Computational Microelectronics

Assignment #2

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1. Matlab Code

```
% set N value
N= ;

% Constant value
h_bar = 6.62607004 * 10^(-34)/(2*pi); % m^2 kg/s
m0 = 9.10938356 * 10^(-31); % electron rest mass kg
m = 0.19*m0; % electron mass
a = 5 * 10^(-9); % m
dx = a/(N-1); % m

A = zeros(N-2,N-2) ;

% First and last line of Laplacian operator
A(1,1) = -2.0; A(1,2) = 1.0 ;
A(N-2,N-3) = 1.0; A(N-2,N-2) = -2.0 ;

% The other line
for ii = 2:N-3
   A(ii,ii-1) = 1.0, A(ii,ii) = -2.0, A(ii,ii+1) = 1.0 ;
end

[V,D] = eig (A);

d = min(D);
d_min = min(abs(d));
k_square = d_min/(dx^2);
E = (k_square)*((h_bar^2)/(2*m));
E_eV = E * 6.242*10^(18);
```

Minimum D

i. N=5→ D = 0.5858

ii. N=50 → D = 0.0041

iii. N=500 → D = 3.9637e-05

2. Find ground state energy

- Condition : a = 5 nm and m=0.19 m_o,

i. N = 5

- $\Delta x = a/N-1 = 1.25$ nm
- $k^2(\Delta x)^2 = 0.5858$
- $E = \frac{\hbar}{2m}k^2 = 0.0753$ eV

ii. N = 50

- $\Delta x = a/N-1 = 0.10204$ nm
- $k^2(\Delta x)^2 = 0.0041$
- $E = \frac{\hbar}{2m}k^2 = 0.0791$ eV

iii. N= 500

- $\Delta x = a/N-1 = 0.01002004$ nm
- $k^2(\Delta x)^2 = 3.9637e-05$
- $E = \frac{\hbar}{2m}k^2 = 0.0792$ eV

3. Error analysis as a function of N

- Analytic solution : 0.0792 eV
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