11. Appendix F - Discrete Equations

11.1 Auxiliary Equations

Numerical Integration:

Bulk: $$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} f(x)dx = f(x_i)\left(\frac{x_{i+1}-x_{i-1}}{2}\right)$$

QW:

$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} f(x)dx = \sum_{j=1}^{S} \int_{j-\frac{1}{2}}^{j+\frac{1}{2}} f(x)dx$$

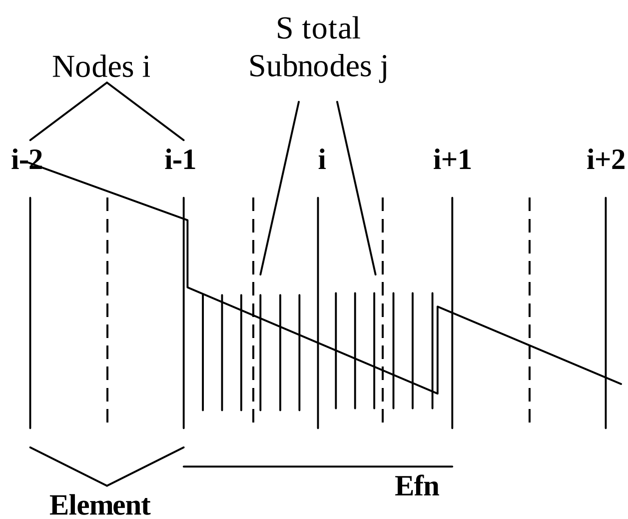

Figure 53 - Arrangement of nodes and subnodes in a quantum well

11.2 Rate Equations

Box Integration Method - See reference [60]

Poisson's Equation: $$\mathbf{D}(i+\tfrac{1}{2}) - \mathbf{D}(i-\tfrac{1}{2}) - \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} r(x)dx = 0$$

Electron Rate Equation:
$$\tfrac{1}{q}(\mathbf{J_n}(i+\tfrac{1}{2})-\mathbf{J_n}(i-\tfrac{1}{2}))-\int_{i-\frac{1}{2}}^{i+\frac{1}{2}}U_{tot}(x)dx=0$$

Hole Rate Equation:
$$\tfrac{1}{q}(\mathbf{J_p}(i+\tfrac{1}{2})-\mathbf{J_p}(i-\tfrac{1}{2}))+\int_{i-\frac{1}{2}}^{i+\frac{1}{2}}U_{tot}(x)dx=0$$

Electron Energy Rate Equation:
$$\mathbf{S}_n^{tot}(i+\tfrac{1}{2})-\mathbf{S}_n^{tot}(i-\tfrac{1}{2})+\int_{i-\frac{1}{2}}^{i+\frac{1}{2}}W_n^{tot}(x)dx=0$$

Hole Energy Rate Equation:
$$\mathbf{S}_p^{tot}(i+\tfrac{1}{2})-\mathbf{S}_p^{tot}(i-\tfrac{1}{2})+\int_{i-\frac{1}{2}}^{i+\frac{1}{2}}W_p^{tot}(x)dx=0$$

Lattice Energy Rate Equation:
$$\mathbf{S}_{lat}(i+\tfrac{1}{2})-\mathbf{S}_{lat}(i-\tfrac{1}{2})-\int_{i-\frac{1}{2}}^{i+\frac{1}{2}}H(x)dx=0$$

Total Energy Rate Equation (for $T_n=T_p=T_{lat}=T$):
$$\begin{aligned}&\mathbf{S}_{lat}(i+\tfrac{1}{2})+\mathbf{S}_n^{tot}(i+\tfrac{1}{2})+\mathbf{S}_p^{tot}(i+\tfrac{1}{2})-\mathbf{S}_{lat}(i-\tfrac{1}{2})-\mathbf{S}_n^{tot}(i-\tfrac{1}{2})-\mathbf{S}_p^{tot}(i-\tfrac{1}{2})\\&\quad+\int_{i-\frac{1}{2}}^{i+\frac{1}{2}}\left(hu_{stim}U_{stim}(x)+E_gU_{b-b}(x)-hu_{opt}G_{opt}(x)\right)dx=0\end{aligned}$$

11.3 Vector Equations

Field:
$$\mathbf{D}(i+\tfrac{1}{2})=-\frac{\in(i+1)+\in(i)}{2}\frac{f(i+1)-f(i)}{x(i+1)-x(i)}$$

Drift-Diffusion Current:

Scharfetter-Gummel Discretization Technique - See References [61-64]
$$A_n=-\left(\left(\tfrac{5}{2}+u\right)\tfrac{F_{3/2+u}(h_c)}{F_{1/2+u}(h_c)}\tfrac{F_{-1/2}(h_c)}{F_{1/2}(h_c)}-\tfrac{3}{2}\right)\Delta kT_n-\tfrac{F_{-1/2}(h_c)}{F_{1/2}(h_c)}\Delta E_C+\tfrac{3kT_n}{2}\Delta\ln(m_n^*)$$

$$\mathbf{J_n}(i+\tfrac{1}{2}) = \frac{m_n \frac{F_{1/2}(h_c)}{F_{-1/2}(h_c)}}{x_{i+1}-x_i}\left\{n(i+1)kT_n(i+1)B\left(\tfrac{A_n}{kT_n(i+1)}\right)-n(i)kT_n(i)B\left(\tfrac{-A_n}{kT_n(i)}\right)\right\}$$

$$A_p = -\left(\left(\tfrac{5}{2}+u\right)\tfrac{F_{3/2+u}(h_v)}{F_{1/2+u}(h_v)}\tfrac{F_{-1/2}(h_v)}{F_{1/2}(h_v)}-\tfrac{3}{2}\right)\Delta kT_p + \tfrac{F_{-1/2}(h_v)}{F_{1/2}(h_v)}\Delta E_V + \tfrac{3kT_p}{2}\Delta\ln(m_p^*)$$

$$\mathbf{J_p}(i+\tfrac{1}{2}) = \frac{-m_p \frac{F_{1/2}(h_v)}{F_{-1/2}(h_v)}}{x_{i+1}-x_i}\left\{p(i+1)kT_p(i+1)B\left(\tfrac{A_p}{kT_p(i+1)}\right)-p(i)kT_p(i)B\left(\tfrac{-A_p}{kT_p(i)}\right)\right\}$$

Thermionic Emission and Tunneling Current:

Same as continuous equations except use:

$$U_{c+} = \Delta E_{c+} - \tfrac{1}{2}(f_- - f_+) \qquad U_{c-} = \Delta E_{c-} - \tfrac{1}{2}(f_+ - f_-)$$

$$U_{v-} = \Delta E_{v-} + \tfrac{1}{2}(f_+ - f_-) \qquad U_{v+} = \Delta E_{v+} + \tfrac{1}{2}(f_- - f_+)$$

Lattice Energy Flow:

$$\mathbf{S}_{lat}(i+\tfrac{1}{2}) = -\frac{k(i)+k(i+1)}{2}\frac{T(i+1)-T(i)}{x(i+1)-x(i)}$$

Carrier "Drift-Diffusion" Energy Flow:

Scharfetter-Gummel Discretization Technique - See References [61-64]

$$A_n' = -\left(\left(\tfrac{7}{2}+u\right)\tfrac{F_{5/2+u}(h_c)}{F_{3/2+u}(h_c)}\tfrac{F_{-1/2}(h_c)}{F_{1/2}(h_c)}-\tfrac{5}{2}\right)\Delta kT_n - \tfrac{F_{-1/2}(h_c)}{F_{1/2}(h_c)}\Delta E_C + \tfrac{3kT_n}{2}\Delta\ln(m_n^*)$$

$$\mathbf{S_n}(i+\tfrac{1}{2}) = \frac{-m_n\left(\tfrac{5}{2}+u\right)\frac{F_{3/2+u}(h_c)}{F_{1/2+u}(h_c)}\frac{F_{1/2}(h_c)}{F_{-1/2}(h_c)}}{q(x_{i+1}-x_i)}\left\{\begin{aligned}n(i+1)(kT_n(i+1))^2B\left(\tfrac{A_n'}{kT_n(i+1)}\right)\\ -n(i)(kT_n(i))^2B\left(\tfrac{-A_n'}{kT_n(i)}\right)\end{aligned}\right\}-\frac{E_c\mathbf{J}_n}{q}$$

$$A_p' = -\left(\left(\tfrac{7}{2}+u\right)\tfrac{F_{5/2+u}(h_v)}{F_{3/2+u}(h_v)}\tfrac{F_{-1/2}(h_v)}{F_{1/2}(h_v)}-\tfrac{5}{2}\right)\Delta kT_p + \tfrac{F_{-1/2}(h_v)}{F_{1/2}(h_v)}\Delta E_V + \tfrac{3kT_p}{2}\Delta\ln(m_p^*)$$

$$\mathbf{S}_p(i+\tfrac{1}{2}) = \frac{-m_p\left(\tfrac{5}{2}+u\right)\frac{F_{3/2+u}(h_v)}{F_{1/2+u}(h_v)}\frac{F_{1/2}(h_v)}{F_{-1/2}(h_v)}}{q(x_{i+1}-x_i)}\left\{\begin{aligned}p(i+1)(kT_p(i+1))^2B\left(\tfrac{A_p'}{kT_p(i+1)}\right)\\ -p(i)(kT_p(i))^2B\left(\tfrac{-A_p'}{kT_p(i)}\right)\end{aligned}\right\}-\frac{E_v\mathbf{J}_p}{q}$$