PHY 505: Final Project
Quantum Dot Eigenstates

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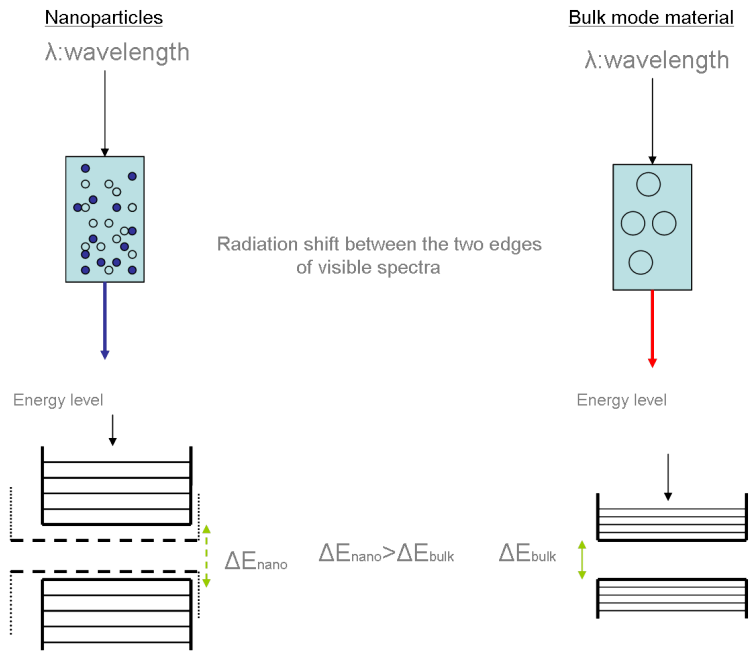
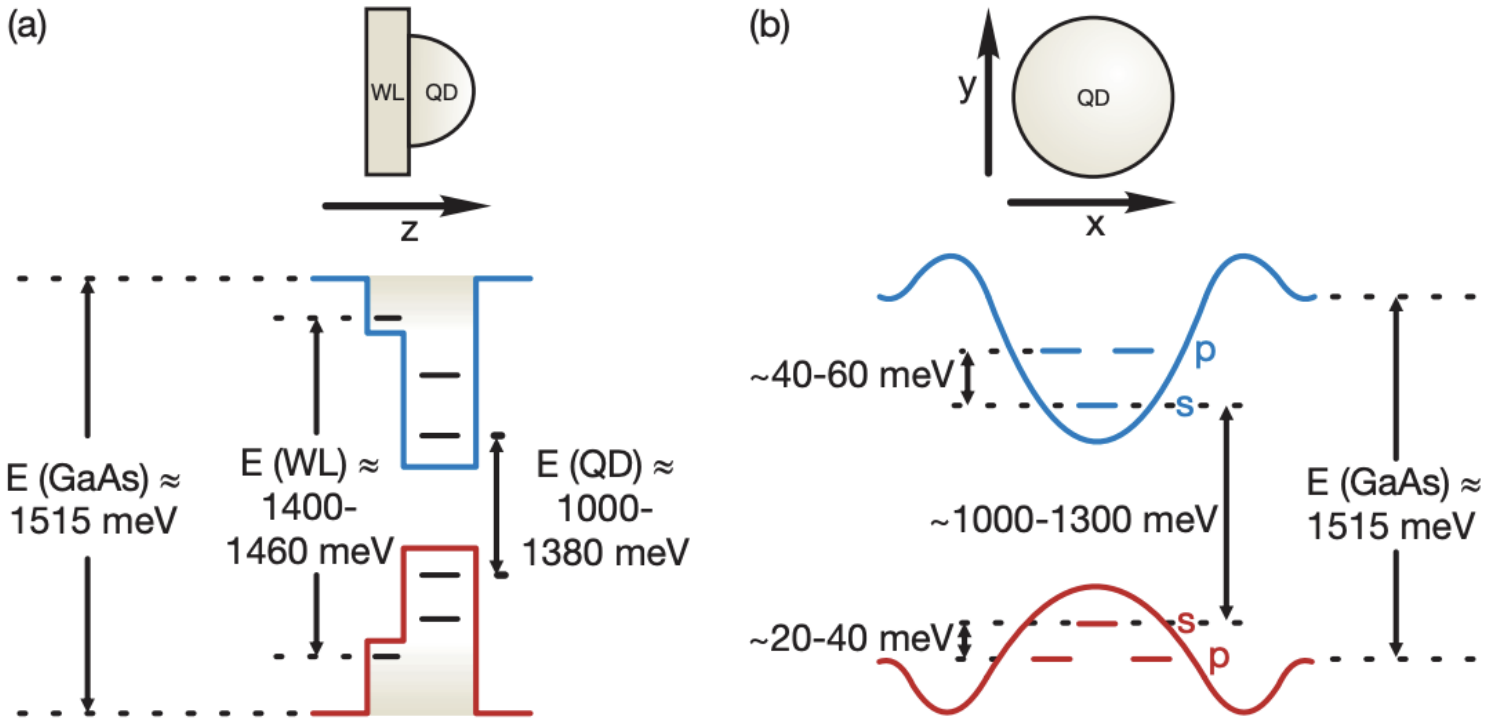
Quantum Dots

- Quantum dots (QDs) are nanometer-scale semiconductor materials
- Display quantum confinement due to small size ($<$10 [nm])
- Numerous applications, such as LEDs, single-electron transistors and solar cells



Quantum Dots Energy Band Structure[1]

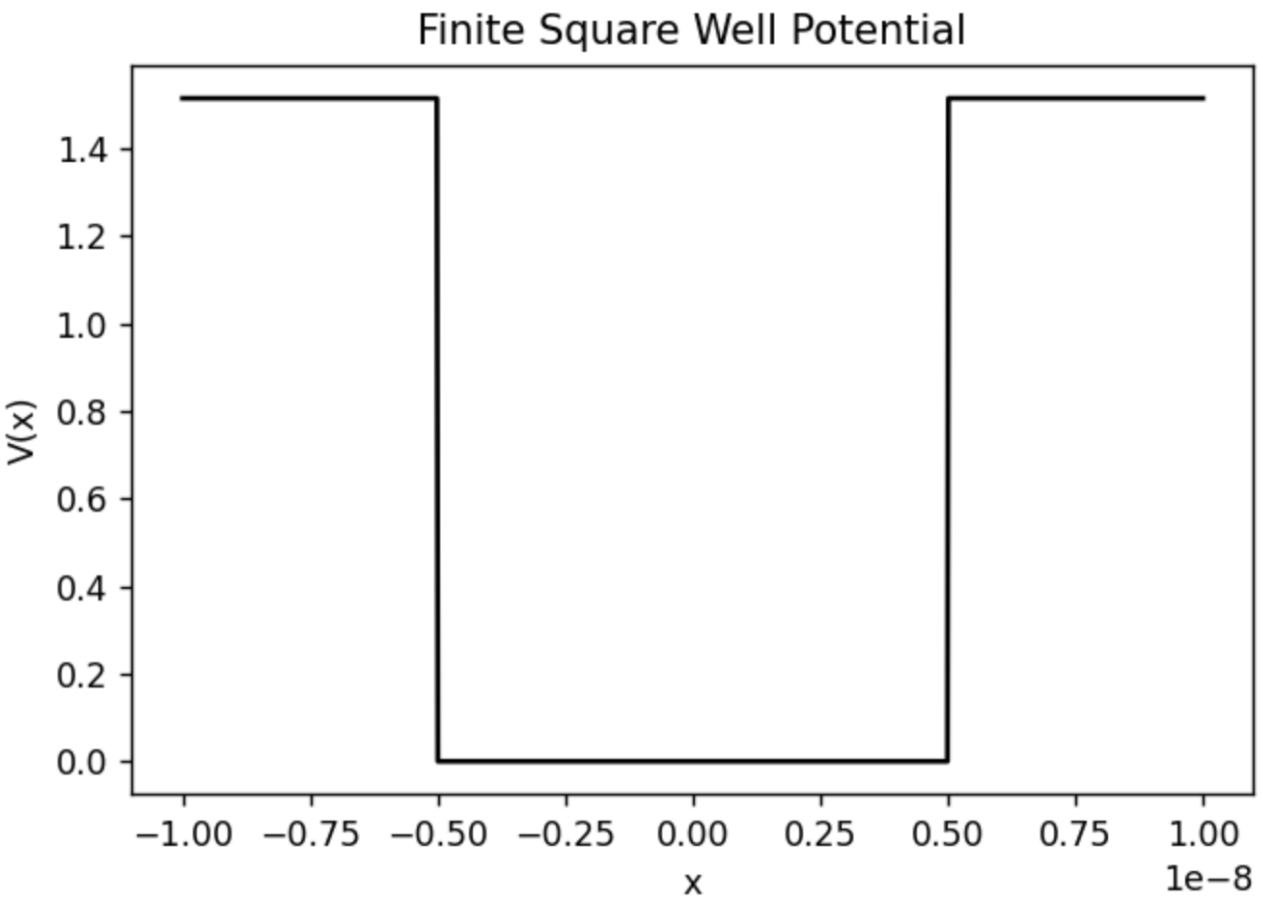


→ **z-direction**: Finite Potential Square Well

→ **x,y-direction**: Weak Parabolic Potential Well

Finite Potential Square Well

$$V(x) = \begin{cases} 0, & for\ -a \leq x \leq a \\ V_0, & for\ |x| > a \end{cases} \tag{1}$$



Time Independent Schrodinger Equation: Analytic Approach[2]

Time Independent Schrödinger Equation,

$$\frac{-\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x) \tag{2}$$

For $x < -a$ and $x > a$,

$$\frac{-\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V_0\Psi(x) = E\Psi(x) \tag{3}$$

For $-a \leq x \leq a$,

$$\frac{-\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = E\Psi(x) \tag{4}$$

The general solution for this system is therefore,

$$\begin{cases} \Psi_1(x) = Ae^{-\alpha x} + Be^{\alpha x} & for x < -a \\ \Psi_2(x) = Csin(\kappa x) + Dcos(\kappa x) & for -a < x < a \\ \Psi_3(x) = Fe^{-\alpha x} + Ge^{\alpha x} & for x > a \end{cases} \tag{5}$$

where,

$$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar^2} \tag{6}$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar^2} \tag{7}$$

Time Independent Schrodinger Equation: Analytic Approach

Applying continuity conditions,

$$\Psi_1(x=-a) = \Psi_2(x=-a), \ \Psi_3(x=a) = \Psi_2(x=a), \tag{8}$$

$$\frac{d\Psi_1}{dx}(x=-a) = \frac{d\Psi_2}{dx}(x=-a), \ \frac{d\Psi_3}{dx}(x=a) = \frac{d\Psi_2}{dx}(x=a), \tag{9}$$

gives the analytic solutions,

$$tan(z) = \sqrt{(z_0/z)^2 - 1} \quad (symmetric\ case) \tag{10}$$

$$-cot(z) = \sqrt{(z_0/z)^2 - 1} \quad (antisymmetric\ case) \tag{11}$$

where,

$$z = \frac{a}{\hbar}\sqrt{2m(V_0 - E)} \tag{12}$$

$$z_0 = \frac{a}{\hbar^2}\sqrt{2mV_0} \tag{13}$$

TRANSCENDENTAL EQUATIONS!
$\Rightarrow$ Use numerical root finding methods

Alternate Approach: Finite Difference Method

Central difference formula for second derivative [3],

$$\Psi''(x) = \frac{\frac{\Psi(x+h)-\Psi(x)}{h} - \frac{\Psi(x)-\Psi(x-h)}{h}}{h}, \tag{14}$$

$$\tag{15}$$

$$= \frac{\Psi(x+h) - 2\Psi(x) + \Psi(x-h)}{h^2}. \tag{16}$$

Plugging into the Schrödinger equation,

$$\frac{-\hbar}{2m}\left(\frac{\Psi(x+h) - 2\Psi(x) + \Psi(x-h)}{h^2}\right) + V(x)\Psi(x) = E\Psi(x). \tag{17}$$

Alternate Approach: Finite Difference Method

Combine all steps into matrix form,

$$-\frac{\hbar^2}{2mh^2}\begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & & \dots & -2 & 1 \\ 0 & & \dots & 1 & -2 \end{pmatrix}\begin{bmatrix} \Psi(x_0) \\ \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_N) \end{bmatrix} + \begin{pmatrix} V(x_0) & & & & \\ & V(x_1) & & & \\ & & V(x_2) & & \\ & & & \ddots & \\ & & & & V(x_N) \end{pmatrix}\begin{bmatrix} \Psi(x_0) \\ \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_N) \end{bmatrix} = E\begin{bmatrix} \Psi(x_0) \\ \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_N) \end{bmatrix}$$

or,

$$-\frac{\hbar^2}{2mh^2}\left(\begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & & \dots & -2 & 1 \\ 0 & & \dots & 1 & -2 \end{pmatrix} + \begin{pmatrix} V(x_0) & & & & \\ & V(x_1) & & & \\ & & V(x_2) & & \\ & & & \ddots & \\ & & & & V(x_N) \end{pmatrix}\right)\begin{bmatrix} \Psi(x_0) \\ \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_N) \end{bmatrix} = E\begin{bmatrix} \Psi(x_0) \\ \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_N) \end{bmatrix}.$$

$\Rightarrow$ Diagonalize Hamiltonian matrix to get eigenstates

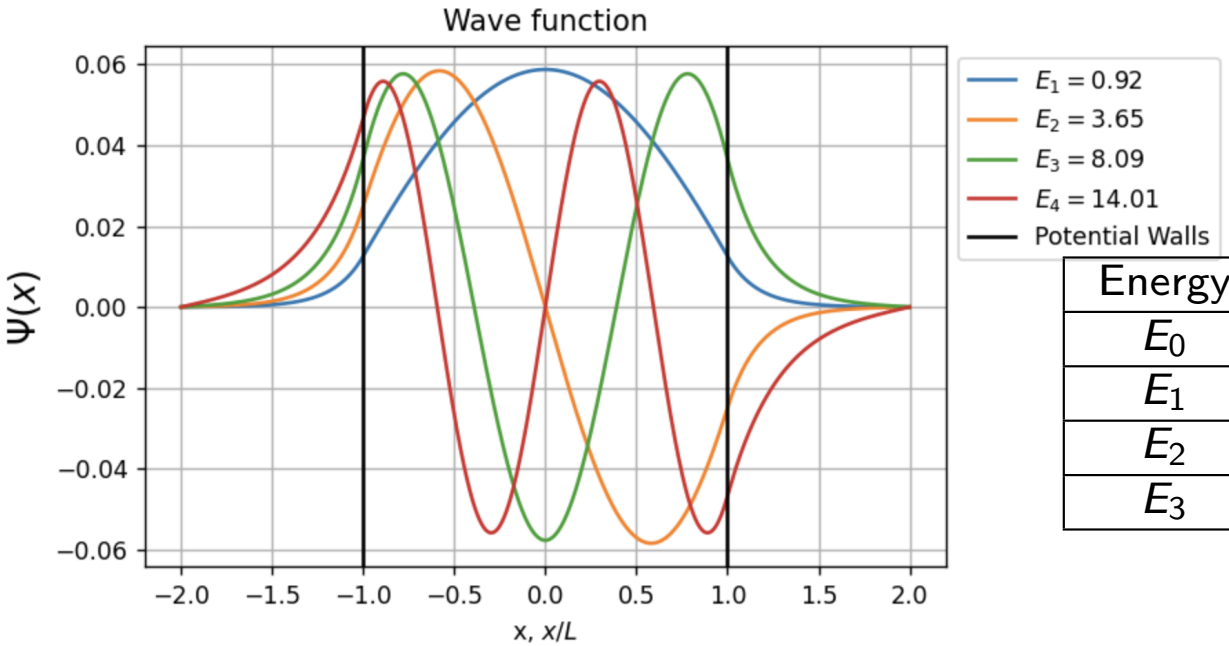
Finite Difference Method Code

```
27      def build_Hamiltonian(self):
28          N = len(self.x)
29          h = abs(self.x[1]-self.x[0])
30          T = np.zeros((N-2)**2).reshape(N-2,N-2)
31          for i in range(N-2):
32              for j in range(N-2):
33                  if i==j:
34                      T[i,j] = -2
35                  elif np.abs(i-j)==1:
36                      T[i,j] = 1
37                  else:
38                      T[i,j] = 0
39          #T = -T/(2*(h**2))
40          T = -((self.hbar**2)/(2*self.m*(h**2))) * T
41          V = np.zeros((N-2)**2).reshape(N-2,N-2)
42          for i in range(N-2):
43              for j in range(N-2):
44                  if i==j:
45                      V[i,j]= self.V_func(self.x[i+1])
46                  else:
47                      V[i,j]=0
48
49          return T + V
50
51      def finite_diff(self, num_eigs):
52          H = self.build_Hamiltonian()
53
54          val,vec=np.linalg.eig(H)
55          eigval_ind = np.argsort(val)
56          eigval_ind = eigval_ind[0:num_eigs]
57          energies = val[eigval_ind]
58
59          wavefunctions = np.zeros((len(val), num_eigs))
60          for i in range(len(eigval_ind)):
61              wavefunctions[:,i] = vec[:,eigval_ind[i]]
62
63          zero_vec = np.zeros(num_eigs)
64          wavefunctions = np.vstack((zero_vec,wavefunctions,zero_vec))
65          wavefunctions[:,0] = abs(wavefunctions[:,0])
66
67          return energies, wavefunctions
```

Energy Comparisons

Check accuracy of FD method using simple inputs

- $V_0 = 20$
- $L = 1$
- $\frac{\hbar^2}{m} = 1$

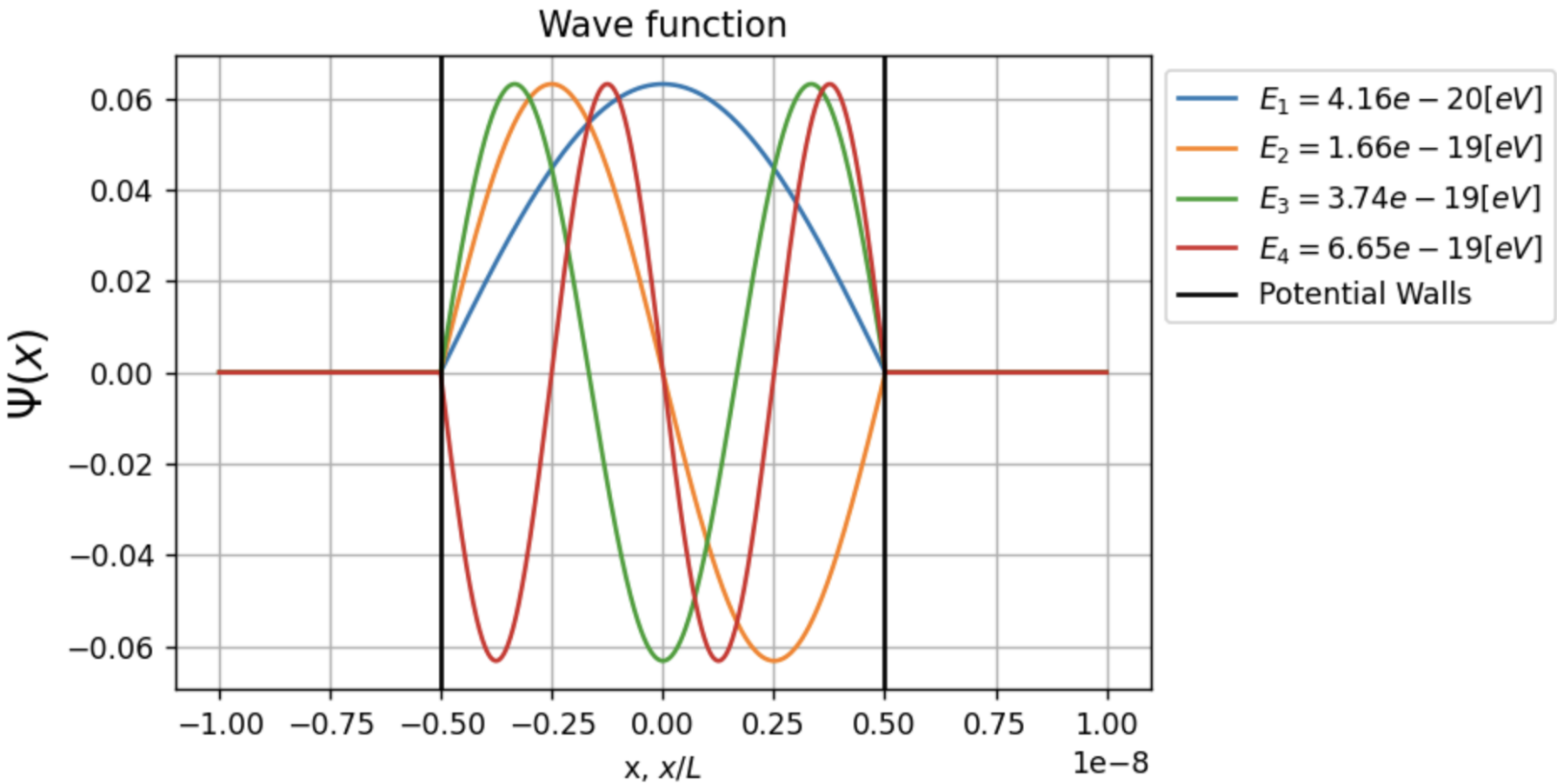


Energy	Analytic	Finite Difference
E_0	0.917870	0.916272
E_1	3.646201	3.639914
E_2	8.092151	8.078635
E_3	14.002160	13.983551

Wavefunctions

Calculate eigenstates for GaAs

- $V_0 = 1.515[eV]$
- $L = 10[nm]$
- $\hbar = 6.582 * 10^{-16}[eV * s]$
- $m = 0.5109[MeV/c^2]$



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