Lecture21

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GIST Lecture on November 26, 2018

Our achievement

- We can now solve the drift-diffusion equation.
  - However, it has been tested only at the equilibrium condition.
- Today's goal
  - Apply our code to nonequilibrium cases.
  - Calculate the current as a function of the voltage.

Implementation (1)

- The bias voltage is considered.

```
res = zeros(2*N,1);
Jaco = sparse(2*N,2*N);
res(1,1) = phi(1,1) - thermal*log(Ndon(1,1)/ni);
Jaco(1,1) = 1.0;
for ii=2:N-1
   res(2*ii-1,1) = eps_si*(phi(ii+1,1)-2*phi(ii,1)+phi(ii-1,1)) + coef*(Ndon(ii,1)-elec(ii,1));
   Jaco(2*ii-1,2*ii+1) =    eps_si;
   Jaco(2*ii-1,2*ii-1) = -2*eps_si;
   Jaco(2*ii-1,2*ii-3) =    eps_si;
   Jaco(2*ii-1,2*ii  ) = -coef;
end
res(2*N-1,1) = phi(N,1) - thermal*log(Ndon(N,1)/ni) – V_applied;
Jaco(2*N-1,2*N-1) = 1.0;
```

Implementation (2)

- The continuity equation (No change at all)

```
for ii=1:N-1 % edge-wise construction
   n_av = 0.5*(elec(ii+1,1)+elec(ii,1));
   dphidx = (phi(ii+1,1)-phi(ii,1))/Deltax;
   delecdx = (elec(ii+1,1)-elec(ii,1))/Deltax;
   Jn = n_av * dphidx – thermal * delecdx;
   res(2*ii,1) = res(2*ii,1) + Jn;
   Jaco(2*ii,2*ii+2) = Jaco(2*ii,2*ii+2) + 0.5*dphidx – thermal / Deltax;
   Jaco(2*ii,2*ii  ) = Jaco(2*ii,2*ii  ) + 0.5*dphidx + thermal / Deltax;
   Jaco(2*ii,2*ii+1) = Jaco(2*ii,2*ii+1) + n_av / Deltax;
   Jaco(2*ii,2*ii-1) = Jaco(2*ii,2*ii-1) - n_av / Deltax;
   res(2*ii+2,1) = res(2*ii+2,1) - Jn;
   Jaco(2*ii+2,2*ii+2) = Jaco(2*ii+2,2*ii+2) - 0.5*dphidx + thermal / Deltax;
   Jaco(2*ii+2,2*ii  ) = Jaco(2*ii+2,2*ii  ) - 0.5*dphidx - thermal / Deltax;
   Jaco(2*ii+2,2*ii+1) = Jaco(2*ii+2,2*ii+1) - n_av / Deltax;
   Jaco(2*ii+2,2*ii-1) = Jaco(2*ii+2,2*ii-1) + n_av / Deltax;
end
```

Implementation (3)

- Overall structure

```
for bias=0:10
   V_applied = 0.05 * bias;
   for newton=1:10
      (Jaco and res are constructed here. Copy-and-paste)
      update = Jaco \ (-res);
      phi = phi + update(1:2:2*N-1,1);
      elec = elec + update(2:2:2*N,1);
      norm(update(1:2:2*N-1,1),inf)
   end
end
```

Terminal current

- We want to calculate the terminal current.
  - Remember the convention for any terminal current.
  - "Incoming current density contributes positively."
  - Therefore, for the right contact located at $x = 600$ nm, the x-component of $\mathbf{J}_n$ contributes negatively.

$$J_{n,x} = -q\mu_n \left(n \frac{d\phi}{dx} - V_T \frac{dn}{dx} \right)$$

  - Finally, the *<u>terminal current per unit area</u>* (for the right contact) is

$$\frac{I_{Right}}{Area} = q\mu_n \left(n \frac{d\phi}{dx} - V_T \frac{dn}{dx} \right)$$

Importance of S-G scheme

- “The equation that started it all”
  - M. Lundstrom, SISPAD 2015 presentation

SISPAD 2015, September 9-11, 2015, Washington, DC, USA

Drift-Diffusion and computational electronics – Still going strong after 40 years!

Reflections on computational electronics and the equation that started it all

Our naïve approach

- Re-arrangement
  - The current density was discretized as

$$\frac{J_{n,i+0.5}}{-q\mu_n} = \frac{n_{i+1}+n_i}{2}\frac{\phi_{i+1}-\phi_i}{\Delta x} - V_T\frac{n_{i+1}-n_i}{\Delta x}$$

  - Simple manipulation gives

$$\frac{J_{n,i+0.5}}{qD_n}\Delta x = -\frac{n_{i+1}+n_i}{2}\frac{\phi_{i+1}-\phi_i}{V_T} + n_{i+1} - n_i$$

  - In terms of n_{i+1} and n_i,

$$\frac{J_{n,i+0.5}}{qD_n}\Delta x = n_{i+1}\left(1 - \frac{\phi_{i+1}-\phi_i}{2V_T}\right) - n_i\left(1 + \frac{\phi_{i+1}-\phi_i}{2V_T}\right)$$

Scharfetter-Gummel

- What happens if $|\phi_{i+1} - \phi_i| > 2V_T$?
  - One of two coefficients for the electron densities becomes negative. Unphysical!

$$\frac{J_{n,i+0.5}}{qD_n}\Delta x = n_{i+1}\left(1 - \frac{\phi_{i+1} - \phi_i}{2V_T}\right) - n_i\left(1 + \frac{\phi_{i+1} - \phi_i}{2V_T}\right)$$

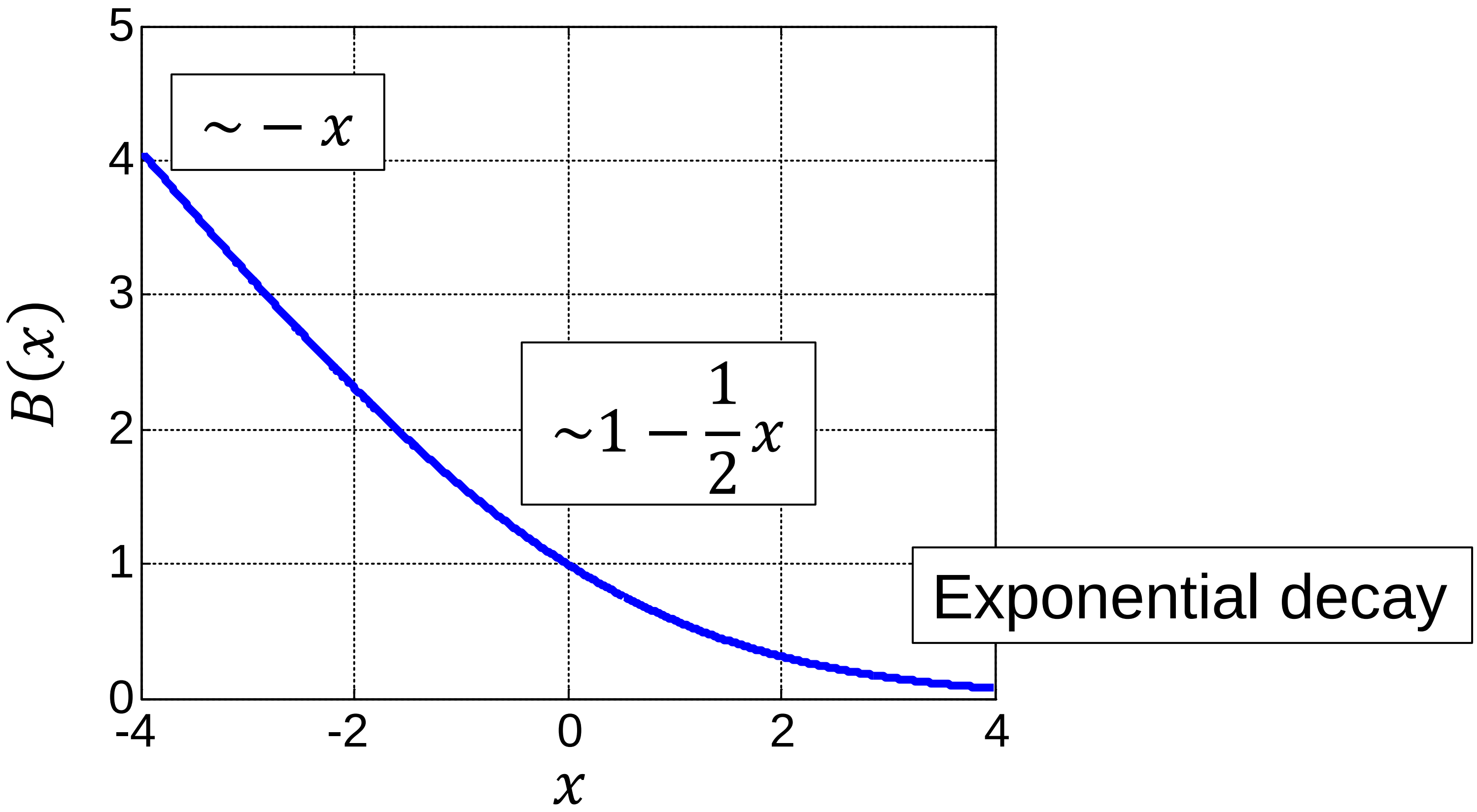
  - The Scharfetter-Gummel scheme

$$\frac{J_{n,i+0.5}}{qD_n}\Delta x = n_{i+1}B\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right) - n_i B\left(\frac{\phi_i - \phi_{i+1}}{V_T}\right)$$

  - Here, the Bernoulli function is

$$B(x) = \frac{x}{e^x - 1}$$

Bernoulli function



Two limits

- When $|\phi_{i+1} - \phi_i| \approx 0$,
  - Our original scheme is obtained.

$$\frac{J_{n,i+0.5}}{qD_n}\Delta x = n_{i+1}\left(1 - \frac{\phi_{i+1} - \phi_i}{2V_T}\right) - n_i\left(1 + \frac{\phi_{i+1} - \phi_i}{2V_T}\right)$$

- When $|\phi_{i+1} - \phi_i| \gg 0$,
  - (Without loss of generality) when $\phi_{i+1} - \phi_i \gg 0$,

$$\frac{J_{n,i+0.5}}{qD_n}\Delta x = -n_i \frac{\phi_{i+1} - \phi_i}{V_T}$$

$$J_{n,i+0.5} = -q\mu_n n_i \frac{\phi_{i+1} - \phi_i}{\Delta x}$$