Newton Method for Root Finding

Consider the eigenenergies, $\varepsilon_\nu$ ($\nu = 1, 2, ...$), of the effective single-electron Hamiltonian in the previous section. We will fill these energy levels with $M$ electrons. (For $N$ silicon atoms, there are $M = 4N$ valence electrons in the outermost shell.) The occupation number, $N_\nu$, of the $\nu$-th level is given by the Fermi distribution function,

$$N_\nu = f(\varepsilon_\nu) = \frac{2}{\exp((\varepsilon_\nu - \mu)/k_B T) + 1}, \quad (1)$$

where $\mu$ is the chemical potential, $k_B$ is the Boltzmann constant, and $T$ is the temperature. In Eq. (1), the factor 2 is due to the spin degeneracy of each eigenenergy.

The chemical potential in Eq. (1) needs to be determined, so that the total number of electrons is $M$, i.e.,

$$\sum_\nu N_\nu = \sum_\nu \frac{2}{\exp((\varepsilon_\nu - \mu)/k_B T) + 1} = M. \quad (2)$$

Equation (2) is a typical root-finding problem, i.e., we need to find the root $\mu$ to satisfy $F(\mu) = 0$ for the nonlinear function,

$$F(\mu) = \sum_\nu \frac{2}{\exp((\varepsilon_\nu - \mu)/k_B T) + 1} - M. \quad (3)$$

NEWTON METHOD

The Newton method for root finding is successive linear approximations to $F(\mu)$. Given an approximate estimate, $\mu_{\text{old}}$, of the root, the method uses the Taylor expansion of $F(\mu)$ around $\mu_{\text{old}}$ to provide an improved estimate, $\mu_{\text{new}}$, of the root:

$$F(\mu) \equiv F(\mu_{\text{old}}) + \frac{dF}{d\mu}_{\mu=\mu_{\text{old}}} (\mu - \mu_{\text{old}}) = 0. \quad (4)$$

By solving Eq. (4) for $\mu$, the improved estimate is given as

$$\mu_{\text{new}} = \mu_{\text{old}} - \frac{F(\mu_{\text{old}})}{dF/d\mu_{\mu=\mu_{\text{old}}}}. \quad (5)$$

This is illustrated in the following figure.
**Newton Method**

1. Begin with an initial guess, $\mu$, of the root.
2. Repeat the recursion

\[
\mu \leftarrow \mu - \frac{F(\mu)}{dF/d\mu}
\]

until the difference, $|F/(dF/d\mu)|$, between successive approximations becomes less than the prescribed error tolerance, $\mu_{\text{tol}}$. 