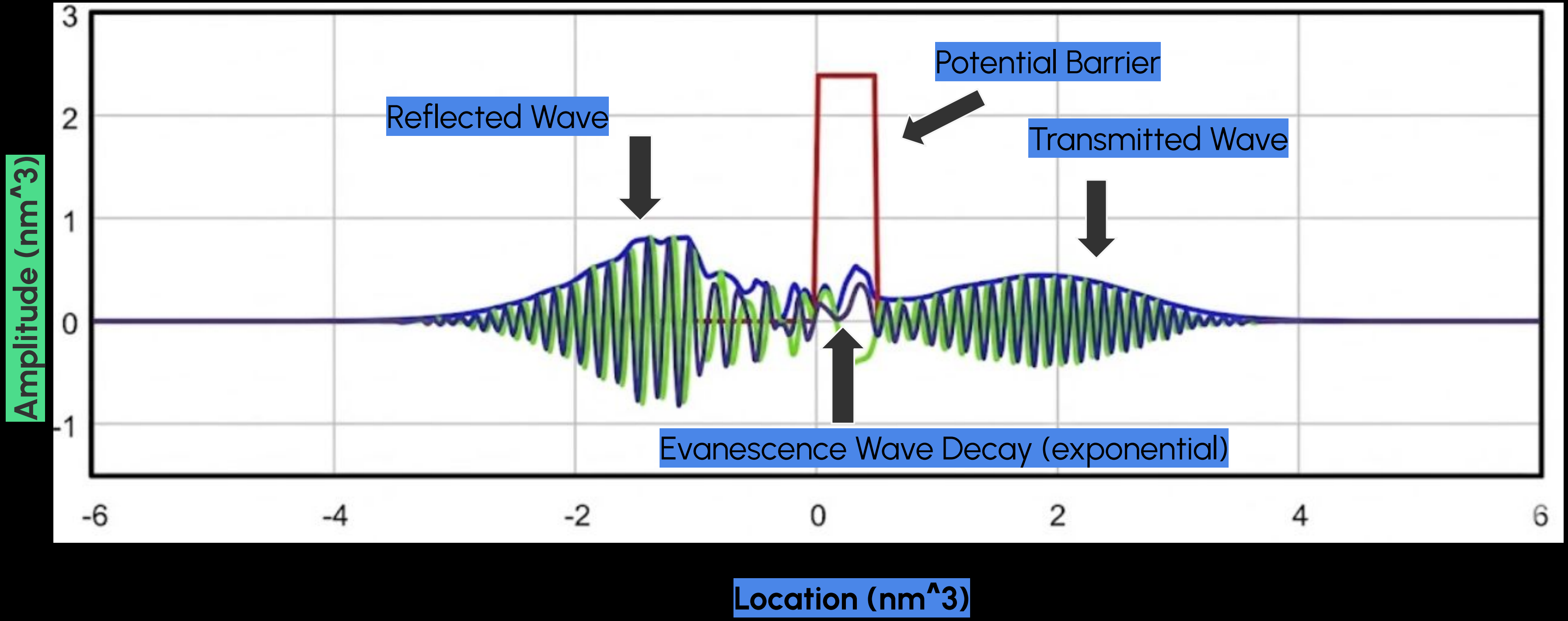


Energy Quantization

1. *Only specific waves will fit at with different barrier energies*
2. *This causes discrete peaks where the barrier forces the wave to take on specific shapes.*
3. *Represented by the integer number of peaks.*

Cubic Potential Barrier (small)
(x,y,z) = (1.50,1.50,1.50)

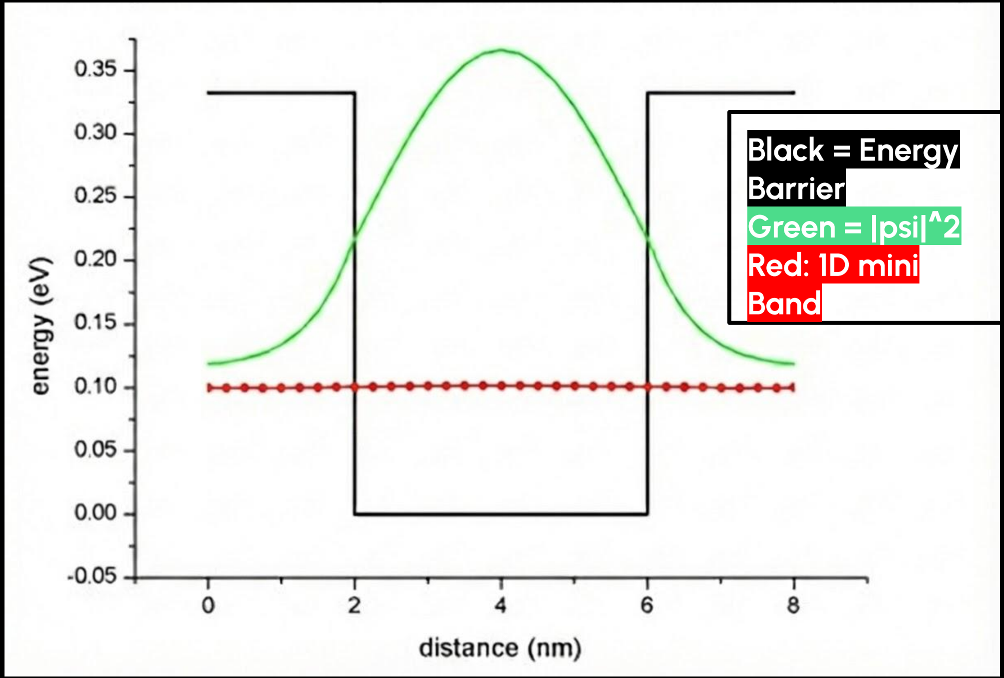
Data:
R = 0.724 (reflect)
T = 0.276 (tunnel)

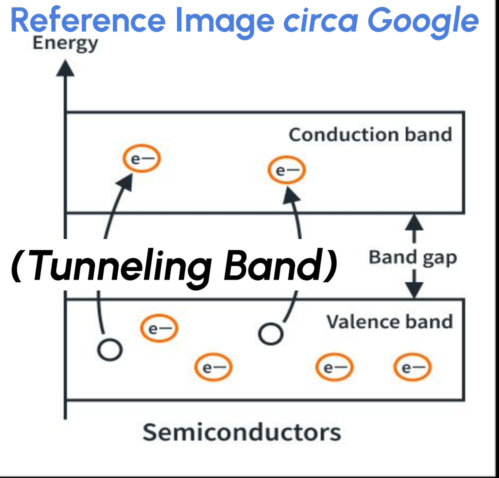


Findings / Principles

Barrier Input Data:
3D Step Barrier
(x,y,z) = (2,4,2)

Superlattice Miniband





1. *When a barrier potential drops (similar to semiconducting bands) it forms a discrete energy wave band*
2. *This graph shows the formation of microstructures in a 1D format*

Applications

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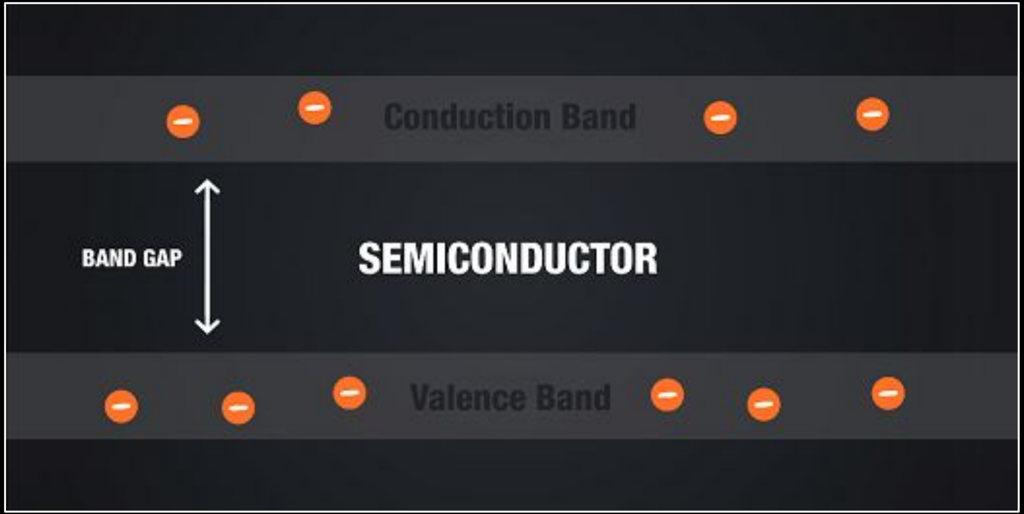
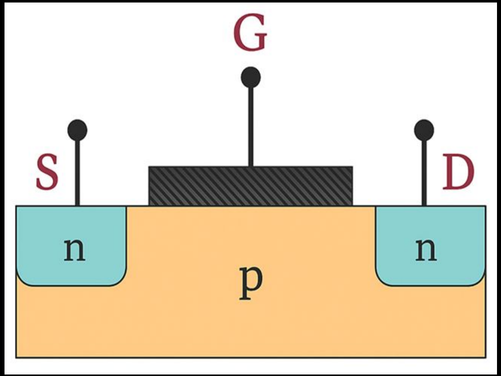
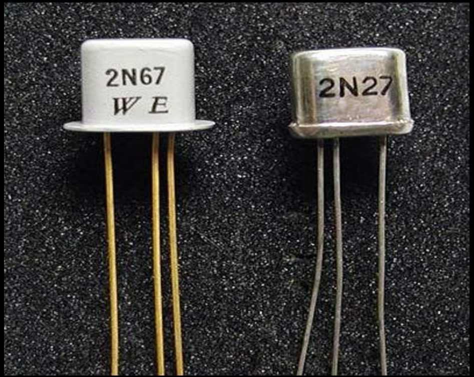
Semiconductor Bands



Transistor Malfunctions (Nobel Prize 2025)





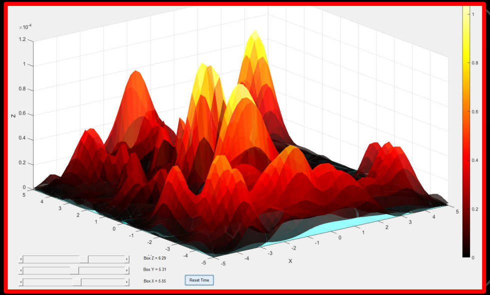
Main Concepts:

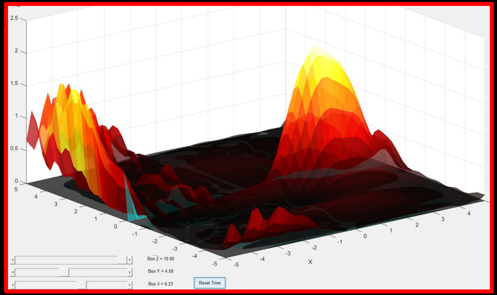
1. **Non-Zero Probability Inside Forbidden Region** (Inside cubic barrier)

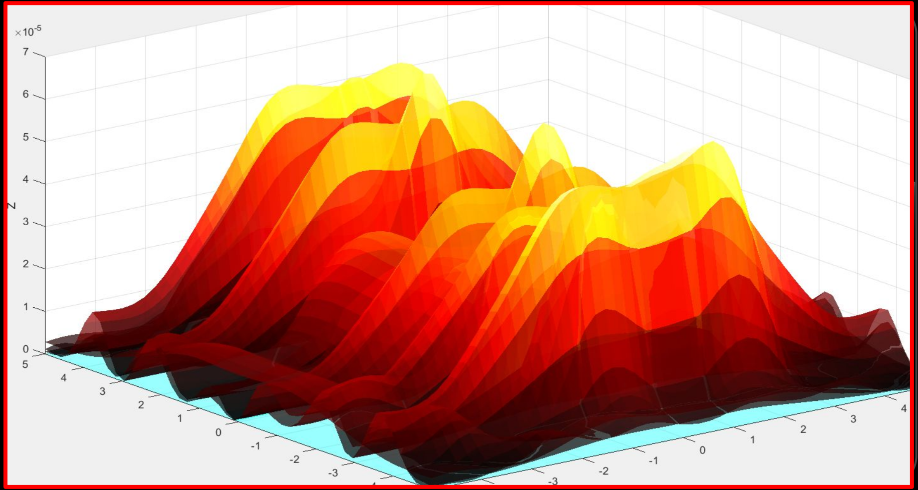
2. **Exponential Decay of Transmission through barrier**

3. **Small Energy Gaps can almost guarantee quantum tunneling**

4. **Step Barrier dimensions can form discrete bands**







Thank you!

References

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