Computational Microelectronics, 2018 Fall

Homework #2

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**Assumption**:

a = 5nm

m = 0.19 m0

**Analytical solution**:

Smallest k2 is 3.94784176043574e+17

Ground state energy is 1.65300981320417e-2

**Numerical solution**:

1. N=5: k2 = 3.74903320081219e+17

Ground state energy = 1.569766e-02 eV

1. N=50: k2 = 3.94648960515371e+17

Ground state energy = 1.652444e-02 eV

1. N=500: k2 = 3.94782872043323e+17

Ground state energy = 1.653004e-02 eV

**Error\***:

1. N=5: k2: 5.04 %

E: 5.04 %

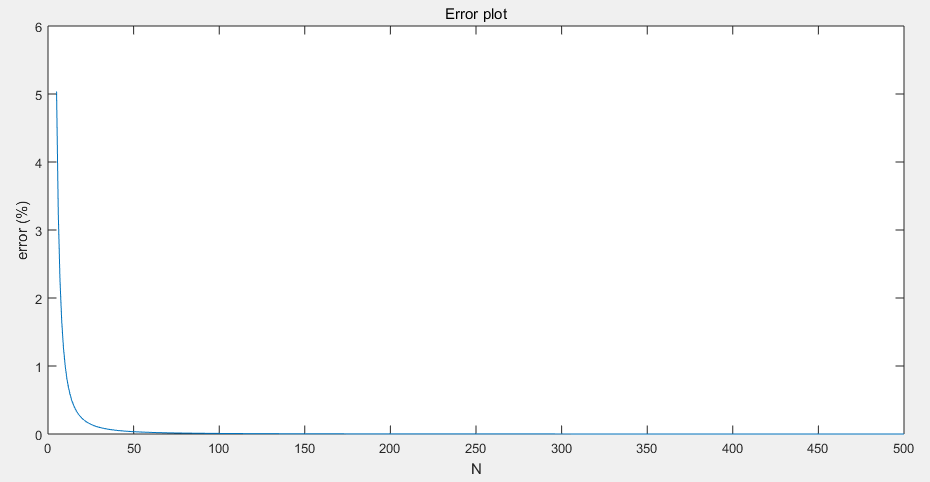
1. N=5: k2: 0.0343 %

E: 0.0343 %

1. N=5: k2: 0.000330 %

E: 0.000352 %

\*:



**Code**

clear all;

hbar = 1.054571800e-34; % Planck constant (J\*s)

m\_elec = 9.10938356e-31; % Mass of electron (kg)

x = 5.0e-9;

N = 5;

m = 0.91\*m\_elec;

dx = x/(N-1);

for i = 1:N-2

if i==1

A(i,i) = -2;

A(i,i+1)= 1;

elseif i==N-2

A(i,i) = -2;

A(i,i-1)= 1;

else

A(i,i-1)=1;

A(i,i) = -2;

A(i,i+1)= 1;

end

end

[eigvec,eigval] = eig(A);

k\_sq = -eigval/(dx^2);

E = (hbar^2)\*k\_sq/(2\*m);

E\_ground = E(N-2,N-2);

E\_ground\_eV = E\_ground\*6.242e+18;

%% wave function

eig\_vec = eigvec(N-2,:); %wave function of n-th excited state =N-2-n (ground state = 0th state)

for i = 1:N-2

x\_val(i) = i\*dx;

end

figure(1)

plot(x\_val,eig\_vec)

%%

fprintf('Ground state energy is %d eV\n',E\_ground\_eV)