中国科学技术大学
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数值代数中 Gummel 迭代方法的补充研究

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Content

考虑引入量子修正效应的半导体器件方程：

$$\begin{cases} f_1: & \varepsilon\Delta\psi + q(p - n + N_D^+ - N_A^-) + \rho_s = 0, \\ f_2: & \frac{1}{q}\nabla\cdot J_n - (U - G) = 0, \\ f_3: & -\frac{1}{q}\nabla\cdot J_p - (U - G) = 0, \\ f_4: & b_n(\Delta\ln n + \frac{1}{2}\varepsilon(\ln n)^2) - \Lambda_n = 0 \\ f_5: & b_p(\Delta\ln p + \frac{1}{2}\varepsilon(\ln p)^2) - \Lambda_p = 0. \end{cases} \tag{1}$$

现在已知第 k 次迭代时自变量 $(\psi, \phi_n, \phi_p, \Lambda_n, \Lambda_p)$ 的值 $(\psi_k, \phi_{n,k}, \phi_{p,k}, \Lambda_{n,k}, \Lambda_{p,k})$，要迭代求出第 $k+1$ 次迭代时自变量 $(\psi, \phi_n, \phi_p, \Lambda_n, \Lambda_p)$ 的值 $(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}, \Lambda_{n,k+1}, \Lambda_{p,k+1})$ 使以下方程组的残差接近于 0。

$$f_i(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}, \Lambda_{n,k+1}, \Lambda_{p,k+1}) = 0, i = 1, 2, 3, 4, 5.$$

假设准费米势 ϕ_n, ϕ_p，量子修正 Λ_n,Λ_p 是静电势 ψ 的函数：

$$n = n\left(\psi, \phi_n, \Lambda_n\right) \tag{2}$$

$$dn = \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n} d\phi_n + \frac{\partial n}{\partial \Lambda_n} d\Lambda_n = \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n}\frac{d\phi_n}{d\psi} d\psi + \frac{\partial n}{\partial \Lambda_n}\frac{d\Lambda_n}{d\psi} d\psi \tag{3}$$

$$= \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n}\alpha_n^k d\psi + \frac{\partial n}{\partial \Lambda_n}\beta_n^k d\psi = \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi \tag{4}$$

原 Possion 方程：$-\frac{\varepsilon\Delta\psi^{k+1}}{q} - p^{k+1} + n^{k+1} - N_D^+ + N_A^- + \frac{\rho_s}{q} = 0.$

普通 Gummel 迭代：令 p^{k+1}, n^{k+1} 分别在 p^k, n^k 处对 ψ 一阶 Taylor 展开：

$$-\frac{\varepsilon\Delta\psi^{k+1}}{q} - \left(p^k + \frac{\partial p}{\partial \psi}\left(\psi^{k+1} - \psi^k\right)\right) + \left(n^k + \frac{\partial n}{\partial \psi}\left(\psi^{k+1} - \psi^k\right)\right) - N_D^+ + N_A^- + \frac{\rho_s}{q} = 0. \tag{5}$$

令 p^{k+1}, n^{k+1} 分别在 p^k, n^k 处对 $\psi, \phi_n, \phi_p, \Lambda_n, \Lambda_p$ 一阶 Taylor 展开：

$$n^{k+1} = n^k\left(\psi^k, \phi_n^k, \Lambda_n^k\right) + \frac{\partial n}{\partial \psi}\left(\psi^{k+1} - \psi^k\right) + \frac{\partial n}{\partial \phi_n}\left(\phi_n^{k+1} - \phi_n^k\right) + \frac{\partial n}{\partial \Lambda_n}\left(\Lambda_n^{k+1} - \Lambda_n^k\right)$$

将 $dn = \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi$ 代入：

$$n^{k+1} = n^k\left(\psi^k, \phi_n^k, \Lambda_n^k\right) + \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi,$$

$$-\frac{\varepsilon \Delta \psi^{k+1}}{q} + n^k - p^k + \left(\frac{\partial n}{\partial \psi} - \frac{\partial p}{\partial \psi}\right)(\psi^{k+1} - \psi^k) + C +$$

$$\left(\alpha_n^k \frac{\partial n}{\partial \phi_n} - \alpha_p^k \frac{\partial p}{\partial \phi_p} + \beta_n^k \frac{\partial n}{\partial \Lambda_n} - \beta_p^k \frac{\partial p}{\partial \Lambda_p}\right)(\psi^{k+1} - \psi^k) = 0$$

更新策略：

$$
\begin{aligned}
\phi_n^{k+1} &= \phi_n^k + \alpha_n^k(\psi^{k+1}-\psi^k), \quad & \phi_p^{k+1} &= \phi_p^k + \alpha_p^k(\psi^{k+1}-\psi^k),\\
\Lambda_n^{k+1} &= \Lambda_n^k + \beta_n^k(\psi^{k+1}-\psi^k), \quad & \Lambda_p^{k+1} &= \Lambda_p^k + \beta_p^k(\psi^{k+1}-\psi^k).\\
n_{k+1} &= n(\psi^{k+1}, \phi_n^{k+1}, \Lambda_n^{k+1}), \quad & p_{k+1} &= p(\psi^{k+1}, \phi_p^{k+1}, \Lambda_p^{k+1}),
\end{aligned}
$$

$$
R_{k+1} = R(\psi^{k+1}, \phi_n^{k+1}, \phi_p^{k+1}, \Lambda_n^{k+1}, \Lambda_p^{k+1}).
$$

$\alpha_p^{k+1}, \alpha_n^{k+1}, \beta_n^{k+1}, \beta_p^{k+1}$ 的更新策略：

$$
dn = \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi \Rightarrow \alpha_n^k = \frac{dn/d\psi - \partial n/\partial\psi - \partial n/\partial\Lambda_n \cdot \beta_n^k}{\partial n/\partial\phi_n}
$$

$$
\beta_n^k = \frac{dn/d\psi - \partial n/\partial\psi - \partial n/\partial\phi_n \cdot \alpha_n^k}{\partial n/\partial\Lambda_n}
$$

1. 对于 ψ 问题：求解 ψ^{k+1} 使得

$$-\frac{\varepsilon\Delta\psi^{k+1}}{q}+n^k-p^k+\left(\frac{\partial n}{\partial\psi}-\frac{\partial p}{\partial\psi}\right)(\psi^{k+1}-\psi^k)+C+$$
$$\left(\alpha_n^k\frac{\partial n}{\partial\phi_n}-\alpha_p^k\frac{\partial p}{\partial\phi_p}+\beta_n^k\frac{\partial n}{\partial\Lambda_n}-\beta_p^k\frac{\partial p}{\partial\Lambda_p}\right)(\psi^{k+1}-\psi^k)=0.$$

2. 对于 ϕ,Λ 问题，更新准费米势以及量子修正：

$$\phi_n^{k+1}=\phi_n^k+\alpha_n^k(\psi^{k+1}-\psi^k),\quad \phi_p^{k+1}=\phi_p^k+\alpha_p^k(\psi^{k+1}-\psi^k),$$
$$\Lambda_n^{k+1}=\Lambda_n^k+\beta_n^k(\psi^{k+1}-\psi^k),\quad \Lambda_p^{k+1}=\Lambda_p^k+\beta_p^k(\psi^{k+1}-\psi^k).$$

3. 更新载流子浓度以及 R:

$$n_{k+1}=n(\psi^{k+1},\phi_n^{k+1},\Lambda_n^{k+1}),\quad p_{k+1}=p(\psi^{k+1},\phi_p^{k+1},\Lambda_p^{k+1}),$$
$$R_{k+1}=R(\psi^{k+1},\phi_n^{k+1},\phi_p^{k+1},\Lambda_n^{k+1},\Lambda_p^{k+1}).$$

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4. **for** $i \in \mathcal{I}$

 4.1 设 $\nabla \cdot \mathbf{J}_n - qR = 0, \nabla \cdot \mathbf{J}_p + qR = 0$ 的离散格式，分别记为 f_n^J 以及 f_p^J，及量子修正方程的离散格式，分别记为 f_n^Q 以及 f_p^Q。

 4.2 更新节点 i 处的 n,p：

$$
\begin{gathered}
n_i^* = f_n^J(N(i), n^{k+1}, R^{k+1}), \ p_i^* = f_p^J(N(i), p^{k+1}, R^{k+1}), \\
\Lambda_{n,i}^* = f_n^Q(N(i), n^{k+1}), \ \Lambda_{p,i}^* = f_p^Q(N(i), p^{k+1}).
\end{gathered}
$$

5. 更新离散节点的 $\alpha_n, \alpha_p, \beta_n, \beta_p$：

$$
\beta_n^{k+1} = \frac{\Lambda_n^* - \Lambda_n^k}{\psi^{k+1} - \psi^k} \simeq \frac{d\Lambda_n}{d\psi}, \alpha_n^{k+1} = \frac{\frac{n^* - n^k}{\psi^{k+1} - \psi^k} - \partial n / \partial \psi - \partial n / \partial \Lambda_n \cdot \beta_n^{k+1}}{\partial n / \partial \phi_n}
$$

$$
\beta_p^{k+1} = \frac{\Lambda_p^* - \Lambda_p^k}{\psi^{k+1} - \psi^k} \simeq \frac{d\Lambda_p}{d\psi}, \alpha_p^{k+1} = \frac{\frac{p^* - p^k}{\psi^{k+1} - \psi^k} - \partial p / \partial \psi - \partial p / \partial \Lambda_p \cdot \beta_n^{k+1}}{\partial p / \partial \phi_p}
$$

观察方程形式：

$$\begin{cases} -\frac{\varepsilon}{q}\Delta\psi + n - p + C = 0 \\ \nabla\cdot\mathbf{J}_n - qR = 0, \mathbf{J}_n = -q\mu_n n\nabla\phi_n \\ \nabla\cdot\mathbf{J}_p + qR = 0, \mathbf{J}_p = -q\mu_p p\nabla\phi_p \end{cases} \tag{6}$$

(1) 考虑对 $\phi_p^{k+1}, d\phi_p$ 的求解：

- **近似牛顿**： $\nabla\cdot[\mu_p p(\nabla d\phi_p + \nabla\phi_p)] = R + \frac{\partial R}{\partial\phi_p}d\phi_p.$
- **MSP-Gummel**： $\nabla\cdot[\mu_p p\nabla\phi_p^{k+1}] = -qR.$

(2) 考虑对 $\psi_1, d\psi_1$ 的求解：

- **近似牛顿**： $-\frac{\varepsilon}{q}(\Delta d\psi_1 + \Delta\psi) + n - p + C - \frac{\partial p}{\partial\psi}d\psi_1 - \frac{\partial p}{\partial\phi_p} = 0$
- **MSP-Gummel**： $-\frac{\varepsilon}{q}\Delta\psi^{k+1} + n - p + C = 0.$

（3）考虑对 $d\phi_n, \phi_n^{k+1}$ 的求解：

- **近似牛顿**：

$$\nabla \cdot [\mu_n n(\nabla d\phi_n + \nabla \phi_n)] = -R - \frac{\partial R}{\partial \phi_n} d\phi_n - \frac{\partial R}{\partial \phi_p} d\phi_p - \mu_n \nabla \cdot [\frac{\partial n}{\partial \psi} \nabla \phi_n d\psi_1].$$

- **MSP-Gummel**：$\nabla \cdot [\mu_n n(\psi^{k+1}, \phi_n^{k+1}) \nabla \phi_n] = -R$, 而 $\psi_{k+1} = g(\phi_{n,k+1}) :=$ $\psi_1 - (\frac{\partial f_0}{\partial \phi_n}\left(\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right))/(\frac{\partial f_0}{\partial \psi}\left(\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right)) \cdot (\phi_{n,k+1} - \phi_{n,k})$.

（4）考虑对 $d\psi, \psi^{k+1}$ 的求解：

- **近似牛顿**：$-\frac{\varepsilon}{q}(\Delta d\psi + \Delta \psi) + n - p + C = \frac{\partial p}{\partial \phi_p} d\phi_p - \frac{\partial n}{\partial \phi_n} d\phi_n - \frac{\partial n}{\partial \psi} d\psi + \frac{\partial p}{\partial \psi} d\psi.$
- **MSP-Gummel**：$-\frac{\varepsilon}{q} \Delta \psi^{k+1} + n - p + C = 0.$

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