Computational Microelectronics
Lecture 20 Continuity Equation

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Scharfetter-Gummel Scheme

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

Derivation (1)

- The electron current density in 1D
  - It is treated as a differential equation for n.

$$J_n = -q\mu_n n \frac{d\phi}{dx} + qD_n \frac{dn}{dx}$$

  - Assumption: J_n is a constant. (Current continuity, $\frac{dJ_n}{dx} = 0$)
  - Assumption: $\frac{d\phi}{dx} \approx \frac{\Delta\phi}{\Delta x}$
  - After simple manipulation,

$$\frac{dn}{dx} - \frac{1}{V_T}\frac{\Delta\phi}{\Delta x} n = \frac{J_n}{qD_n}$$

Treated as contants

Derivation (2)

$$J_n = -\frac{qD_n}{V_T}\frac{\Delta\phi}{\Delta x}C_2$$

- First-order differential equation
  - The solution has the following form:

$$n(x) = \underbrace{C_1 \exp\left(\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x\right)}_{\text{Homogeneous solution}} + C_2$$

  - We must find out two contants, C_1 and C_2, to satisfy

$$n(x_i) = n_i$$
$$n(x_{i+1}) = n_{i+1}$$

Derivation (3)

- Boundary values
  - At two boundaries,

$$n_i = C_1 \exp\left(\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i\right) + C_2$$

$$n_{i+1} = C_1 \exp\left(\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_{i+1}\right) + C_2$$

  - Taking the difference,

$$n_{i+1} - n_i = C_1 \exp\left(\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i\right) \times \left(\exp\frac{\Delta\phi}{V_T} - 1\right)$$

  - Now, we know C_1.

Derivation (4)

- Calculate C_2.
  - Recall that

$$C_2 = n_i - C_1 \exp\left(\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i\right)$$

  - By using C_1,

$$C_2 = n_i - \frac{n_{i+1} - n_i}{\exp\frac{\Delta\phi}{V_T} - 1} = n_i \frac{\exp\frac{\Delta\phi}{V_T}}{\exp\frac{\Delta\phi}{V_T} - 1} - n_{i+1}\frac{1}{\exp\frac{\Delta\phi}{V_T} - 1}$$

  - From $J_n = -\frac{qD_n}{V_T}\frac{\Delta\phi}{\Delta x}B$,

Derivation (5)

- We are almost there.
  - From $J_n = -\frac{qD_n}{V_T}\frac{\Delta\phi}{\Delta x}C_2$,

$$J_n = \frac{qD_n}{\Delta x}\left(n_{i+1}\frac{\frac{\Delta\phi}{V_T}}{\exp\frac{\Delta\phi}{V_T} - 1} - n_i\frac{\frac{\Delta\phi}{V_T}\exp\frac{\Delta\phi}{V_T}}{\exp\frac{\Delta\phi}{V_T} - 1} \right)$$

  - With the Bernoulli function, $B(x) = \frac{x}{\exp x - 1}$,

$$J_n = \frac{qD_n}{\Delta x}\left[n_{i+1}B\left(\frac{\Delta\phi}{V_T}\right) - n_iB\left(-\frac{\Delta\phi}{V_T}\right) \right]$$

Comparison

- Electron current density

$$J_n(x_{i+0.5}) = \frac{qD_n}{x_{i+1}-x_i}\left[(n_{i+1}-n_i) - \frac{1}{V_T}\frac{n_{i+1}+n_i}{2}(\phi_{i+1}-\phi_i)\right]$$

$$J_n(x_{i+0.5}) = \frac{qD_n}{x_{i+1}-x_i}\left[n_{i+1}B\left(\frac{\phi_{i+1}-\phi_i}{V_T}\right) - n_iB\left(-\frac{\phi_{i+1}-\phi_i}{V_T}\right)\right]$$

- Hole current density

$$J_p(x_{i+0.5}) = -\frac{qD_p}{x_{i+1}-x_i}\left[(p_{i+1}-p_i) + \frac{1}{V_T}\frac{p_{i+1}+p_i}{2}(\phi_{i+1}-\phi_i)\right]$$

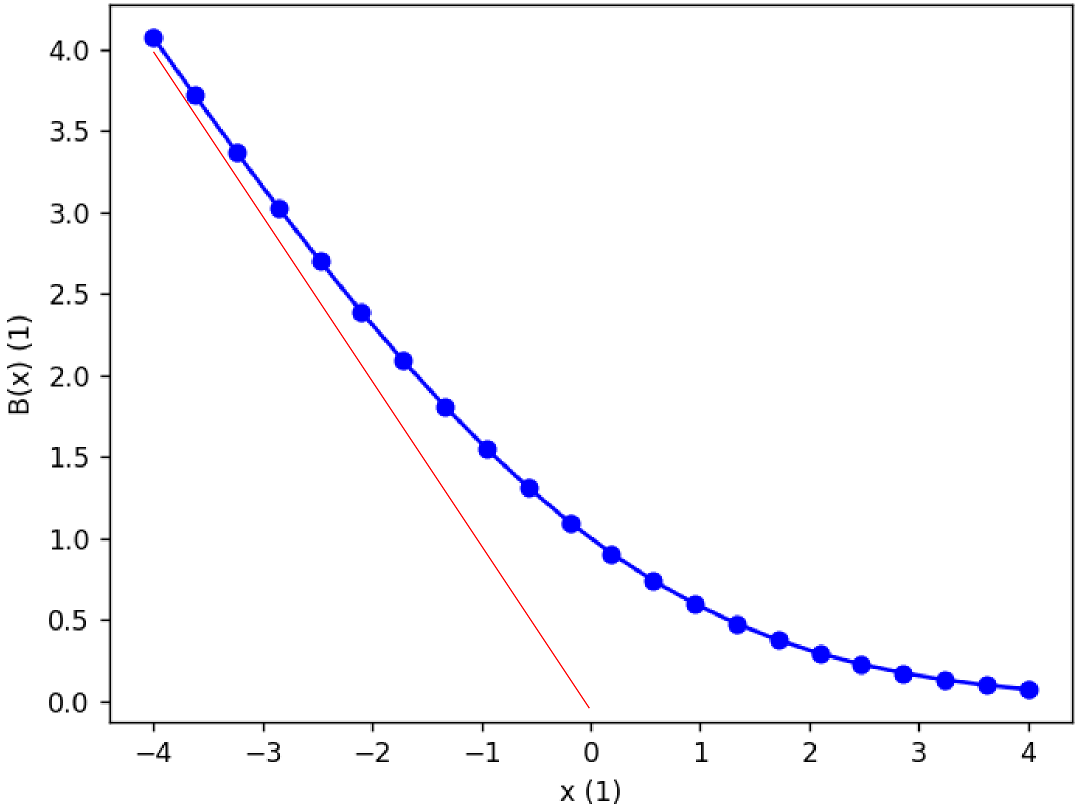
$$J_p(x_{i+0.5}) = -\frac{qD_p}{x_{i+1}-x_i}\left[p_{i+1}B\left(-\frac{\phi_{i+1}-\phi_i}{V_T}\right) - p_iB\left(\frac{\phi_{i+1}-\phi_i}{V_T}\right)\right]$$

Bernoulli function, B

- A nonlinear function

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

  - 0) $B(x) > 0$ everywhere
  - 1) $B(0) = 1$
  - 2) $B(x) \sim x \exp(-x)$ when $x \to \infty$
  - 3) $B(x) \sim -x$ when $x \to -\infty$
  - 4) Monotonically decreasing
  - 5) $B'(0) = -\frac{1}{2}$
  - Careful implementation is needed.

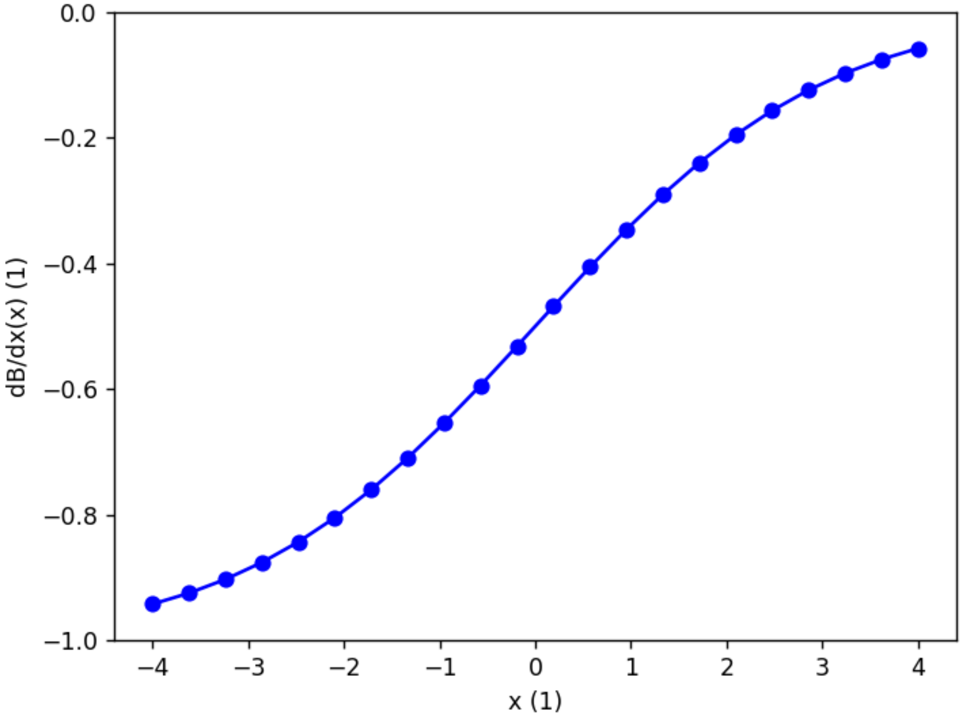


Its derivative, B'

- We also need its derivative.

$$B'(x) = \frac{1}{\exp x - 1} - B(x)\frac{\exp x}{\exp x - 1}$$

  - It can be implemented with $B(x)$ and $\frac{1}{\exp x - 1}$.



Jacobian, electron dependence

- Electron current density

$$J_n(x_{i+0.5}) = \frac{qD_n}{x_{i+1} - x_i}\left[n_{i+1}B\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right) - n_i B\left(-\frac{\phi_{i+1} - \phi_i}{V_T}\right)\right]$$

  – Components of Jacobian matrix are given as

$$\frac{\partial J_n(x_{i+0.5})}{\partial n_{i+1}} = \frac{qD_n}{x_{i+1} - x_i}\left[B\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right)\right] > 0$$

$$\frac{\partial J_n(x_{i+0.5})}{\partial n_i} = \frac{qD_n}{x_{i+1} - x_i}\left[-B\left(-\frac{\phi_{i+1} - \phi_i}{V_T}\right)\right] < 0$$

Jacobian, potential dependence

- Electron current density

$$J_n(x_{i+0.5}) = \frac{qD_n}{x_{i+1} - x_i}\left[n_{i+1}B\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right) - n_i B\left(-\frac{\phi_{i+1} - \phi_i}{V_T}\right)\right]$$

  – Components of Jacobian matrix are given as

$$\frac{\partial J_n(x_{i+0.5})}{\partial \phi_{i+1}} = \frac{qD_n}{x_{i+1} - x_i}\left[n_{i+1}B'\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right) + n_i B'\left(-\frac{\phi_{i+1} - \phi_i}{V_T}\right)\right]\frac{1}{V_T}$$

$$\frac{\partial J_n(x_{i+0.5})}{\partial \phi_i} = \frac{qD_n}{x_{i+1} - x_i}\left[-n_{i+1}B'\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right) - n_i B'\left(-\frac{\phi_{i+1} - \phi_i}{V_T}\right)\right]\frac{1}{V_T}$$

Thank you!