Newton Method for Root Finding

Consider the eigenenergies, $\varepsilon_v$ ($v = 1, 2, \ldots$), 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, $N_v$, of the $v$-th level is given by the Fermi distribution function,

$$N_v = f(\varepsilon_v) = \frac{2}{\exp\left(\frac{(\varepsilon_v - \mu)}{k_B T}\right) + 1},$$

(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.,

$$\sum_v N_v = \sum_v \frac{2}{\exp\left(\frac{(\varepsilon_v - \mu)}{k_B T}\right) + 1} = M.$$  

(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,

$$F(\mu) = \sum_v \frac{2}{\exp\left(\frac{(\varepsilon_v - \mu)}{k_B T}\right) + 1} - M.$$  

(3)

NEWTON METHOD

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

$$F(\mu) \approx F(\mu_{old}) + \frac{dF}{d\mu}\bigg|_{\mu=\mu_{old}} (\mu - \mu_{old}) = 0.$$  

(4)

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

$$\mu_{new} = \mu_{old} - \frac{F(\mu_{old})}{\frac{dF}{d\mu}\bigg|_{\mu=\mu_{old}}}.$$  

(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, $\mu_{tol}$.