Lecture12

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Potential energy

- In the case of the infinite potential well, the potential energy is 0 eV.
  - Of course, in the realistic case, the potential energy is provided from the Poisson equation.
  - When the electro potential, $\phi(z)$, is given, the potential energy is written as

$$V(z) = -q\phi(z) + (E_c - E_i)$$

$E_c - E_i$: Constant for a given material

Schrödinger equation

- For the z-directional Schrodinger equation,
  - We have the following form:

$$-\frac{\hbar^2}{2m_{zz}}\frac{d^2}{dz^2}\psi_{z,n}(z)+V(z)\,\psi_{z,n}(z)=E_{z,n}\psi_{z,n}(z)$$

  - After a simple manipulation,

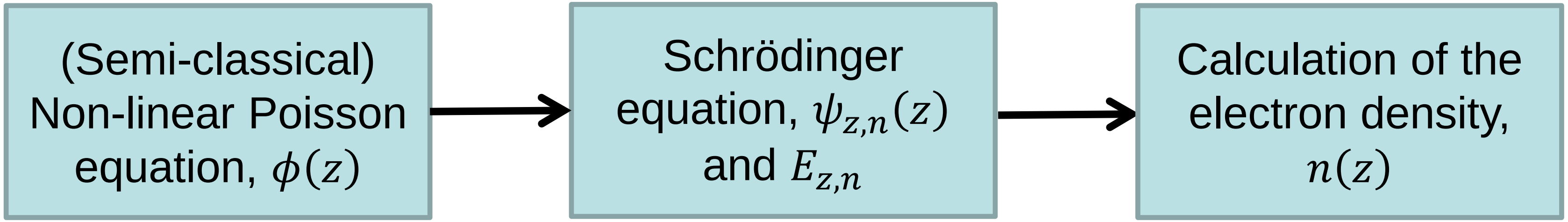
$$\frac{d^2}{dz^2}\psi_{z,n}(z)-\frac{2m_{zz}}{\hbar^2}V(z)\,\psi_{z,n}(z)=-\frac{2m_{zz}}{\hbar^2}E_{z,n}\psi_{z,n}(z)$$

  - Discretized version

$$\psi_{z,n,i+1}-2\psi_{z,n,i}+\psi_{z,n,i-1}-\frac{2m_{zz}}{\hbar^2}V(z_i)(\Delta z)^2\psi_{z,n,i}=-\frac{2m_{zz}}{\hbar^2}E_{z,n}(\Delta z)^2\psi_{z,n,i}$$

Simulation flow

- Anyway, we need the initial solution.
  - It can be obtained from the semi-classical simulation.
  - Then, under the given potential energy, we can calculate the electron density.



(Semi-classical) Non-linear Poisson equation, $\phi(z)$

Schrödinger equation, $\psi_{z,n}(z)$ and $E_{z,n}$

Calculation of the electron density, $n(z)$

  - Of course, the electron density is not fully consistent with the Poisson equation. It should be improved later.

MATLAB example (1)

- Defining variables

```
h = 6.626176e-34; % Planck constant, J s
hbar = h / (2*pi); % Reduced Planck constant, J s
q = 1.602192e-19; % Elementary charge, C
m0 = 9.109534e-31; % Electron rest mass, kg
k_B = 1.380662e-23; % Boltzmann constant, J/K
eps0 = 8.854187817e-12; % Vacuum permittivity, F/m
T = 300.0; % Temperature, K
thermal = k_B*T/q; % Thermal voltage, V
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
Deltaz = 0.1e-9; % 0.1 nm spacing
Nz = 61; % 6 nm thick
z = Deltaz*transpose([0:Nz-1]); % real space, m
interface1 = 6; % At z=0.5 nm
interface2 = 56; % At z=5.5 nm
eps_si = 11.7; eps_ox = 3.9; % Relative permittivity
Nacc = 1e24; % 1e18 /cm^3
ni = 1.075e16; % 1.075e10 /cm^3
coef = Deltaz*Deltaz*q/eps0;
Ec_Ei = 0.561004; % E_c – E_i, eV
```

MATLAB example (2)

- Semi-classical nonlinear Poisson solver

```
phi = zeros(Nz,1);
phi(:,1) = 0.33374;
for newton=1:10
   res = zeros(Nz,1);
   Jaco = sparse(Nz,Nz);
   res(1,1) = phi(1,1) - 0.33374;
   Jaco(1,1) = 1.0;
   res(Nz,1) = phi(Nz,1) - 0.33374;
   Jaco(Nz,Nz) = 1.0;
   for ii=2:Nz-1
      if     (ii< interface1 || ii> interface2)
         res(ii,1) = eps_ox*phi(ii+1,1) - 2*eps_ox*phi(ii,1) + eps_ox*phi(ii-1,1);
         Jaco(ii,ii-1) = eps_ox; Jaco(ii,ii) = -2*eps_ox;        Jaco(ii,ii+1) = eps_ox;
      elseif (ii==interface1)
         res(ii,1) = eps_si*phi(ii+1,1) - (eps_si+eps_ox)*phi(ii,1) + eps_ox*phi(ii-1,1);
         Jaco(ii,ii-1) = eps_ox; Jaco(ii,ii) = -(eps_si+eps_ox); Jaco(ii,ii+1) = eps_si;
      elseif (ii==interface2)
         res(ii,1) = eps_ox*phi(ii+1,1) - (eps_ox+eps_si)*phi(ii,1) + eps_si*phi(ii-1,1);
         Jaco(ii,ii-1) = eps_si; Jaco(ii,ii) = -(eps_ox+eps_si); Jaco(ii,ii+1) = eps_ox;
      else
         res(ii,1) = eps_si*phi(ii+1,1) - 2*eps_si*phi(ii,1) + eps_si*phi(ii-1,1);
         Jaco(ii,ii-1) = eps_si; Jaco(ii,ii) = -2*eps_si;        Jaco(ii,ii+1) = eps_si;
      end
   end
```

MATLAB example (3)

- Semi-classical nonlinear Poisson solver (continued)

```
   for ii=interface1:interface2
      if     (ii==interface1)
         res(ii,1) = res(ii,1) - coef*(Nacc+ni*exp(phi(ii,1)/thermal))*0.5;
         Jaco(ii,ii) = Jaco(ii,ii) - coef*ni*exp(phi(ii,1)/thermal)/thermal*0.5;
      elseif (ii==interface2)
         res(ii,1) = res(ii,1) - coef*(Nacc+ni*exp(phi(ii,1)/thermal))*0.5;
         Jaco(ii,ii) = Jaco(ii,ii) - coef*ni*exp(phi(ii,1)/thermal)/thermal*0.5;
      else
         res(ii,1) = res(ii,1) - coef*(Nacc+ni*exp(phi(ii,1)/thermal));
         Jaco(ii,ii) = Jaco(ii,ii) - coef*ni*exp(phi(ii,1)/thermal)/thermal;
      end
   end
   update = Jaco \ (-res);
   phi = phi + update;
end
```

MATLAB example (3)

- Schrödinger solver
  - Now we have the electrostatic potential. The potenti energy is

```
V = q*Ec_Ei - q*phi; % Potential energy, J
```

  - Only for bulk silicon nodes, the Hamiltonian is constructured.

```
Nbulk = interface2-interface1-1; % Number of bulk silicon nodes
Hamil = zeros(Nbulk,Nbulk);
Hamil(1,1) = -2; Hamil(1,2) = 1;
for ii=2:Nbulk-1
   Hamil(ii,ii+1) =  1;
   Hamil(ii,ii  ) = -2;
   Hamil(ii,ii-1) =  1;
end
Hamil(Nbulk,Nbulk) = -2; Hamil(Nbulk,Nbulk-1) = 1;
```

MATLAB example (4)

- Schrödinger solver (continued)
  - The potential energy is added.

```
for ii=1:Nbulk
   Hamil(ii,ii) = Hamil(ii,ii) -2*mzz*m0*(Deltaz/hbar)^2*V(ii+interface1,1);
end
```

  - Get the solution.

```
[eigenvectors,eigenvalues] = eig(Hamil);
```

  - Scale the eigenenergies.

```
Ez = diag(eigenvalues)/(-2*mzz*m0*(Deltaz/hbar)^2); % Eigenenergy, J
```

  - The wavefunction should be scaled.

Normalization of $\psi_{z,n}(z)$

- Its normalization condition
  - Intergration form

$$\int_0^{L_z} dz\left|\psi_{z,n}(z)\right|^2 = 1$$

  - Discretized version

$$\sum_i \Delta z\, \left|\psi_{z,n,i}\right|^2 = 1$$

  - Eigenfunctions should be normalized accordingly.

Modified MATLAB code (1)

- Defining variables (1)

```
h = 6.626176e-34; % Planck constant, J s
hbar = h / (2*pi); % Reduced Planck constant, J s
q = 1.602192e-19; % Elementary charge, C
m0 = 9.109534e-31; % Electron rest mass, kg
k_B = 1.380662e-23; % Boltzmann constant, J/K
eps0 = 8.854187817e-12; % Vacuum permittivity, F/m
T = 300.0; % Temperature, K
thermal = k_B*T/q; % Thermal voltage, V
```

Modified MATLAB code (2)

- Defining variables (2)

```
Lx = 100e-9; Ly = 100e-9; % Lenghs, m
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
Deltaz = 0.1e-9; % 0.1 nm spacing
Nz = 61; % 6 nm thick
z = Deltaz*transpose([0:Nz-1]); % real space, m
interface1 = 6; % At z=0.5 nm
interface2 = 56; % At z=5.5 nm
eps_si = 11.7; eps_ox = 3.9; % Relative permittivity
Nacc = 1e24; % 1e18 /cm^3
ni = 1.075e16; % 1.075e10 /cm^3
coef_Poi = Deltaz*Deltaz*q/eps0;
coef_Sch = 2*Lx*Ly/(2*pi)*sqrt(mxx*myy)*m0/(hbar^2)*(k_B*T);
Ec_Ei = 0.561004; % E_c – E_i, eV
```

Modified MATLAB code (3)

- Semi-classical nonlinear Poisson solver

```
phi = zeros(Nz,1);
phi(:,1) = 0.33374;
for newton=1:10
   res = zeros(Nz,1);
   Jaco = sparse(Nz,Nz);
   res(1,1) = phi(1,1) - 0.33374;
   Jaco(1,1) = 1.0;
   res(Nz,1) = phi(Nz,1) - 0.33374;
   Jaco(Nz,Nz) = 1.0;
```

Modified MATLAB code (4)

- Semi-classical nonlinear Poisson solver

```
for ii=2:Nz-1
    if     (ii< interface1 || ii> interface2)
       res(ii,1) = eps_ox*phi(ii+1,1) - 2*eps_ox*phi(ii,1) + eps_ox*phi(ii-1,1);
       Jaco(ii,ii-1) = eps_ox; Jaco(ii,ii) = -2*eps_ox;        Jaco(ii,ii+1) = eps_ox;
    elseif (ii==interface1)
       res(ii,1) = eps_si*phi(ii+1,1) - (eps_si+eps_ox)*phi(ii,1) + eps_ox*phi(ii-1,1);
       Jaco(ii,ii-1) = eps_ox; Jaco(ii,ii) = -(eps_si+eps_ox); Jaco(ii,ii+1) = eps_si;
    elseif (ii==interface2)
       res(ii,1) = eps_ox*phi(ii+1,1) - (eps_ox+eps_si)*phi(ii,1) + eps_si*phi(ii-1,1);
       Jaco(ii,ii-1) = eps_si; Jaco(ii,ii) = -(eps_ox+eps_si); Jaco(ii,ii+1) = eps_ox;
    else
       res(ii,1) = eps_si*phi(ii+1,1) - 2*eps_si*phi(ii,1) + eps_si*phi(ii-1,1);
       Jaco(ii,ii-1) = eps_si; Jaco(ii,ii) = -2*eps_si;        Jaco(ii,ii+1) = eps_si;
    end
 end
```

Modified MATLAB code (5)

- Semi-classical nonlinear Poisson solver (continued)

```
   for ii=interface1:interface2
      if     (ii==interface1)
         res(ii,1) = res(ii,1) - coef_Poi*(Nacc+ni*exp(phi(ii,1)/thermal))*0.5;
         Jaco(ii,ii) = Jaco(ii,ii) - coef_Poi*ni*exp(phi(ii,1)/thermal)/thermal*0.5;
      elseif (ii==interface2)
         res(ii,1) = res(ii,1) - coef_Poi*(Nacc+ni*exp(phi(ii,1)/thermal))*0.5;
         Jaco(ii,ii) = Jaco(ii,ii) - coef_Poi*ni*exp(phi(ii,1)/thermal)/thermal*0.5;
      else
         res(ii,1) = res(ii,1) - coef_Poi*(Nacc+ni*exp(phi(ii,1)/thermal));
         Jaco(ii,ii) = Jaco(ii,ii) - coef_Poi*ni*exp(phi(ii,1)/thermal)/thermal;
      end
   end
   update = Jaco \ (-res);
   phi = phi + update;
end
```

Modified MATLAB code (6)

- Schrödinger solver

```
V = q*Ec_Ei - q*phi; % Potential energy, J
Nbulk = interface2-interface1-1; % Number of bulk silicon nodes
Hamil = zeros(Nbulk,Nbulk);
Hamil(1,1) = -2; Hamil(1,2) = 1;
for ii=2:Nbulk-1
   Hamil(ii,ii+1) =  1;
   Hamil(ii,ii  ) = -2;
   Hamil(ii,ii-1) =  1;
end
Hamil(Nbulk,Nbulk) = -2; Hamil(Nbulk,Nbulk-1) = 1;
for ii=1:Nbulk
   Hamil(ii,ii) = Hamil(ii,ii) -2*mzz*m0*(Deltaz/hbar)^2*V(ii+interface1,1);
end
```

MATLAB example (1)

- Continued discussion
  - Get the solution.

```
[eigenvectors,eigenvalues] = eig(Hamil);
```

  - Scale the eigen-energies.

```
scaledEz = diag(eigenvalues)/(-2*mzz*m0*(Deltaz/hbar)^2); % Eigenenergy, J
```

  - Sort the eigen-energies.

```
[sortedEz,sortedIndex] = sort(scaledEz);
```

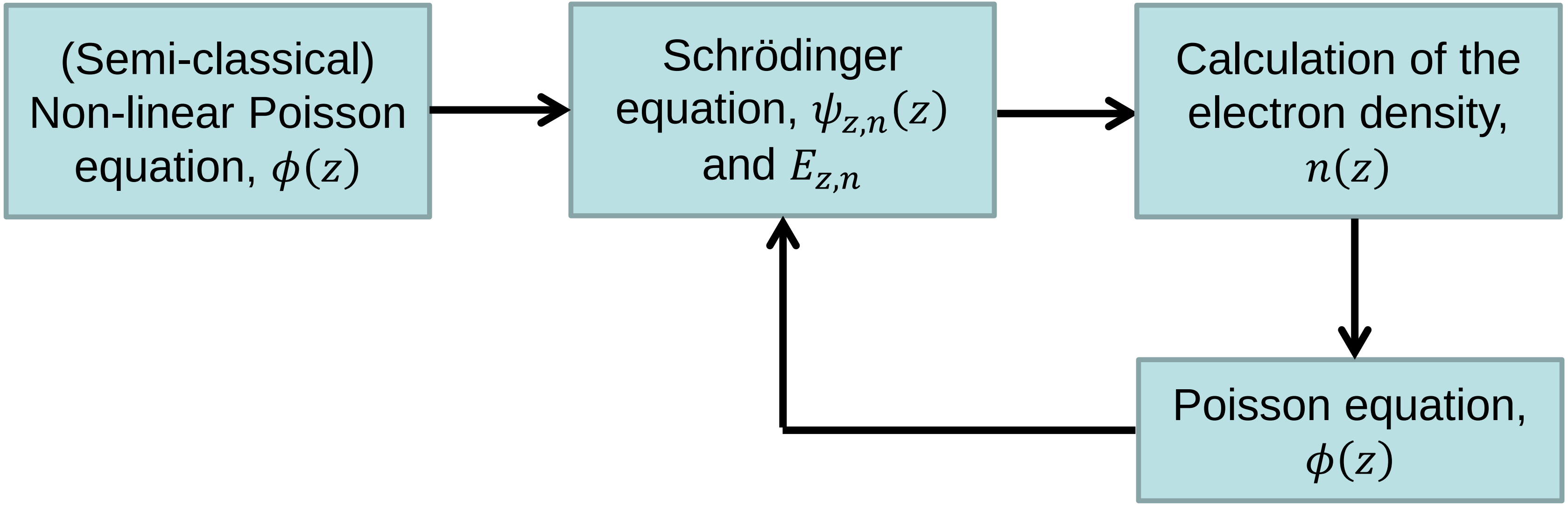
MATLAB example (2)

- Calculation of the electron density

```
nSubband = 10;
elec = zeros(Nz,1); % Electron density, /m^3
totalNumber = 0;
for n=1:nSubband
  Ez = sortedEz(n,1);
  wavefunction2 = eigenvectors(:,sortedIndex(n)).^2;
  normalization = sum(wavefunction2)*Deltaz;
  wavefunction2 = wavefunction2 / normalization;
  subbandNumber = coef_Sch*log(1+exp(-Ez/(k_B*T)));
  totalNumber = totalNumber + subbandNumber;
  elec(interface1+1:interface2-1,1) = elec(interface1+1:interface2-1,1) +
1/(Lx*Ly)*wavefunction2*subbandNumber;
end
```

Simulation flow

- Self-consistency
  - The electron density is not consistent with the Poisson equation.
  - Better way?



(Semi-classical) Non-linear Poisson equation, $\phi(z)$

Schrödinger equation, $\psi_{z,n}(z)$ and $E_{z,n}$

Calculation of the electron density, $n(z)$

Poisson equation, $\phi(z)$

6 valleys in silicon

- Up to now, we have considered only one band.
  - In silicon, we need to consider three valley pairs.
  - They can be characterized by (for a certain channel direction)

$$m_{xx} = 0.91m_0, m_{yy} = 0.19m_0, m_{zz} = 0.19m_0$$
$$m_{xx} = 0.19m_0, m_{yy} = 0.91m_0, m_{zz} = 0.19m_0$$
$$m_{xx} = 0.19m_0, m_{yy} = 0.19m_0, m_{zz} = 0.91m_0$$

  - Each of them has two-fold degeneracy.

MATLAB example

- Pseudocode

```
(Defining constants. Copy-and-paste)
(Semi-classical nonlinear Poisson equation. Copy-and-paste)
for iNewton = 1:20
   totalNumber = 0;
   elec = zeros(Nz,1); % Electron density, /m^3
   for iValley = 1:3
      mass = ones(3)*0.19;
      mass(iValley) = 0.91;
      coef_Sch = 2*Lx*Ly/(2*pi)*sqrt(mass(1)*mass(2))*m0/(hbar^2)*(k_B*T);
      (Schrodinger solver. Now mzz becomes mass(3).)
      (Calculation of electron density. Add it to elec.)
   end
   (Poisson equation)
end
```