Simulating the Energy Spectrum of Quantum Dots

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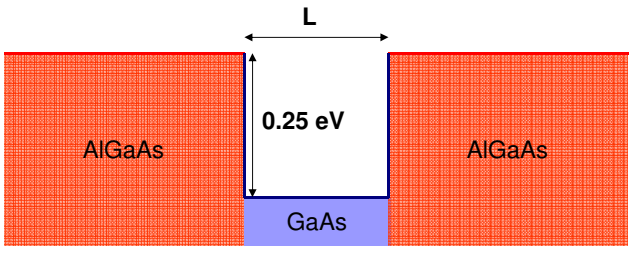
PROBLEM 1. Calculate the electron energy spectrum of a 1D GaAs/AlGaAs QD as a function of the size.

Hint: consider GaAs effective mass all over the structure.



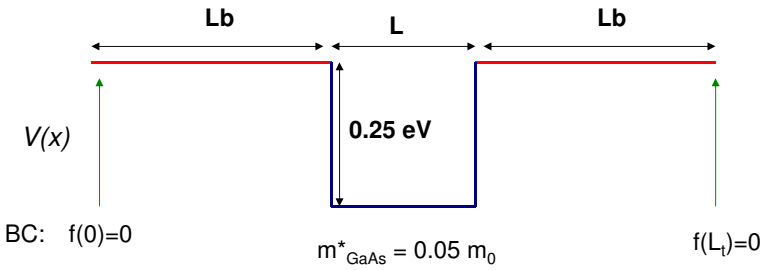
$m^*_{GaAs} = 0.05\ m_0$

The single-band effective mass equation:

$$[-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2} + V(x)]\,f(x) = E\,f(x)$$

Let us use atomic units ($\hbar = m_0 = e = 1$)

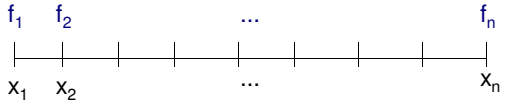
$$[-\frac{1}{2(m^*/m_0)}\frac{d^2}{dx^2} + V(x)]\,f(x) = E\,f(x)$$



Numerical integration of the differential equation: *finite differences*

$$[-\frac{1}{2m^*}\frac{d^2}{dx^2} + V(x)]\,f(x) = E\,f(x)$$

Discretization grid

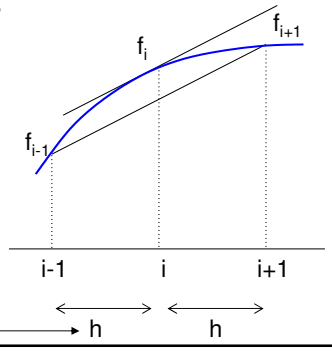


How do we approximate the derivatives at each point?

$$f'(x_i) = f_i' = \frac{f_{i+1} - f_{i-1}}{2h}$$

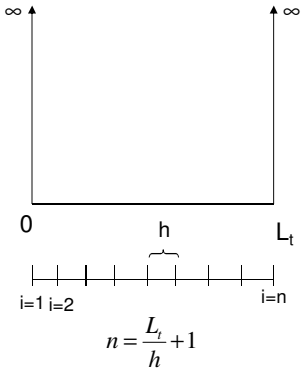
$$f''(x_i) = f_i'' = \frac{f_{i+1}' - f_{i-1}'}{2h} =$$

$$= \ldots = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$



FINITE DIFFERENCES METHOD

$$[-\frac{1}{2m^*}\frac{d^2}{dx^2} + V(x)]\,f(x) = E\,f(x) \quad + \quad BCs: \begin{vmatrix} f(0)=0 \\ f(L_t)=0 \end{vmatrix}$$



$$n = \frac{L_t}{h} + 1$$

1. Define discretization grid
2. Discretize the equation:

$$-\frac{1}{2m^*} f_i'' + V_i f_i = E\,f_i$$

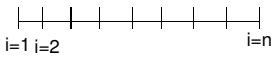
$$-\frac{1}{2m^* h^2}[f_{i+1} - 2f_i + f_{i-1}] + V_i f_i = E\,f_i$$

3. Group coefficients of fwd/center/bwd points

$$\left(-\frac{1}{2m^*h^2}\right)f_{i-1} + \left(\frac{1}{m^*h^2} + V_i\right)f_i + \left(-\frac{1}{2m^*h^2}\right)f_{i+1} = E\,f_i$$

$$\beta_{i-1}\,f_{i-1} + a_i\,f_i + b_{i+1}\,f_{i+1} = E\,f_i$$

$$\beta_{i-1}\,f_{i-1} + a_i\,f_i + b_{i+1}\,f_{i+1} = E\,f_i$$



Trivial eqs: $f_1 = 0$, $f_n = 0$.

Extreme eqs:

$$\begin{vmatrix} i=2 & \rightarrow & \beta_1 \cancel{f_1}^{\,0} & + a_2 f_2 & + b_3 f_3 = E f_2 \\ \ldots. & & \ldots. & \ldots. & \ldots. \quad \ldots. \\ i=n-1 & \rightarrow & \beta_{n-2} f_{n-2} & + a_{n-1} f_{n-1} & + b_n \cancel{f_n}_{\,0} = E f_{n-1} \end{vmatrix}$$

Matriz (n-2) x (n-2) - sparse

We now have a standard diagonalization problem (dim n-2):

$$\begin{bmatrix} a_2 & b_3 & & & \\ \beta_2 & a_3 & b_4 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & a_{n-2} & b_{n-1} \\ & & & \beta_{n-2} & a_{n-1} \end{bmatrix} \cdot \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix} = E \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix}$$

```
% INPUT DATA

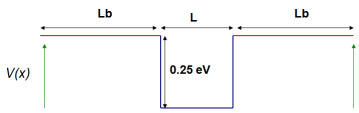
L_nm=40.0;      % box length (nm)
Lb_nm=20.0;     % length of the barrier (nm)
m=0.05;         % electron effective mass (times m0)
Vin_eV=0.00;    % potential energy in the box (eV)
Vout_eV=0.1;    % potential energy in the barrier (eV)
n=321;          % grid nodes
neig=4;         % number of states to be calculated (starting from ground state)


% 1) Convert into atomic units
kdist=0.0529177; % kdist nm = 1 bohr radius
kener=27.21138;  % kener eV = 1 hartree

L=L_nm/kdist;
Lb=Lb_nm/kdist;
Vin=Vin_eV/kener;
Vout=Vout_eV/kener;

% 2) Define grid

Lt= 2*Lb + L;       % total length
h=Lt/(n-1)          % grid step
```

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% 3) Calculate potential V(x)

for i=1:n
    x(i)= (i-1)*h-Lt/2; % position at i-th grid point
    if (abs(x(i))<=L/2)
        V(i)=Vin;  % inside the box
    else
        V(i)=Vout; % in the barrier
    end;

end;


% 4) Define coefficients of f(i), f(i+/-1)
a=zeros(n,1);
for i=1:n
    a(i)=1/(m*h^2)+V(i); % coef of f(i) -depends on i
end;
b=-1/(2*m*h^2);          % coef. of f+ and f-
```

$$\begin{bmatrix} a_2 & b & & & \\ b & a_3 & b & & \\ & \ddots & \ddots & \ddots & \\ & & b & a_{n-2} & b \\ & & & b & a_{n-1} \end{bmatrix}$$

```
   [di    dc    ds]
    2     2     2
    3     3     3
    4     4     4
    5     5     5

mat=spdiags([di dc ds],[-1, 0, 1],4,4)

    2     3     0     0
    2     3     4     0
    0     3     4     5
    0     0     4     5
```

$$\beta_{i-1} f_{i-1} + a_i f_i + b_{i+1} f_{i+1} = E f_i$$

$$\begin{bmatrix} a_2 & b_3 & & & \\ \beta_2 & a_3 & b_4 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & a_{n-2} & b_{n-1} \\ & & & \beta_{n-2} & a_{n-1} \end{bmatrix}$$

β_2	a_2	0
β_3	a_3	b_3
...	...	b_4
...	...	...
...	...	...
β_{n-2}	a_{n-2}	b_{n-2}
0	$a_{(n-1)}$	b_{n-1}

```
% 5) Build the Hamiltonian matrix

% define the three diagonals (vectors)

dc=a(2:n-1);    % main diagonal f(i)
di=[ones(n-3,1)*b;0]; % or just di=ones(n-2,1)*b; subdiagonal f(i-1)
ds=[0;ones(n-3,1)*b]; % or just ds=ones(n-2,1)*b; superdiagonal f(i+1)

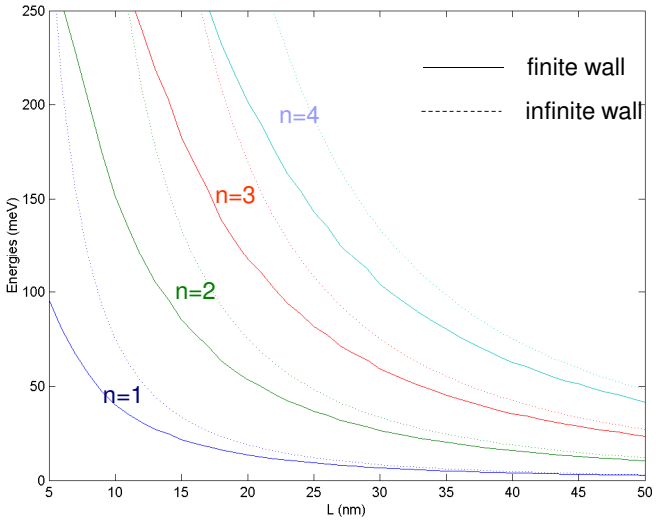
% introduce them into a sparse, tridiagonal matrix
matrix=spdiags([di,dc,ds],[-1,0,1],n-2,n-2);

% 6) Diagonalize the matrix
[P,D]=eigs(matrix,neig,'sa');
eners=diag(D)*kener;        % grep energy and convert to eV


% ploting potential vs. x (nm)
figure;plot(x*kdist,V*kener);
% ploting the neig low-lying eigenfunctions vs. x (nm)
figure;plot(x(2:n-1)*kdist,P(:,1:neig));

% write neig low-lying energy meV
'Lowest energies  meV ', eners
```

The result should look like this:



Exercices:

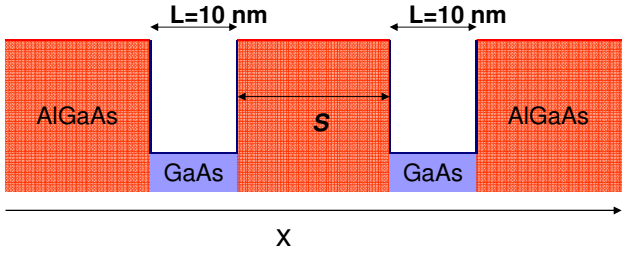
a) Compare the converged energies with those of the particle-in-the-box with infinite walls for the n=1,2,3 states.

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$$

b) Plot the 3 lowest eigenstates for L=15 nm, L_b=10 nm. What is different from the infinite wall eigenstates?

HOME WORK:

Calculate the electron energy spectrum of two coupled QDs as a function of their separation S. Plot the two lowest states for S=1 nm and S=10 nm.



The result should look like this: