

Grand-reaction ensemble.

Grand canonical ensemble

The free energy of the grand-canonical ensemble for single particle type

$$\Omega = E - TS + \mu N$$

The entropy S expands via Boltzmann formula

$$S = k_B \ln \frac{V^N}{N!} \qquad \Omega = E - k_B T \ln \frac{V^N}{N!} + \mu N$$

The change of free energy associated with a single particle exchange is

$$\Delta\Omega = k_B T \ln \left(V^\xi \frac{N!}{(N+\xi)!} \right) + \xi\mu + \Delta E$$

accept if $\mathcal{R}^\xi < e^{\Delta\Omega/k_B T}$