Lecture8

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Residue and Jacobian matrix

- In silicon regions, consider the integrated Poisson equation.
  - The i-th entry of the residue vector reads

$$r_i = \frac{\epsilon_{si}}{\Delta x}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) - (\Delta x) q N_{acc} - (\Delta x) q n_i \exp\left(\frac{q\phi_i}{k_B T}\right)$$

  - The i-th row of the Jacobian matrix reads

$$J_{i,i+1} = \frac{\epsilon_{si}}{\Delta x}$$

$$J_{i,i} = -2\frac{\epsilon_{si}}{\Delta x} - (\Delta x) q n_i \frac{q}{k_B T} \exp\left(\frac{q\phi_i}{k_B T}\right)$$

$$J_{i,i-1} = \frac{\epsilon_{si}}{\Delta x}$$

MATLAB example (1)

- Defining variables

```
q = 1.602192e-19; % Elementary charge, C
eps0 = 8.854187817e-12; % Vacuum permittivity, F/m
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
thermal = k_B*T/q; % Thermal voltage, V
Deltax = 0.1e-9; % 0.1 nm spacing
N = 61; % 6 nm thick
x = Deltax*transpose([0:N-1]); % real space, m
interface1 = 6; % At x=0.5 nm
interface2 = 56; % At x=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 = Deltax*Deltax*q/eps0;
```

MATLAB example (2)

- `Jaco` and `res` should be constructed.
  - Boundary conditions

```
res = zeros(N,1);
Jaco = sparse(N,N);
res(1,1) = phi(1,1) - 0.33374;
Jaco(1,1) = 1.0;
res(N,1) = phi(N,1) - 0.33374;
Jaco(N,N) = 1.0;
```

MATLAB example (3)

- Laplacian part

```
for ii=2:N-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 (4)

- Charge part

```
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
```

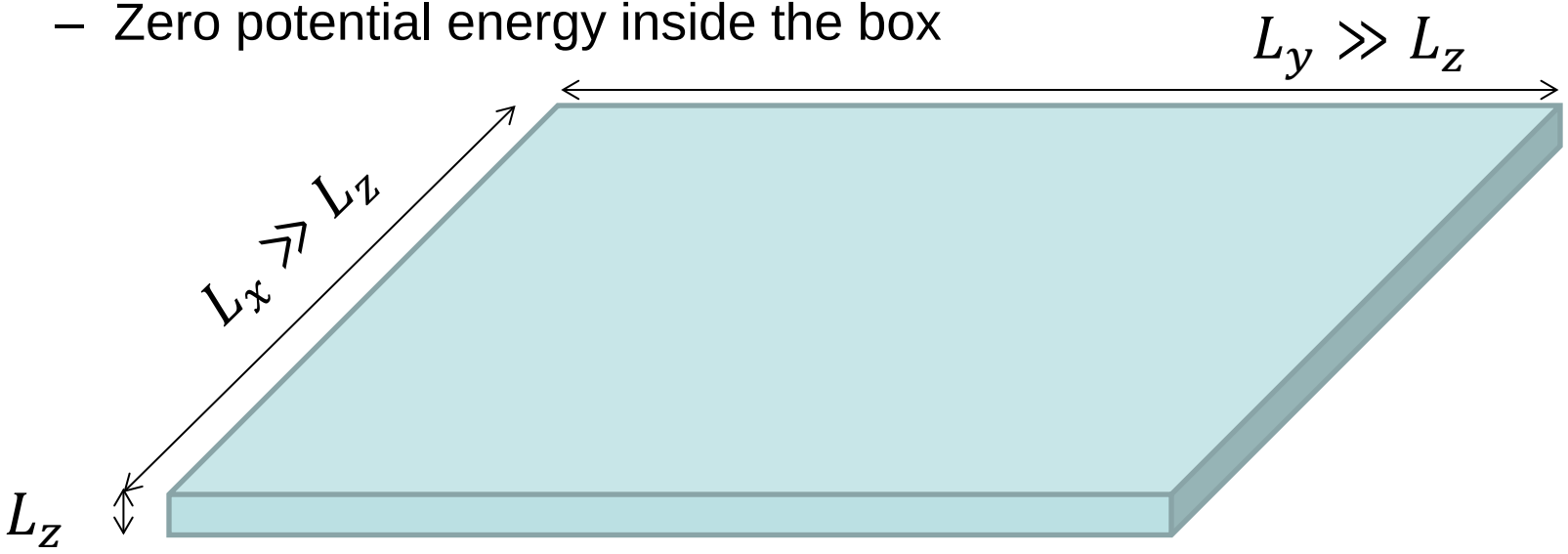
MATLAB example (5)

- Full code

```
(Defining variables. Copy-and-paste)
phi = zeros(N,1);
phi(:,1) = 0.33374;
for newton=1:10
   (Jaco and res are constructed here. Copy-and-paste)
   update = Jaco \ (-res);
   phi = phi + update;
end
plot(x,phi);
```

Thin and wide box

- Consider a thin and wide box. (3D infinite potential well)
  - Length along the confinement direction, L_z
  - At all six surfaces, the wavefunction vanishes.
  - Zero potential energy inside the box



Eigen-energy?

- Hamiltonian operator

$$H = -\frac{\hbar^2}{2m_{xx}}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{yy}}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{zz}}\frac{\partial^2}{\partial z^2}$$

  - We can find the following solution:

$$\psi_{l,m,n}(x,y,z) = A_{l,m,n}\sin\left(\frac{l\pi}{L_x}x\right)\sin\left(\frac{m\pi}{L_y}y\right)\sin\left(\frac{n\pi}{L_z}z\right)$$

  - Of course, the eigen-energy is given by

$$E_{l,m,n} = \frac{\hbar^2}{2m_{xx}}\frac{l^2\pi^2}{L_x^2} + \frac{\hbar^2}{2m_{yy}}\frac{m^2\pi^2}{L_y^2} + \frac{\hbar^2}{2m_{zz}}\frac{n^2\pi^2}{L_z^2}$$

Fermi-Dirac distribution

- Let us assume that there is a state whose eigen-energy is $E_{l,m,n}$.
  - Still, the Fermi level is located at 0 eV.
  - Then, the Fermi-Dirac distribution is given by

$$f_{FD} = \frac{1}{1 + \exp\left(\frac{E_{l,m,n}}{k_B T}\right)}$$

Total number?

- Number of electrons at a certain state
  - For a state with (l, m, n), the number of electrons is $2 \times f_{FD}\left(E_{l,m,n}\right)$. The factor of 2 is due to the spin degeneracy.
- There are many states.
  - The total number is given by

$$2 \times \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} f_{FD}\left(E_{l,m,n}\right)$$

MATLAB example (1)

- Let us consider $L_x = L_y = 100\ \mathrm{nm}$ and $L_z = 5\ \mathrm{nm}$.
  - In practical sense, L_z is reasonable. L_x and L_y are somewhat large.
  - Also, assume that $m_{xx} = m_{yy} = 0.19\, m_0$ and $m_{zz} = 0.91\, m_0$.
  - First, define some constants.

```
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
T = 300.0; % Temperature, K
```

MATLAB example (2)

- What is the number?
  - Set the box size and the masses.

```
Lx = 100e-9; Ly = 100e-9; Lz = 5e-9; % Lenghs, m
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
```

  - Calcultate the total number. How large is it?

```
lmax = 50; mmax = 50; nmax = 50;
totalNumber = 0;
for l=1:lmax
   for m=1:mmax
      for n=1:nmax
         E = (hbar*pi)^2/2/m0*(1/mxx*(l/Lx)^2 + 1/myy*(m/Ly)^2 + 1/mzz*(n/Lz)^2);
         totalNumber = totalNumber + 2/(1+exp(E/(k_B*T)));
      end
   end
end
```

Homework#6

- Due: AM08:00, October 15
- Problem#1
  - Write the nonlinear Poisson solver for the double-gate structure.
  - Consider the same double-gate structure in Homework#4.
  - Calculate the integrated electron density as a function of the gate voltage. (You must use the self-consistent solution.)
  - Suggested voltage range: From 0 V to 1 V