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数值代数 Gummel 迭代法在基于 quasi-Fermi leve 自变量的 TCAD 方程下的应用

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考虑没有引入量子修正效应的半导体器件方程：

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

现在已知第 k 次迭代时自变量 (ψ, ϕ_n, ϕ_p) 的值 $(\psi_k, \phi_n, k, \phi_p, k)$，要迭代求出第 $k+1$ 次迭代时自变量 (ψ, ϕ_n, ϕ_p) 的值 $(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1})$ 使下列方程组的残差为 0.

$$\begin{cases} f_1(\varepsilon; \psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}) = 0, \\ f_2(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}) = 0, \\ f_3(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}) = 0. \end{cases} \tag{2}$$

原始 Gummel 迭代

1. f_3：求解 $\phi_{p,k+1}$
   - 固定 $\psi_{k+1}=\psi_k;\phi_{n,k+1}=\phi_{n,k}$；迭代方程：$f_3(\psi_{k+1}=\psi_k,\phi_{n,k+1}=\phi_{n,k},\phi_{p,k+1})$。

   得到 $\phi_{p,k+1}=\phi_1$。
2. f_2：求解 $\phi_{n,k+1}$
   - 固定 $\psi_{k+1}=\psi_k,\phi_{p,k+1}=\phi_1$；求解方程 $f_2(\psi_{k+1}=\psi_k,\phi_{n,k+1},\phi_{p,k+1}=\phi_1)=0$。

   得到 $\phi_{n,k+1}=\phi_2$。
3. f_1：求解 ψ_{k+1}
   - 固定 $\phi_{n,k+1}=\phi_2,\phi_{p,k+1}=\phi_1$；求解方程 $f_1(\varepsilon;\psi_{k+1},\phi_{n,k+1}=\phi_2,\phi_{p,k+1}=\phi_1)=0$。

   得到 ψ_{k+1}。
4. $n_{k+1}=n(\psi_{k+1},\phi_{p,k+1},\phi_{n,k+1})$，$p_{k+1}=p(\psi_{k+1},\phi_{p,k+1},\phi_{n,k+1})$。

1. f_3：求解 $\phi_{p,k+1}$
   - 固定 $\psi_{k+1}=\psi_k; \phi_{n,k+1}=\phi_{n,k}$；迭代方程：$f_3(\psi_{k+1}=\psi_k, \phi_{n,k+1}=\phi_{n,k}, \phi_{p,k+1})$。

   得到 $\phi_{p,k+1}=\phi_1$。
2. f_1：求解 $\psi_{k+\frac{1}{2}}$
   - 方案 A：求解方程组 $f_1(\varepsilon; \psi_{k+1}; \phi_{n,k+1}=\phi_{n,k}; \phi_{p,k+1}=\phi_{p,k}=\phi_1)=0$
   - 方案 B：求解方程组 $f_1(0; \psi_{k+1}, \phi_{n,k}, \phi_1)=0$，此时为对角矩阵线性求解。

   得到 $\psi_{k+\frac{1}{2}}=\psi_1$。
3. f_2：求解 $\phi_{n,k+1}$
   - 固定 $\psi_{k+1}=g(\phi_{n,k+1}), \phi_{p,k+1}=\phi_1$；令 $f_0(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}):=f_1(\varepsilon=0; \psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1})$，求解方程 $f_2(\psi_{k+1}=g(\phi_{n,k+1}), \phi_{n,k+1}, \phi_{p,k+1}=\phi_1)=0$，而 $\psi_{k+1}=g(\phi_{n,k+1}):=\psi_1-(\frac{\partial f_0}{\partial \phi_n}\left(\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right))/(\frac{\partial f_0}{\partial \psi}\left(\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right))\cdot(\phi_{n,k+1}-\phi_{n,k})$.

补充 Step3 的推导：对于 $f_1(\varepsilon=0;\psi_{k+1},\phi_{n,k+1},\phi_{p,k+1})$，在 $\psi_{k+\frac{1}{2}}$、$\phi_{n,k}$ 处进行一阶二元 Taylor 展开：

$$\left(\psi_{k+1}-\psi_{k+\frac{1}{2}}\right)\times\frac{\partial f_1(0;\psi_{k+\frac{1}{2}},\phi_{n,k},\phi_{p,k+1})}{\partial\psi}+(\phi_{n,k+1}-\phi_{n,k})\times\frac{\partial f_1(0;\psi_{k+\frac{1}{2}},\phi_{n,k},\phi_{p,k+1})}{\partial\phi_n}=0.$$

从而解出 ψ_{k+1}，代入要求解的 $f_2(\psi_{k+1}=g(\phi_{n,k+1}),\phi_{n,k+1},\phi_{p,k+1}=\phi_1)=0$ 即可得到 $\phi_{n,k+1}$。

4. f_1：求解 ψ_{k+1}
   - 固定 $\phi_{n,k+1}=\phi_2,\phi_{p,k+1}=\phi_1$；求解方程 $f_1(\varepsilon;\psi_{k+1},\phi_{n,k+1}=\phi_2,\phi_{p,k+1}=\phi_1)=0$。

   得到 $\psi_{k+1}=\psi_2$。
5. $n_{k+1}=n(\psi_{k+1},\phi_{p,k+1},\phi_{n,k+1})$，$p_{k+1}=p(\psi_{k+1},\phi_{p,k+1},\phi_{n,k+1})$。

- 原始 Gummel 迭代与 MSP-Gummel 的对比:

在原始 Gummel 迭代时，迭代求解自变量 $\phi_{n,k+1}$ 时，$\phi_p = \phi_{p,k+1} = \phi_1, \psi_{k+1} = \psi_k$ 均为常值；在 MSP-Gummel 迭代中，$\phi_p = \phi_{p,k+1} = \phi_1$，而 ψ_{k+1} 取值为由 Possion 方程推导得出的表达式 $\psi_{k+1} = g_{\phi_n,k+1} :=$ $\psi_1 - (\frac{\partial f_0}{\partial \phi_n}\left[\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right])/(\frac{\partial f_0}{\partial \psi}\left[\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right]) \cdot (\phi_{n,h+1} - \phi_{n,h})$。

算法原理:

$$-f\left(x^k\right)=f\prime\left(x^k\right)dx\Rightarrow -F_i\left(w^k\right)=\nabla F_i\left(w^k\right)dw=d\left[F_i\left(w^k\right)\right]=-b_i.$$

$$-b_3\triangleq -F_3(w_k)=\nabla F_3(w_k)\cdot dw=dF_3(w_k)=q\mu_p\nabla\cdot[dp(\psi,\phi_p)\nabla\phi_p+p(\psi,\phi_p)\nabla d\phi_p]-qdR \tag{3}$$

因此对于 F_3 对应的求解变量 $d\phi_p$，其更新公式如下:

$$-F_3\left(w^k\right)=dF_3\left(w^k\right),\mu_p dp(\psi,\phi_p)\nabla\phi_p, dR=\frac{\partial R}{\partial\phi_p}d\phi_p,$$

$$-q\nabla\cdot\left[\mu_p p\left(\psi,\phi_p\right)\nabla\phi_p\right]+qR=q\nabla\cdot\left[\mu_p dp\left(\psi,\phi_p\right)\nabla\phi_p+\mu_p p\left(\psi,\phi_p\right)\nabla d\phi_p\right]-qdR,$$

$$-b_3=\underline{q\nabla\cdot\left[\mu_p p\nabla d\phi_p\right]-qdR},$$

$$\Rightarrow -\frac{b_3}{q}=\nabla\cdot\left[\mu_p p\nabla d\phi_p\right]-\frac{\partial R}{\partial\phi_p}d\phi_p.$$

算法流程：($f(x_i) + (x_{i+1} - x_i)f'(x_i) = 0$)

1. 计算牛顿法的右端项：

$$b_1 = -\frac{\varepsilon}{q}\Delta\psi^k + n^k - p^k + C, \tag{4}$$

$$b_2 = q^k\nabla\cdot[J_n^k] + qR^k,\ b_3 = q^k\nabla\cdot[J_p^k] - qR^k. \tag{5}$$

2. 求解 $d\phi_p$ 使得满足

$$\nabla\cdot[\mu_p p^k\nabla d\phi_p^k] - \frac{\partial R^k}{\partial\phi_p^k}d\phi_p^k = -\frac{b_3}{q^k}. \tag{6}$$

3. 求解 $d\psi_1$ 使得满足

$$\frac{\varepsilon}{q}\Delta d\psi_1 - \frac{\partial p^k}{\partial\psi}d\psi_1 = \frac{\partial p^k}{\partial\phi_p} - b_1. \tag{7}$$

4. 求解 $d\phi_n$ 使得满足

$$\mu_n \nabla \cdot [n^k \nabla d\phi_n] + \frac{\partial R^k}{\partial \phi_n} d\phi_n = -\mu_n \nabla \cdot [\frac{\partial n^k}{\partial \psi} \nabla \phi_n d\psi_1] - \frac{\partial R^k}{\partial \phi_p} d\phi_p - \frac{b_2}{q}. \tag{8}$$

5. 求解 $d\psi$ 使得满足

$$-\frac{\varepsilon}{q} \Delta d\psi_1 + \frac{\partial n^k}{\partial \psi} d\psi - \frac{\partial p^k}{\partial \phi} d\psi = \frac{\partial p^k}{\partial \phi_p} d\phi_p - \frac{\partial n^k}{\partial \phi_n} d\phi_n - b_1. \tag{9}$$

6. 更新 parameters： $\psi^{k+1} = \psi^k + d\psi, \phi_n^{k+1} = \phi_n^k + d\phi_n, \phi_p^{k+1} = \phi_p^k + d\phi_p$。

考虑引入量子修正效应的半导体器件方程:

$$\begin{cases} f_1: & \varepsilon\Delta\psi + (p - n + N_D^+ - N_A^-) + \rho_s = 0, \\ f_2: & \frac{1}{q}\nabla\cdot J_n - (U - G) = 0, \\ f_3: & -\frac{1}{q}\nabla\cdot J_p - (U - G) = 0, \\ f_4: & b_n(\Delta \ln n + \frac{1}{2}\varepsilon(\ln n)^2) - \Lambda_n = 0 \\ f_5: & b_p(\Delta \ln p + \frac{1}{2}\varepsilon(\ln p)^2) - \Lambda_p = 0. \end{cases} \tag{10}$$

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。

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

(1)、将静电势 ψ_{k+1} 作为待求解自变量，在每个 gridpoint 上求解 4×4 的 Jacobi 矩阵 $J_k = \frac{\partial(f_2,f_3,f_4,f_5)}{\partial(\phi_n,\phi_p,\Lambda_n,\Lambda_p)}|_{(\psi_k,\phi_{n,k},\phi_{p,k},\Lambda_{n,k},\Lambda_{p,k})}$。
作变量替换:

$$\begin{pmatrix} \phi_{n,k+1}(\psi_{k+1}) \\ \phi_{p,k+1}(\psi_{k+1}) \\ \Lambda_{n,k+1}(\psi_{k+1}) \\ \Lambda_{p,k+1}(\psi_{k+1}) \end{pmatrix} = \begin{pmatrix} \phi_{n,k} \\ \phi_{p,k} \\ \Lambda_{n,k} \\ \Lambda_{p,k} \end{pmatrix} - J_k^{-1} \begin{pmatrix} \partial f_2/\partial\psi \\ \partial f_3/\partial\psi \\ \partial f_4/\partial\psi \\ \partial f_5/\partial\psi \end{pmatrix} |_P (\psi_{k+1}-\psi_k) - J_k^{-1} \begin{pmatrix} f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix} |_P.$$

求解方程组

$$f_1(\psi_{k+1}, \phi_{n,k+1}(\psi_{k+1}), \phi_{p,k+1}(\psi_{k+1}), \Lambda_{n,k+1}(\psi_{k+1}), \Lambda_{p,k+1}(\psi_{k+1})) = 0,$$

得到自变量 ψ_{k+1} 的解 ψ_1。此时可进行参数更新，令 $\psi_{k+1}=\psi_1$，与自变量 ψ 相关的参数也同时更新；依次求解 $\Lambda_{p,k+1}, \Lambda_{n,k+1}, \psi_{p,k+1}, \psi_{n,k+1}$。

如何理解 Jacobi 矩阵的迭代方案？ **Newton Iteration Method:**

$$x^{k+1} = x^k - \frac{f(x^k)}{f'(x^k)},$$

$$f'(x_n) = \frac{f(x_n) - 0}{x_n - x_{n+1}}, f(x_n) + (x_{n+1} - x_n)f'(x_n) = 0.$$

将 Jacobi 矩阵左乘后，单独分析矩阵第一行的元素：

$$\frac{\partial f_2}{\partial \phi_n}[\phi_{n,k+1} - \phi_{n,k}] + \frac{\partial f_2}{\partial \phi_p}[\phi_{p,k+1} - \phi_{p,k}] + \frac{\partial f_2}{\partial \Lambda_n}[\Lambda_{n,k+1} - \Lambda_{n,k}] + \frac{\partial f_2}{\partial \Lambda_p}[\Lambda_{p,k+1} - \Lambda_{p,k}] + f_2 = 0$$

$$J_k = J_k = \frac{\partial(f_2, f_3, f_4, f_5)}{\partial(\phi_n, \phi_p, \Lambda_n, \Lambda_p)}\Big|_{(\psi_k,\phi_{n,k},\phi_{p,k},\Lambda_{n,k},\Lambda_{p,k})} = \begin{bmatrix} \frac{\partial f_2}{\partial \phi_n} & \frac{\partial f_2}{\partial \phi_p} & \frac{\partial f_2}{\partial \Lambda_n} & \frac{\partial f_2}{\partial \Lambda_p} \\ \frac{\partial f_3}{\partial \phi_n} & \frac{\partial f_3}{\partial \phi_p} & \frac{\partial f_3}{\partial \Lambda_n} & \frac{\partial f_3}{\partial \Lambda_p} \\ \frac{\partial f_4}{\partial \phi_n} & \frac{\partial f_4}{\partial \phi_p} & \frac{\partial f_4}{\partial \Lambda_n} & \frac{\partial f_4}{\partial \Lambda_p} \\ \frac{\partial f_5}{\partial \phi_n} & \frac{\partial f_5}{\partial \phi_p} & \frac{\partial f_5}{\partial \Lambda_n} & \frac{\partial f_5}{\partial \Lambda_p} \end{bmatrix}$$

$$J_k \begin{pmatrix} \phi_{n,k+1}(\psi_{k+1}) \\ \phi_{p,k+1}(\psi_{k+1}) \\ \Lambda_{n,k+1}(\psi_{k+1}) \\ \Lambda_{p,k+1}(\psi_{k+1}) \end{pmatrix} = J_k \begin{pmatrix} \phi_{n,k} \\ \phi_{p,k} \\ \Lambda_{n,k} \\ \Lambda_{p,k} \end{pmatrix} - \begin{pmatrix} \partial f_2/\partial\psi \\ \partial f_3/\partial\psi \\ \partial f_4/\partial\psi \\ \partial f_5/\partial\psi \end{pmatrix}\Big|_P (\psi_{k+1} - \psi_k) - \begin{pmatrix} f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix}\Big|_P.$$

把第一行相乘结果详细展开：

$$\frac{\partial f_2}{\partial \phi_n}\phi_{n,k+1} + \frac{\partial f_2}{\partial \phi_p}\phi_{p,k+1} + \frac{\partial f_2}{\partial \Lambda_n}\Lambda_{n,k+1} + \frac{\partial f_2}{\partial \Lambda_p}\Lambda_{p,k+1} = \frac{\partial f_2}{\partial \phi_n}\phi_{n,k} +$$

$$\frac{\partial f_2}{\partial \phi_p}\phi_{p,k} + \frac{\partial f_2}{\partial \Lambda_n}\Lambda_{n,k} + \frac{\partial f_2}{\partial \Lambda_p}\Lambda_{p,k} - f_2 - \frac{\partial f_2}{\partial \psi}(\psi_{k+1} - \psi_k)$$

(1)、将静电势 ψ_{k+1} 作为待求解自变量，在每个 gridpoint 上求解 4×4 的 Jacobi 矩阵 $J_k = \frac{\partial(f_2,f_3,f_4,f_5)}{\partial(\phi_n,\phi_p,\Lambda_n,\Lambda_p)}\big|_{(\psi_k,\phi_{n,k},\phi_{p,k},\Lambda_{n,k},\Lambda_{p,k})}$。，求解方程组

$$f_1(\psi_{k+1},\phi_{n,k+1}(\psi_{k+1}),\phi_{p,k+1}(\psi_{k+1}),\Lambda_{n,k+1}(\psi_{k+1}),\Lambda_{p,k+1}(\psi_{k+1}))=0,$$

得到自变量 ψ_{k+1} 的解 ψ_1。

(2) 将空穴量子修正量 $\Lambda_{p,k+1}$ 作为待求解自变量，求解方程组 $f_5(\psi_1,\phi_{n,k+1/2},\phi_{p,k+1/2},\Lambda_{n,k+1/2},\Lambda_{p,k+1})=0$，得到 $\Lambda_{p,k+1}$ 的值 Λ_1。

(3) 将电子量子修正量 $\Lambda_{n,k+1}$ 作为待求解自变量，求解方程组 $f_4(\psi_1,\phi_{n,k+1/2},\phi_{p,k+1/2},\Lambda_{n,k+1},\Lambda_1)=0$，得到 $\Lambda_{n,k+1}$ 的值 Λ_2。

(4) 将空穴准费米势 $\phi_{p,k+1}$ 作为待求解自变量，求解方程组 $f_3(\psi_1,\phi_{n,k+1/2},\phi_{p,k+1},\Lambda_2,\Lambda_1)=0$，得到 $\phi_{p,k+1}$ 的值 ϕ_1。

(5) 将电子准费米势 $\phi_{n,k+1}$ 作为待求解自变量，求解方程组 $f_2(\psi_1,\phi_{n,k+1},\phi_1,\Lambda_2,\Lambda_1)=0$，得到 $\phi_{n,k+1}$ 的值 ϕ_2。

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：

$$n = n\left(\psi, \phi_n, \Lambda_n\right) \tag{11}$$

$$dn = \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n} d\phi_n + \frac{\partial n}{\partial \Lambda_n} d\Lambda_n = \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n}\frac{d\phi_n}{d\psi} d\psi + \frac{\partial n}{\partial \Lambda_n}\frac{d\Lambda_n}{d\psi} d\psi \tag{12}$$

$$= \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n}\alpha_n^k d\psi + \frac{\partial n}{\partial \Lambda_n}\beta_n^k d\psi = \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi \tag{13}$$

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：

$$-\frac{\varepsilon \Delta \psi^{k+1}}{q} - \left(p^k + \frac{\partial p}{\partial \psi}\left(\psi^{k+1} - \psi^k\right)\right) + \left(n^k + \frac{\partial n}{\partial \psi}\left(\psi^{k+1} - \psi^k\right)\right) - N_D^+ + N_A^- + \frac{\rho_s}{q} = 0. \tag{14}$$

广义 Gummel 线性化

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：

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

更新策略：

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

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

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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