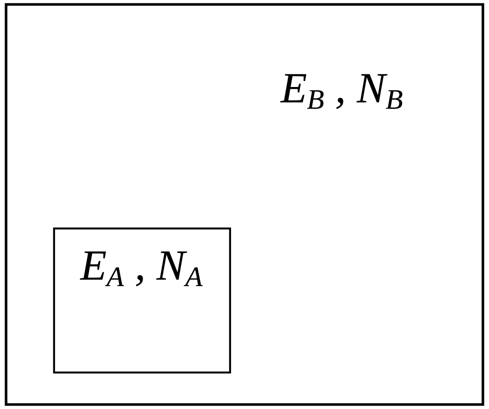
Chapter 4.1: Grand Canonical Ensemble

Assumption: total system isolated and large (microcanonical) $\Omega_{tot}(E_{tot} = E_A + E_B, N_{tot} = N_A + N_B)$
Consider small part A of the system, which is not isolated, $E_A << E_B$ and $N_A << N_B$ not conserved)



What is probability to find system A in one microstate with E_A, N_A?

Def. 4.1:

The chemical potential $\mu = -k_B T\alpha = -\frac{\alpha}{\beta}$ is given in terms of the equilibrium parameter $\alpha = \left(\frac{\partial \ln \Omega}{\partial N}\right)_E$.

The fugacity is given by $z = e^{-\alpha} = e^{\beta\mu}$

Def. 4.2:

The grand canonical partition function is

$$\mathbf{Z} = \sum_{N=0}^{\infty} e^{-\alpha N} \sum_{\{r\}} e^{-\beta E(\{r\})}$$

The grand canonical potential is

$$\Phi = -k_B T \ln \mathbf{Z}$$

Calculation of expectation values using the canonical ensemble

1.) Determine $\mathbf{Z} = \sum_{N=0}^{\infty} e^{-\alpha N} \sum_{\{r\}} e^{-\beta E(\{r\})}$ and $P(N, E(\{r\})) = \dfrac{e^{-\beta E(\{r\})} e^{-\alpha N}}{\mathbf{Z}}$

2.) Determine expectation values (and their derivatives)

Calculation of generalized forces and thermodynamic relations