

## Statistical mechanical ensembles

property	microcanonical	canonical	grand canonical	isothermal-isobaric
constant conditions	$E, V, N$	$T, V, N$	$T, V, \mu$	$T, P, N$
fluctuations	none	$E$	$E, N$	$E, V$
microstate probabilities	$\wp_m = \frac{\delta_{E_m=E}}{\Omega(E, V, N)}$	$\wp_m = \frac{e^{-\beta E_m}}{Q(T, V, N)}$	$\wp_m = \frac{e^{-\beta E_m + \beta \mu N_m}}{\Xi(T, V, \mu)}$	$\wp_m = \frac{e^{-\beta E_m - \beta P V_m}}{\Delta(T, P, N)}$
partition function	$\Omega(E, V, N) = \sum_n \delta_{E_n=E}$	$Q(T, V, N) = \sum_n e^{-\beta E_n}$	$\Xi(T, V, \mu) = \sum_N \sum_n e^{-\beta E_n + \beta \mu N}$	$\Delta(T, P, N) = \sum_V \sum_n e^{-\beta E_n - \beta P V}$
relations to other partition functions	---	$Q = \sum_E e^{-\beta E} \Omega$	$\Xi = \sum_N \lambda^N Q$ $= \sum_N \sum_E \lambda^N e^{-\beta E} \Omega$ $\lambda \equiv \exp[\beta \mu]$	$\Delta = \sum_V e^{-\beta P V} Q$ $= \sum_V \sum_E e^{-\beta E - \beta P V} \Omega$
thermodynamic potential	$S = k_B \ln \Omega(E, V, N)$	$A = -k_B T \ln Q(T, V, N)$	$PV = k_B T \ln \Xi(T, V, \mu)$	$G = -k_B T \ln \Delta(T, P, N)$
classical partition function	$\Omega = \frac{1}{h^{3N} N!} \int \delta[H(\mathbf{p}^N, \mathbf{r}^N) - E] d\mathbf{p}^N d\mathbf{r}^N$	$Q = \frac{Z(T, V, N)}{\Lambda(T)^{3N} N!}$ $Z \equiv \int e^{-\beta U(\mathbf{r}^N)} d\mathbf{r}^N$ $\Lambda \equiv (h^2 / 2\pi m k_B T)^{\frac{1}{2}}$	$\Xi = \sum_{N=0}^{\infty} \frac{\lambda^N Z(T, V, N)}{\Lambda(T)^{3N} N!}$ $\lambda \equiv \exp[\beta \mu]$	$\Delta = \frac{1}{\Lambda(T)^{3N} N!} \int_0^{\infty} e^{-\beta P V} Z(T, V, N) dV$

\*\*Sums over  $n$  correspond to sums over all microstates at a given  $V$  and  $N$ .

\*\*Sums over  $N$  are from 0 to  $\infty$ , for  $V$  from 0 to  $\infty$ , and for  $E$  from  $-\infty$  to  $\infty$ .