# 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,

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

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.,

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

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,

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

**NEWTON METHOD**

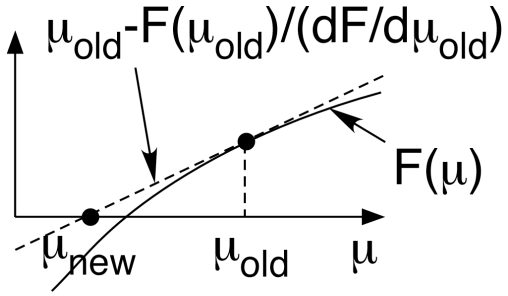
The Newton method for root finding is successive linear approximations to $F(\mu)$. Given an approximate estimate, $\mu_{old}$, of the root, the method uses the Taylor expansion of $F(\mu)$ around $\mu_{old}$ to provide an improved estimate, $\mu_{new}$, of the root:

$$F(\mu) \cong F(\mu_{old}) + \left.\frac{dF}{d\mu}\right|_{\mu=\mu_{old}} (\mu - \mu_{old}) = 0 . \tag{4}$$

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

$$\mu_{new} = \mu_{old} - \frac{F(\mu_{old})}{dF/d\mu\big|_{\mu=\mu_{old}}} . \tag{5}$$

This is illustrated in the following figure.



**Newton Method**

1. Begin with an initial guess, μ, of the root.
2. Repeat the recursion

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

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