

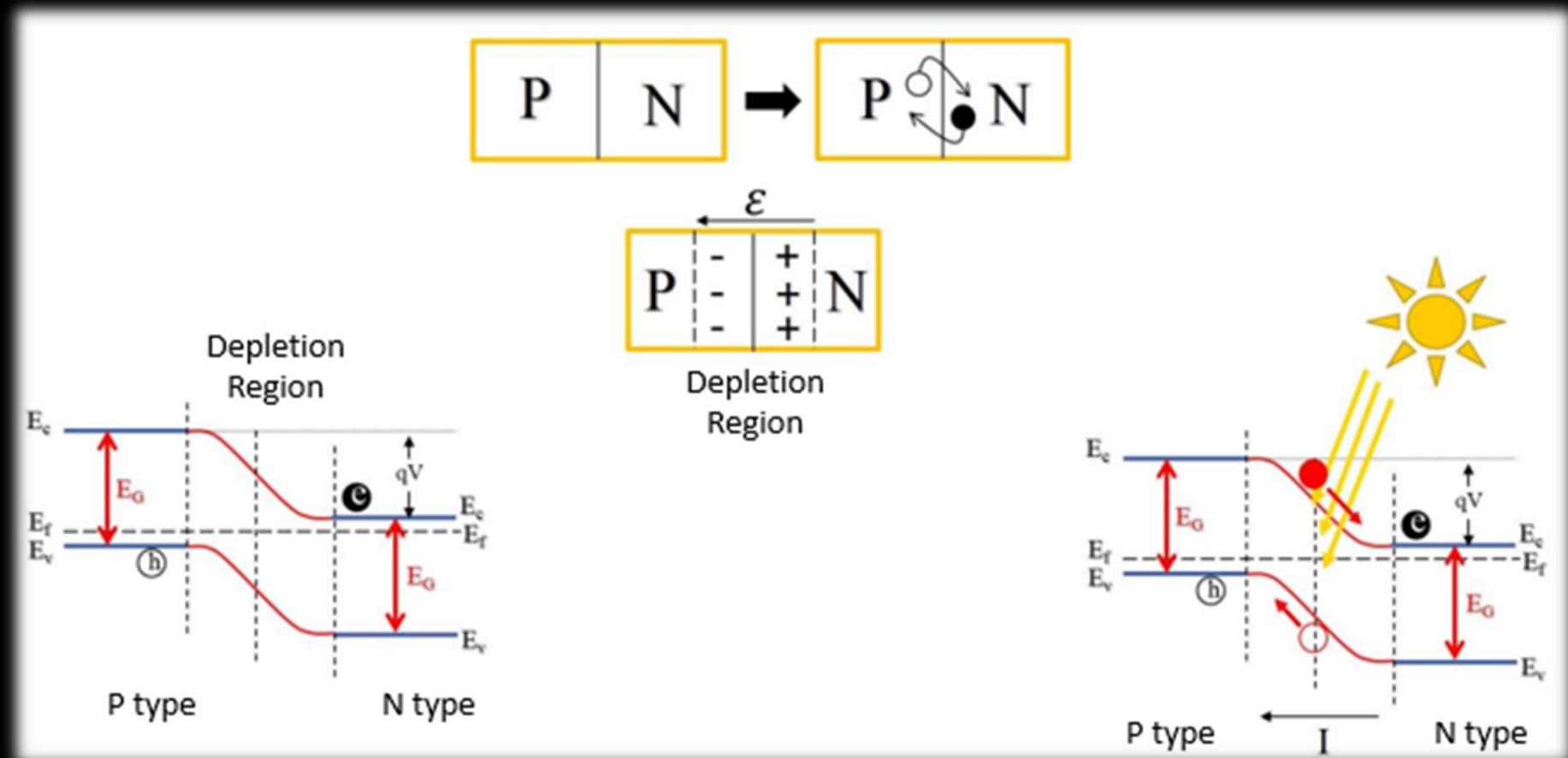
# QUANTUM DOT & MORE EFFICIENT SOLAR CELL

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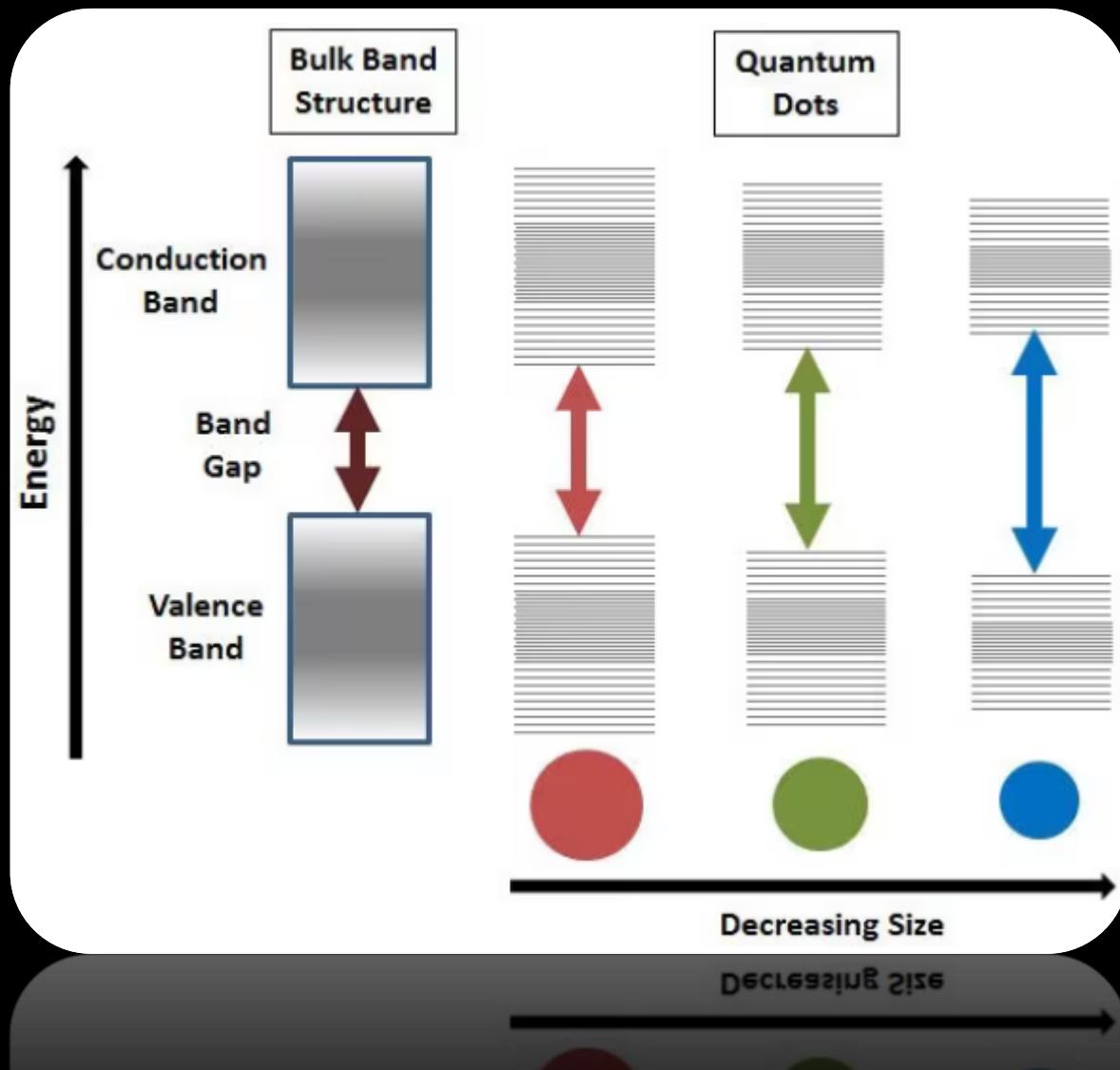
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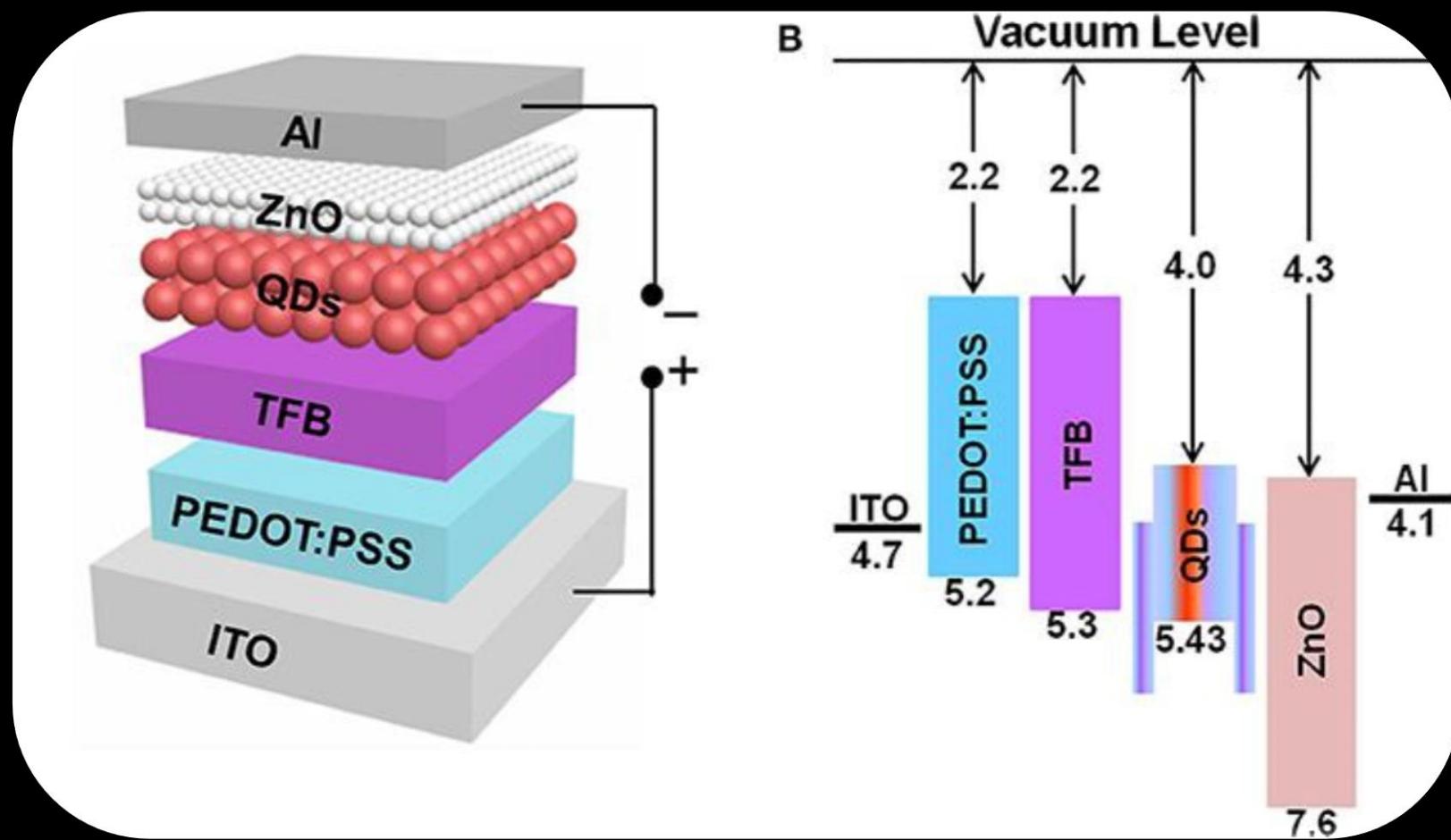
# SOLAR CELL



# WHAT IS QUANTUM DOT?



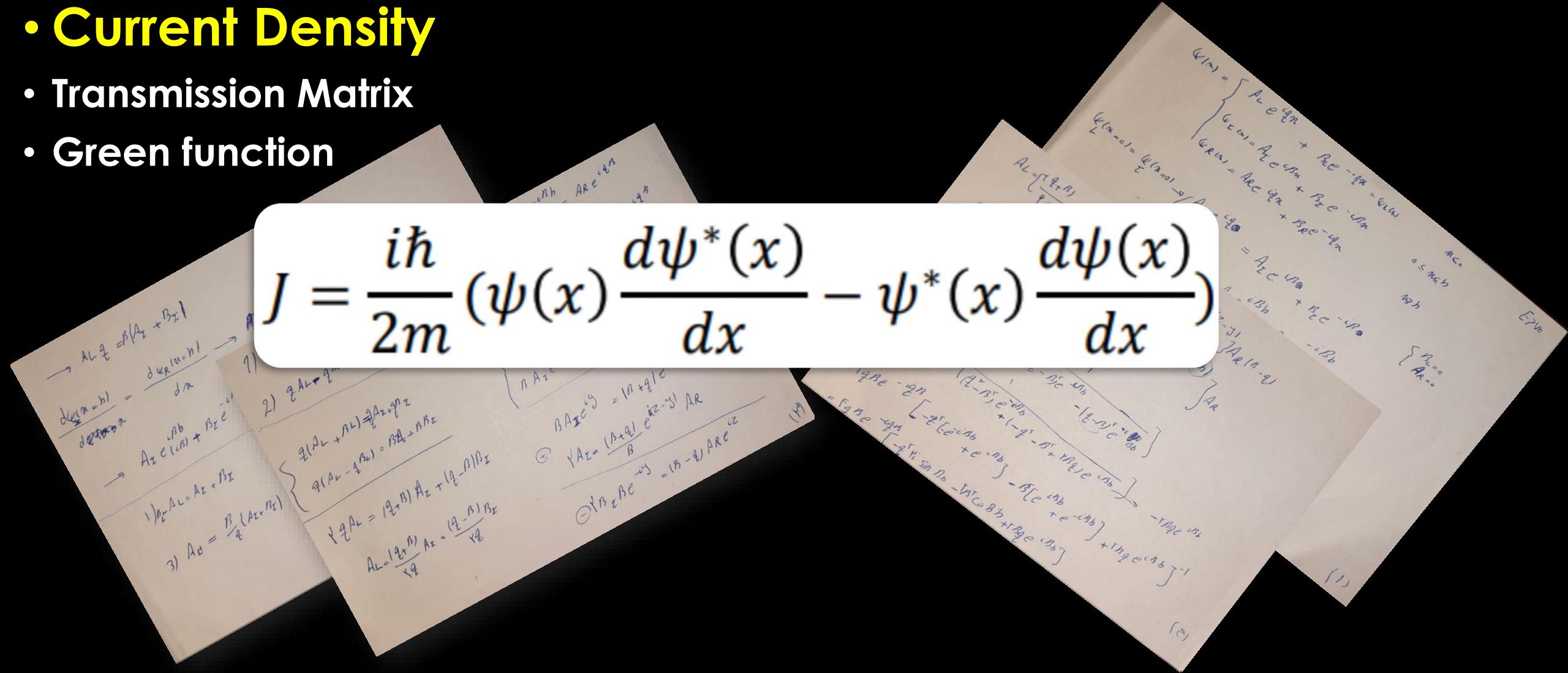
# WHY DO WE NEED QUANTUM DOTS?



# CALCULATING TRANSPORT

- Current Density
- Transmission Matrix
- Green function

$$J = \frac{i\hbar}{2m} (\psi(x) \frac{d\psi^*(x)}{dx} - \psi^*(x) \frac{d\psi(x)}{dx})$$



# CALCULATING TRANSPORT

- Current Density
- **Transmission Matrix**
- Green function, Calculating the Hamiltonian

$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = M(E) \begin{pmatrix} A_L \\ B_L \end{pmatrix} = \begin{bmatrix} m_{11}(E) & m_{12}(E) \\ m_{21}(E) & m_{22}(E) \end{bmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

$\frac{\partial A_L}{\partial E} = A_L - \frac{1}{T_2} B_L$   
 $\frac{\partial B_L}{\partial E} = B_L - \frac{1}{T_2} A_L$

$A_L = \frac{A_0 + A_2 e^{i\theta_0}}{T_2}$   
 $B_L = \frac{B_0 - B_2 e^{i\theta_0}}{T_2}$

$A_2 = \frac{A_0 - A_2 e^{i\theta_0}}{T_2}$   
 $B_2 = \frac{B_0 + B_2 e^{i\theta_0}}{T_2}$

$A_2 e^{i\theta_0} + A_2 e^{-i\theta_0} = A_2 c_{12}$   
 $B_2 e^{i\theta_0} - B_2 e^{-i\theta_0} = B_2 s_{12}$

$m_{11} = \begin{cases} A_0 c_{12} - B_0 s_{12} \\ A_0 s_{12} + B_0 c_{12} \end{cases}$   
 $m_{21} = \begin{cases} B_0 c_{12} - A_0 s_{12} \\ B_0 s_{12} + A_0 c_{12} \end{cases}$

$M = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}$   
 $M = M^H = A^T + B^H = M^*$

$m_{12} = \frac{A_2 c_{12} - B_2 s_{12}}{T_2}$   
 $m_{22} = \frac{B_2 c_{12} - A_2 s_{12}}{T_2}$

$A_2 = \frac{A_0 - A_2 e^{i\theta_0}}{T_2}$   
 $B_2 = \frac{B_0 + B_2 e^{i\theta_0}}{T_2}$

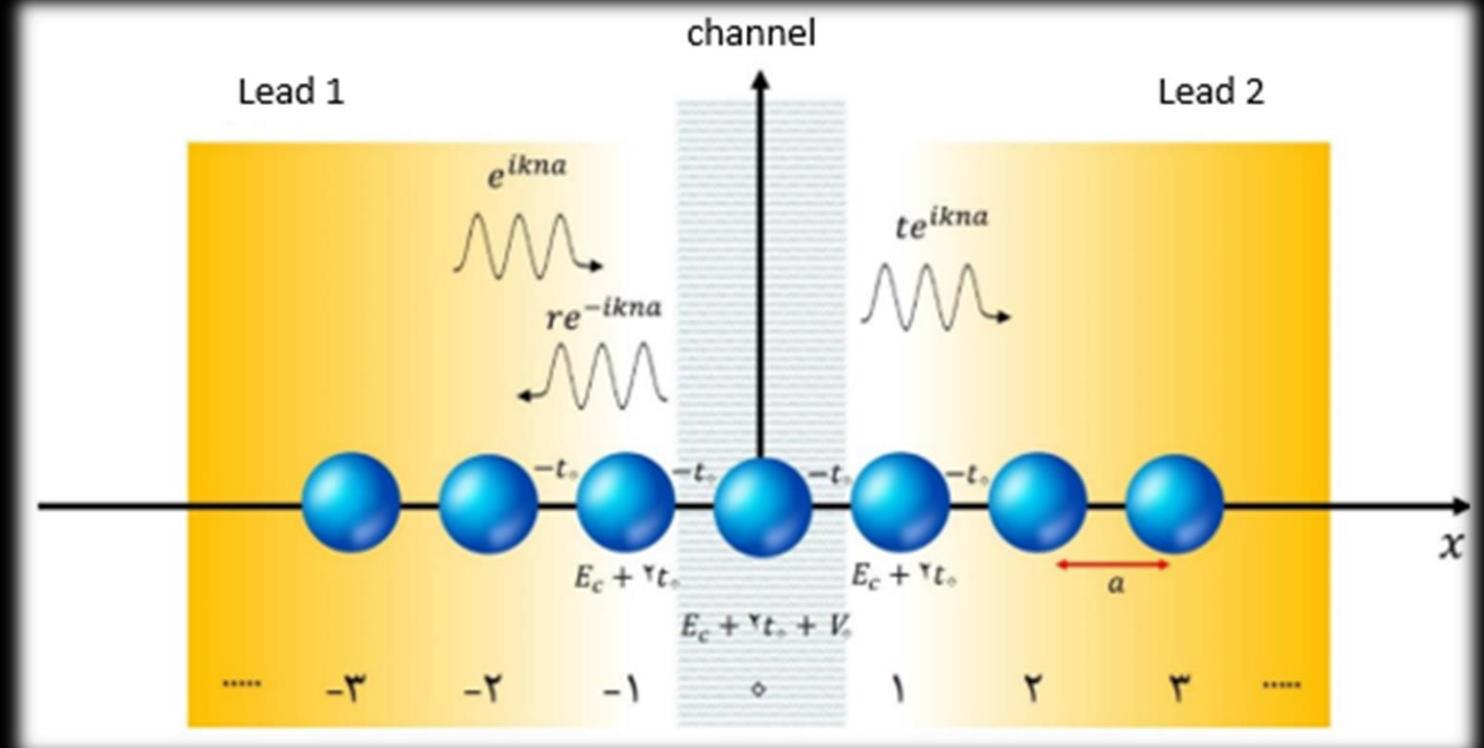
$A_2 c_{12} - B_2 s_{12} = \frac{A_0 c_{12} - B_0 s_{12}}{T_2}$   
 $B_2 c_{12} - A_2 s_{12} = \frac{B_0 c_{12} - A_0 s_{12}}{T_2}$

$m_{12} = \frac{A_0 c_{12} - B_0 s_{12}}{T_2} = A_0 c_{12} c_{22} - B_0 s_{12} s_{22}$   
 $m_{22} = \frac{B_0 c_{12} - A_0 s_{12}}{T_2} = B_0 c_{12} c_{22} - A_0 s_{12} s_{22}$

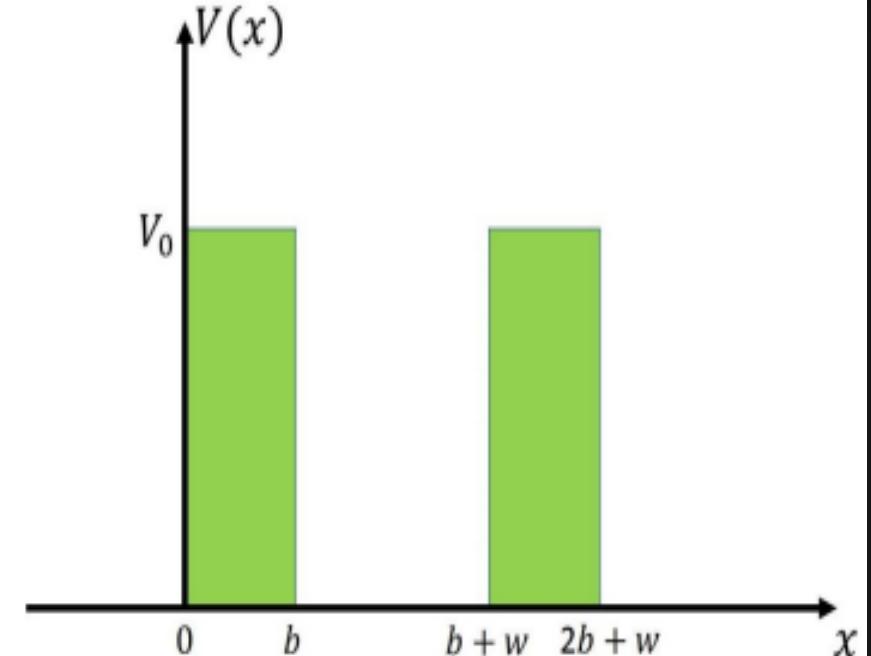
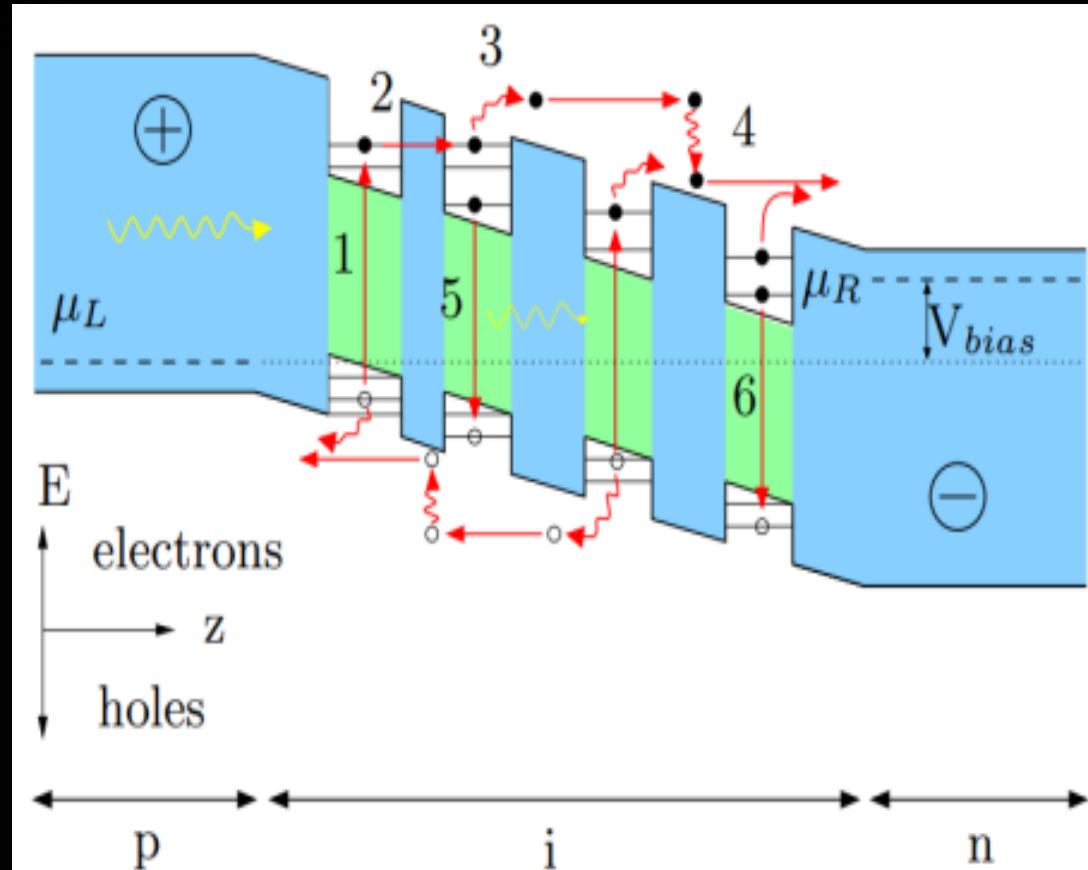
# CALCULATING TRANSPORT

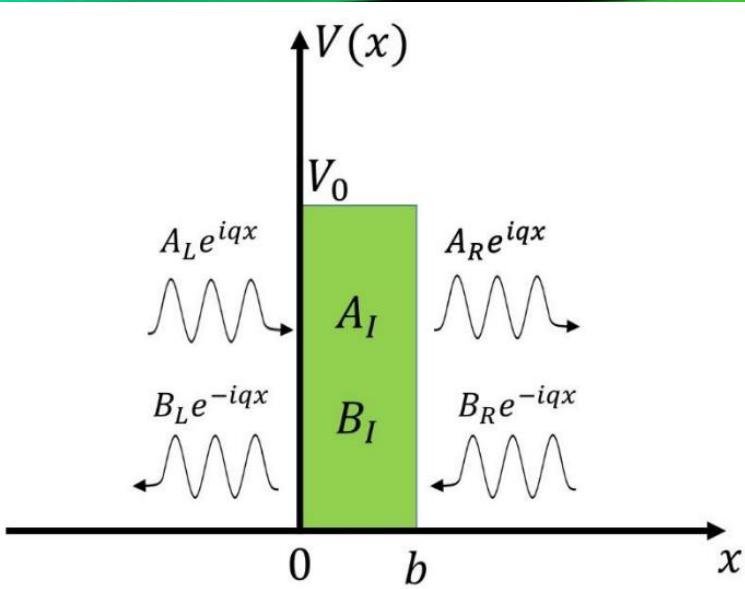
- Current Density
- Transmission Matrix
- Green function, Calculating the Hamiltonian: Hubbard

$$G = \frac{1}{[E - H + i\eta - \Sigma_1 - \Sigma_2]}$$



# More steps...

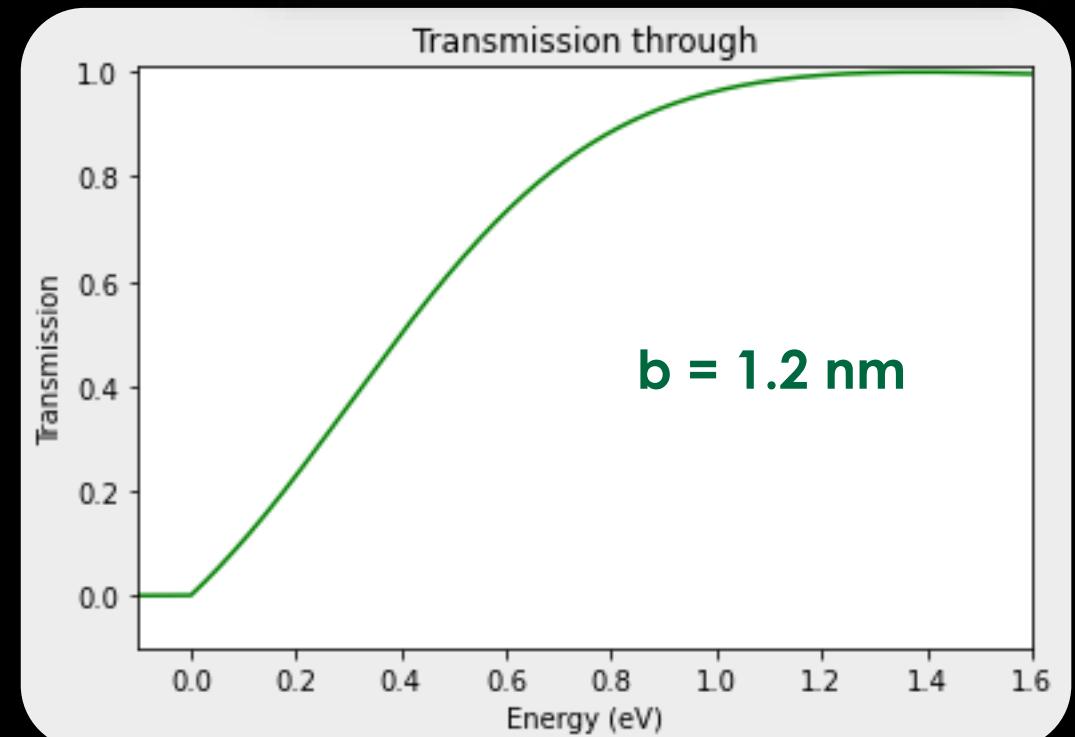
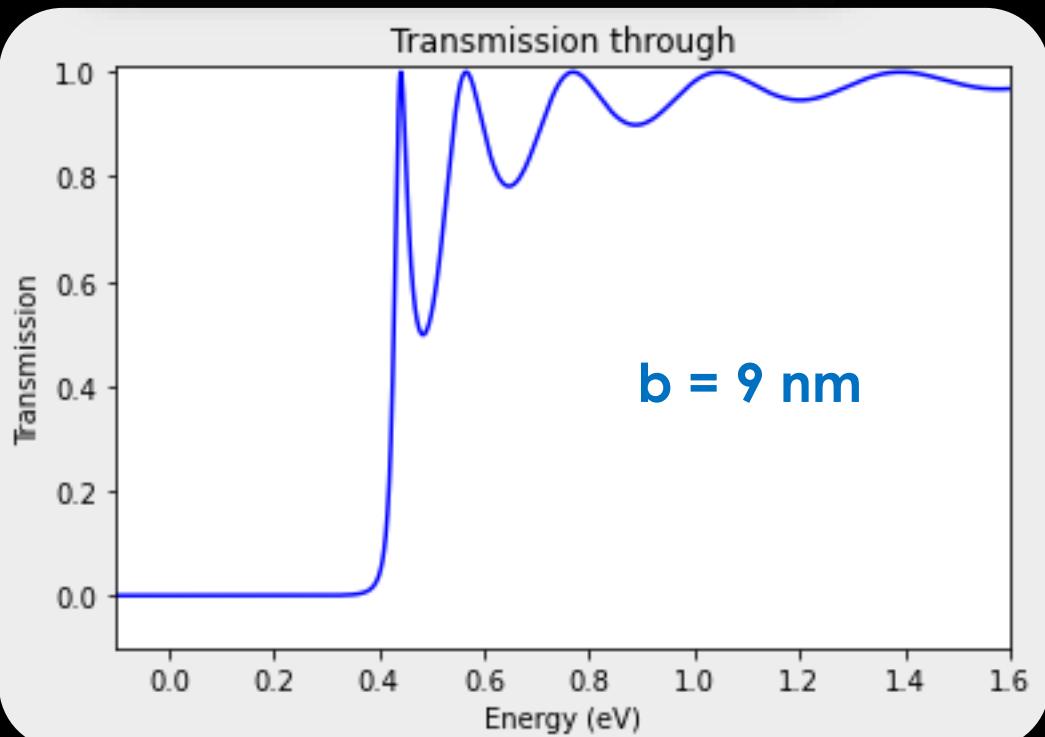
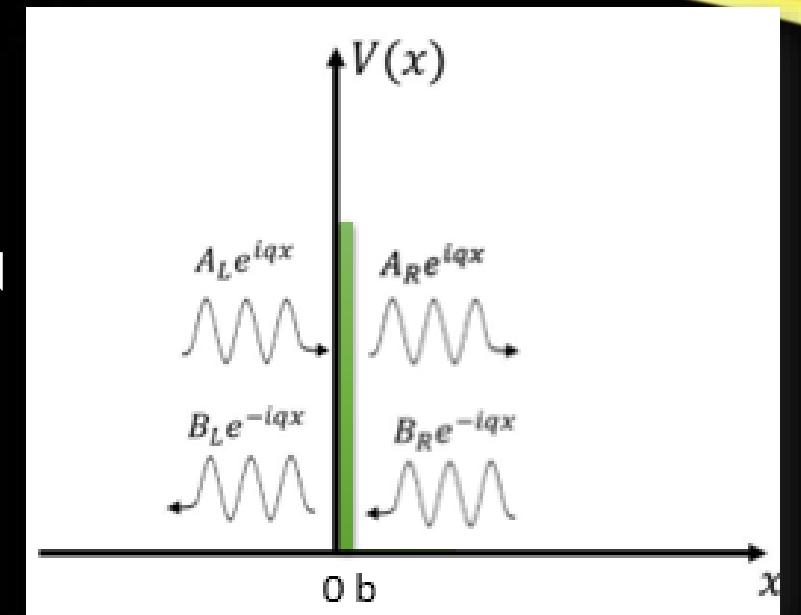




## RESULTS

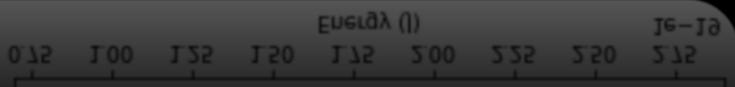
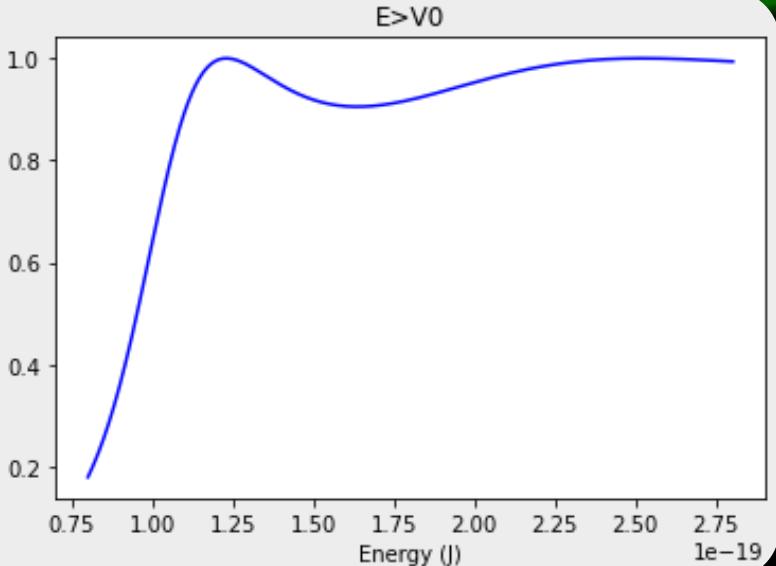
METHOD : GREEN FUNCTION

$$V = 0.4 \text{ eV}$$



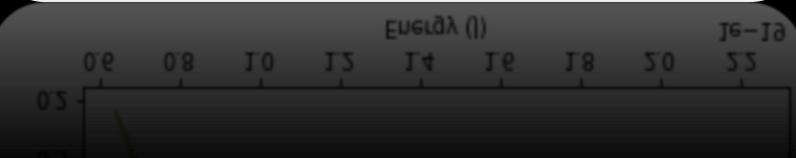
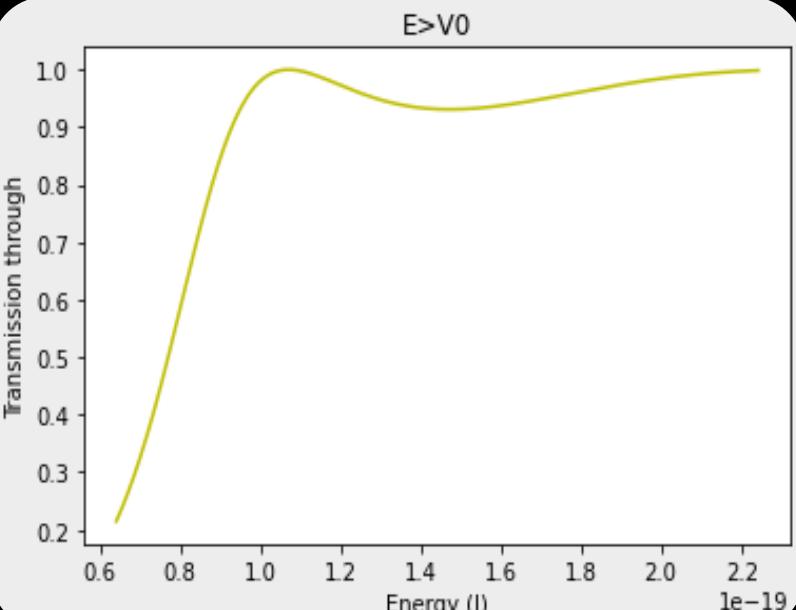
## method : Current Density

```
sigma1 = np.zeros((N,N), dtype = complex)
sigma2 = np.zeros((N,N), dtype = complex)
TM = []
for i in E:
    sigma1[0][0] = -t0*np.exp(1j*(np.arccos(1-((i+Etta0)/(2*t0)))))  
    sigma2[49][49] = -t0*np.exp(1j*(np.arccos(1-((i+Etta0)/(2*t0)))))  
    EE = i*np.eye(N)  
    g = EE - H + Etta - sigma1 - sigma2  
    Gamma1 = -2*np.imag(sigma1)  
    Gamma2 = -2*np.imag(sigma2)  
    G = linalg.inv(EE - H + Etta - sigma1 - sigma2)  
    G_dag = G.conjugate().transpose()  
    TM1 = np.dot(Gamma1,G)  
    TM2 = np.dot(TM1,Gamma2)  
    TM3 = np.dot(TM2,G_dag)  
    TM.append(np.real(TM3.trace()))
plt.plot(E,TM , 'r')
plt.title('Transmission through')
plt.xlabel('Energy (ev)')
plt.ylabel('Transmission')
plt.xlim(-0.1, u0*4)
plt.ylim(-0.1 , 1.01)
plt.show()
```

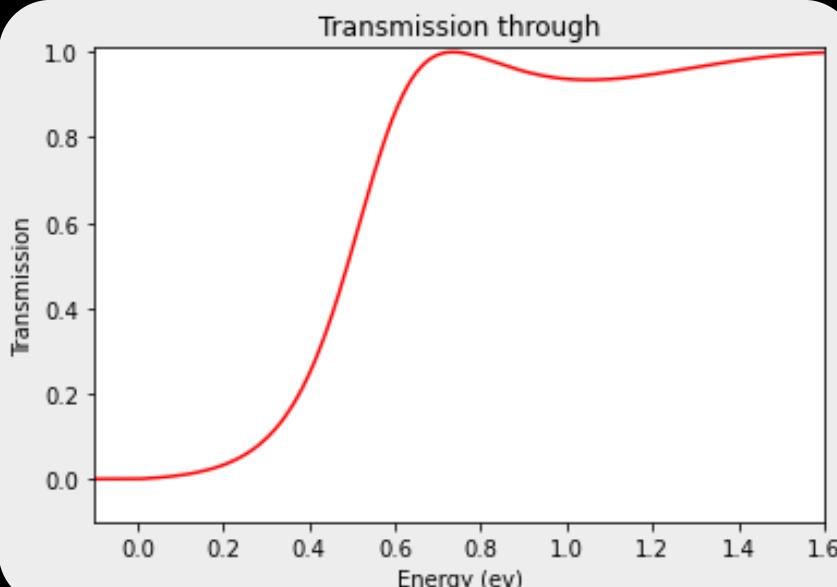


## Results

### method : Transmission Matrix



### method : Green function



```
import numpy as np
import matplotlib.pyplot as plt
from scipy import linalg
from ipywidgets import interact , interactive , fixed , interact_manual
import ipywidgets as widgets
matplotlib inline
a = 3*10**(-10)
E = np.linspace(-0.2 , 1.6 , 5001)
hbar = 1.054*10**(-34)
t0 = 0.4
charge = 1.602*10**(-19)
n = 0.25*9.1*10**(-31)
theta = (hbar**2)/(2*m*a**2)/charge
N = int(input('N:'))
T1 = (-t0)*np.eye(N , k=1)
T2 = 2*t0*np.eye(N)
T3 = (-t0)*np.eye(N , k=-1)
T = T1+T2+T3
Etta0 = 1e-12*1j
Etta = Etta0*np.eye(50)
n1 = int(input('n1:'))
n2 = int(input('n2:'))
n3 = N - n1 - n2
U1 = np.zeros((1,n1), dtype = complex)
U2 = u0*np.ones((1,n2), dtype = complex)
U3 = np.zeros((1,n3), dtype = complex)
U = np.concatenate((U1 , U2 , U3), axis = 1)
U = U.transpose()
U = U*np.eye(U.shape[0])
T =
```

# REFERENCES:

1. J. Grosso Vaj. Pastori Paravicini. Solid state physics. Translated by P. Sahib-Sara Volume 1, Isfahan University of Technology" 2018(0)2. N. Zettili, "Quantum mechanics: concepts and applications," (2003).
3. S. Datta., "Quantum Transport:Atom to Transistor", Cambridge University Press (2005).
4. H. Bruus, and E. Karsten., "Many-body quantum theory in condensed matter physics: an introduction", OUP Oxford (2004).