HW12. Scharfetter Gummel scheme derivation

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$$J_n = q\mu_n n \mathcal{E} + qD_n \nabla n = -q\mu_n n \nabla\phi + qD_n \nabla n$$

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

By Einstein's theorem $\frac{D}{\mu} = \frac{kT}{q} = V_T$ (thermal voltage)

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

n_{i+1} 과 n_i의 term에 대해 정리하면

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

if $|\phi_{i+1}-\phi_i| > 2V_T$ 인 경우 electron density는 negative가 되고 이는 unphysical 하다.

Bernoulli function $B := \frac{x}{e^x - 1}$ 를 도입하여 이를 재정리하면

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

At steady state $\frac{dJ}{dx} = 0 \Rightarrow J_{n,i+0.5} - J_{n,i-0.5} = 0$

$$J_{n,i+0.5} = n_{i+1}(\ A\ ) - n_i(\ B\ )$$

$$J_{n,i-0.5} = n_i(\ C\ ) - n_{i-1}(\ D\ )$$

$A, B, C, D \geq 0$

A, B, C, D is same sign

$$J_{n,i+0.5} - J_{n,i-0.5} = 0$$

$$n_{i+1}(\ A\ ) - n_i(\ B+C\ ) + n_{i-1}(\ D\ ) = 0$$

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

$$\frac{dJ_n}{dx} = 0 \rightarrow J_n = \text{constant}$$

$$\frac{dn}{dx} - \frac{1}{V_T}\frac{d\phi}{dx} n = \underbrace{\frac{J_n}{qD_n}}_{\text{Constant}} \xrightarrow{\text{linear approximation}} \frac{dn}{dx} - \frac{1}{V_T}\frac{\Delta\phi}{\Delta x} n = \frac{J_n}{qD_n}$$

* homogeneous solution

$$n = \underbrace{A\, e^{\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x}}_{\text{homogeneous}} + C_2$$

* Boundary condition

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

$$\left.\begin{aligned} n_{i+1} &= A e^{\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_{i+1}} + C_2 \\ n_i &= A e^{\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i} + C_2 \end{aligned}\right\} \rightarrow n_{i+1} - n_i = A e^{\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i}\left(e^{\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}(x_{i+1}-x_i)} - 1\right)$$

$$= A e^{\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i}\left(e^{\frac{\Delta\phi}{V_T}} - 1\right)$$

$$A e^{\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i} = \frac{n_{i+1} - n_i}{e^{\frac{\Delta\phi}{V_T}} - 1}$$

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

$$J_n = -\frac{qD_n}{\Delta x}\frac{\Delta\phi}{V_T} C_2 = \frac{qD_n}{\Delta x}\left[n_{i+1}\boxed{\frac{\frac{\Delta\phi}{V_T}}{e^{\frac{\Delta\phi}{V_T}} - 1}} - n_i \frac{\frac{\Delta\phi}{V_T}\, e^{\frac{\Delta\phi}{V_T}}}{e^{\frac{\Delta\phi}{V_T}} - 1}\right]$$

$B(x)$: Bernoulli function 도입

$\rightarrow$ $x = \frac{\Delta\phi}{V_T}$ 이면 $\frac{x}{e^x - 1}$ = Bernoulli function

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

$\therefore$ "$B(x)$" ; Bernoulli function , $B(x) = \frac{x}{e^x - 1}$

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

둘중 하나가 (-)여도 Bernoulli function은 항상 > 0 이기에

입력값이 < 0 이여도 density의 계수는 항상 > 0 이다.

J_n 과 동일한 flow로 J_p를 진행하면

$$J_p = -q\mu_p p \nabla\phi - q p D_p \frac{dp}{dx}$$

$$\frac{dp}{dx} + \frac{1}{V_T}\frac{d\phi}{dx} p = -\frac{J_p}{q D_p}$$

* General solution

$$p = C_1 e^{-\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x} + C_2$$

$$p_{i+1} = C_1 e^{-\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_{i+1}} + C_2$$

$$p_i = C_1 e^{-\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i} + C_2$$

* Boundary condition

$$p(x_{i+1}) = p_{i+1}$$
$$p(x_i) = p_i$$

$$p_{i+1} - p_i = C_1 e^{-\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i}\left(e^{-\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}(x_{i+1}-x_i)} - 1\right)$$
$$= C_1 e^{-\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i}\left(e^{-\frac{\Delta\phi}{V_T}} - 1\right)$$

$$\frac{p_{i+1} - p_i}{e^{-\frac{\Delta\phi}{V_T}} - 1} = C_1 e^{-\frac{1}{V_T}\frac{\Delta\phi}{\Delta x}x_i}$$

$$p_i - \frac{p_{i+1} - p_i}{e^{-\frac{\Delta\phi}{V_T}} - 1} p_i = C_2 = -p_{i+1}\frac{1}{e^{-\frac{\Delta\phi}{V_T}} - 1} + p_i \frac{e^{-\frac{\Delta\phi}{V_T}}}{e^{-\frac{\Delta\phi}{V_T}} - 1}$$

$$J_p = \frac{-qD_p}{\Delta x}\frac{\Delta\phi}{V_T} C_2 = \frac{qD_p}{\Delta x}\left[-p_{i+1}\frac{-\frac{\Delta\phi}{V_T}}{e^{-\frac{\Delta\phi}{V_T}} - 1} + p_i \frac{\frac{\Delta\phi}{V_T} e^{-\frac{\Delta\phi}{V_T}}}{e^{-\frac{\Delta\phi}{V_T}} - 1}\right]$$

$$B := \frac{x}{e^x - 1} \quad \text{(Bernoulli function)}$$

$$J_p = \frac{qD_p}{\Delta x}\left[-p_{i+1} B\left(-\frac{\Delta\phi}{V_T}\right) + p_i B\left(\frac{\Delta\phi}{V_T}\right)\right]$$

$$\therefore J_p = \frac{qD_p}{\Delta x}\left[p_i B\left(\frac{\Delta\phi}{V_T}\right) - p_{i+1} B\left(-\frac{\Delta\phi}{V_T}\right)\right]$$