Newton Method for Root Finding

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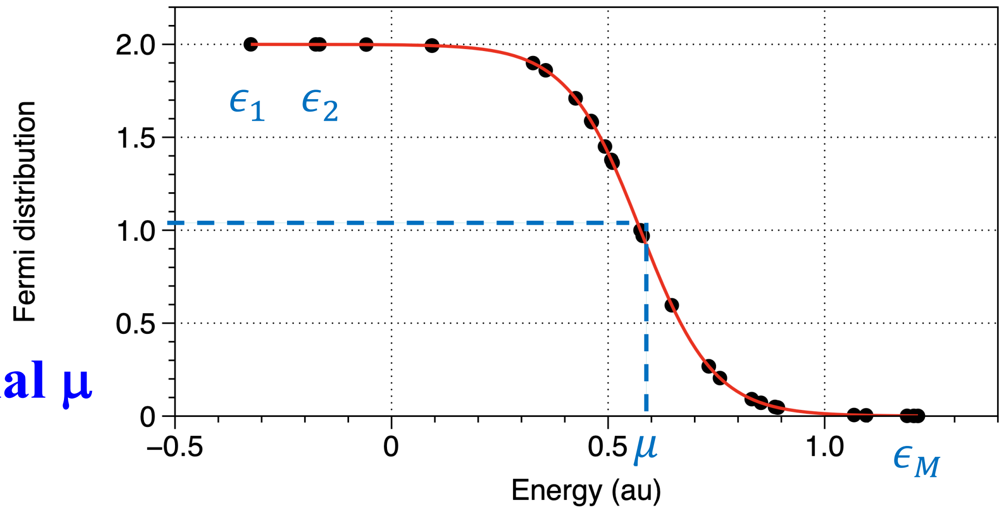
Chemical Potential

- **Fermi distribution**

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



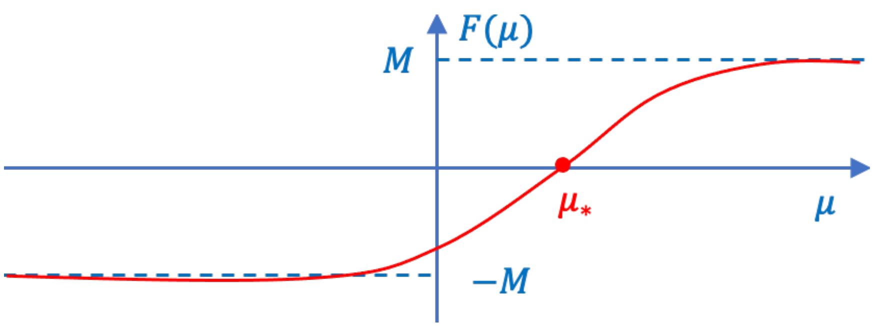
- **Determination of chemical potential μ**

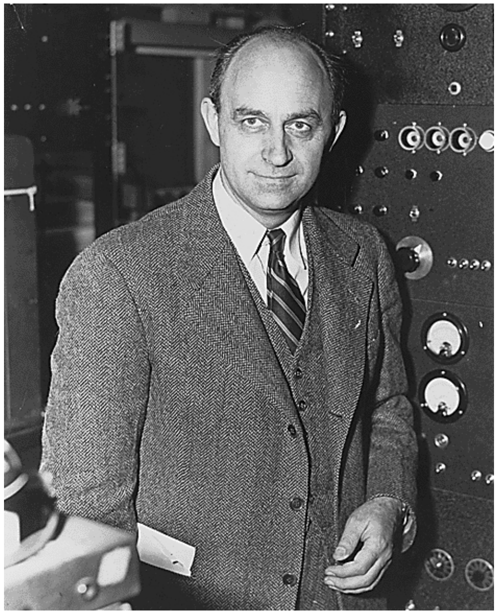
$$\sum_\nu N_\nu = \sum_\nu \frac{2}{\exp((\varepsilon_\nu - \mu)/k_B T) + 1} = M$$

Total # of electrons $M = 4n_{\text{Atom}}$ for Si valence electrons

- **Root finding**

$$F(\mu) = \sum_\nu \frac{2}{\exp((\varepsilon_\nu - \mu)/k_B T) + 1} - M = 0$$

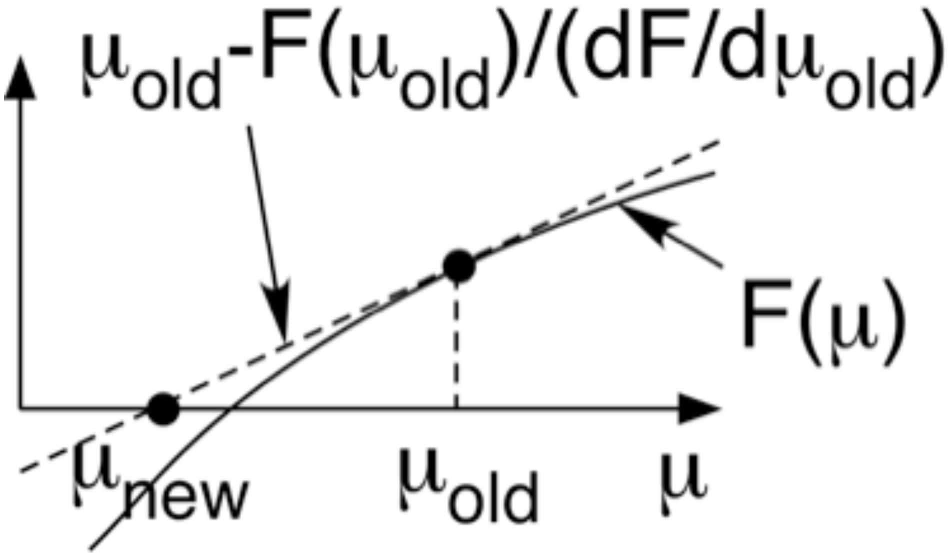


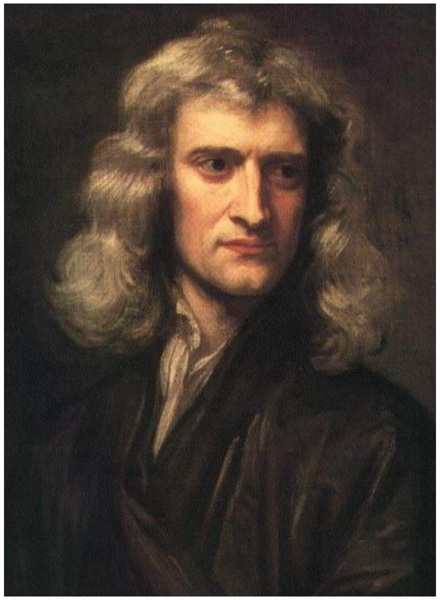


Newton Method

- **Repeated linear approximation**

$$F(\mu) \cong F(\mu_{\text{old}}) + \left.\frac{dF}{d\mu}\right|_{\mu=\mu_{\text{old}}} (\mu - \mu_{\text{old}}) = 0 \rightarrow \mu_{\text{new}} = \mu_{\text{old}} - \frac{F(\mu_{\text{old}})}{dF/d\mu|_{\mu=\mu_{\text{old}}}}$$





- **Algorithm**

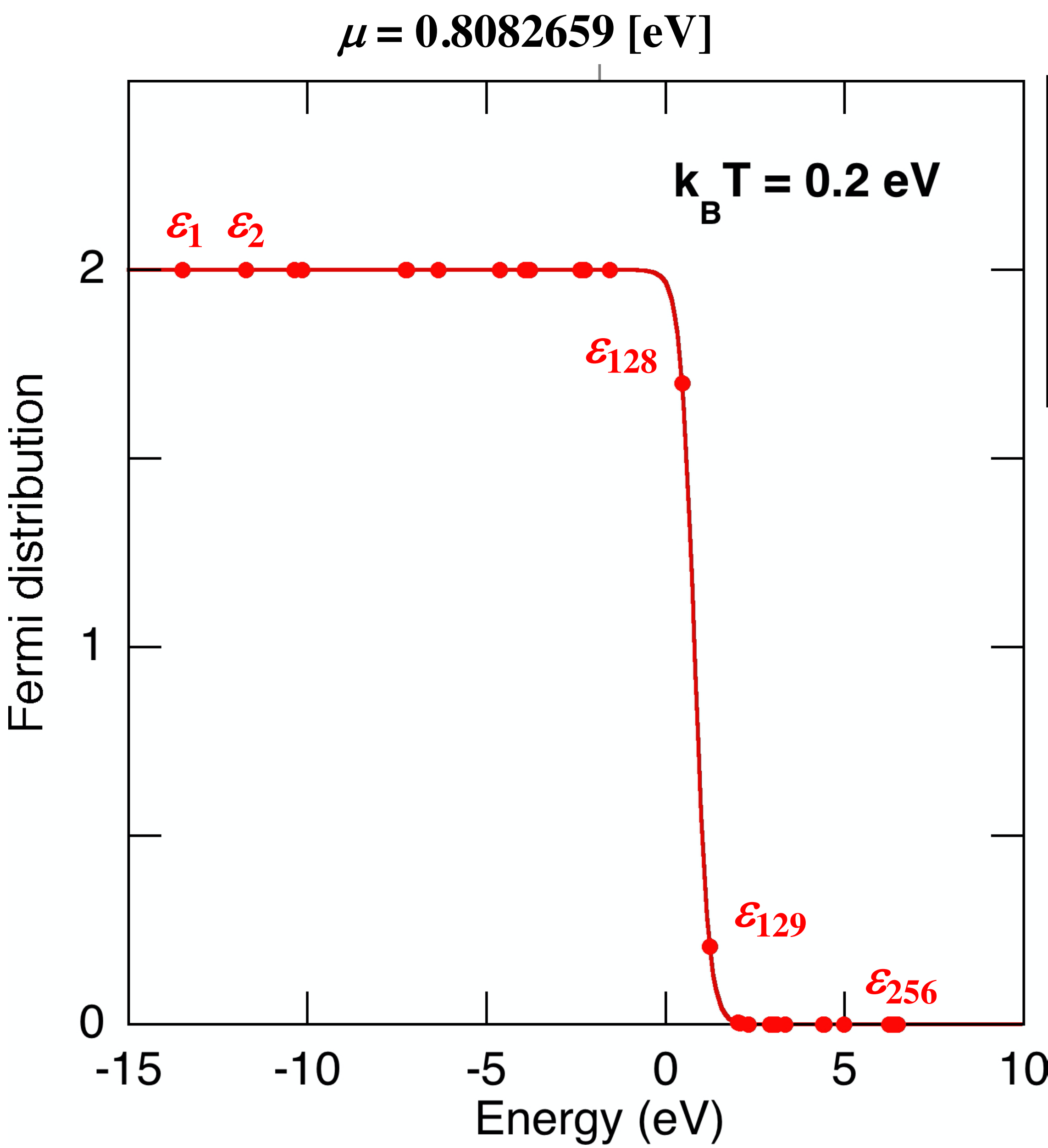
1. Begin with an initial guess, μ, of the root
2. Repeat the recursion

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

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

Example: Silicon Crystal

- **Tight-binding energy eigenvalues for $M = 4\times64 = 256$**



1. $\mu \leftarrow \mu_{\text{guess}} = \varepsilon_{M/2}$
2. Repeat

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

until $|F/(dF/d\mu)| < \mu_{\text{tol}} = 10^{-10}$

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

$$dF/d\mu = ?$$