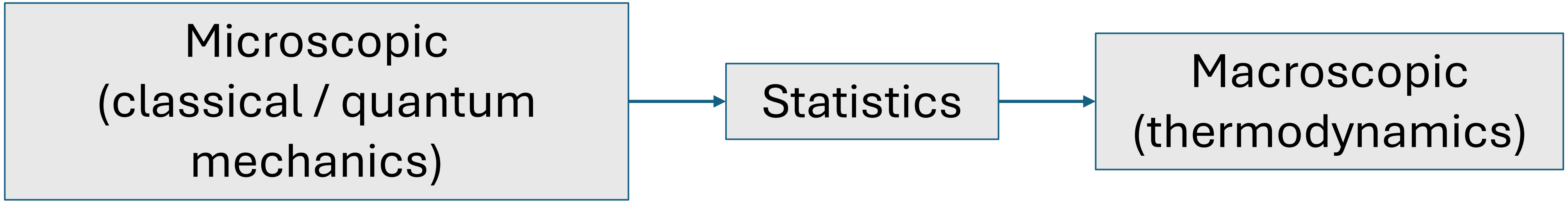
# MSE-421
# Exercise session 1

06.03.2025

# Statistical mechanics




**Revision (weeks 1-2)**

- Thermodynamics
- Probability

**Theory (weeks 3-6)**

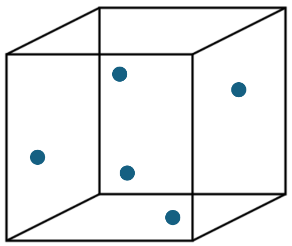
- Microcanonical ensemble
- Canonical ensemble
- Grand-canonical ensemble

**Applications (weeks 7-13)**

- Solids (phonons and electrons)
- Phase transitions and magnetism
- Liquids
- Polymers

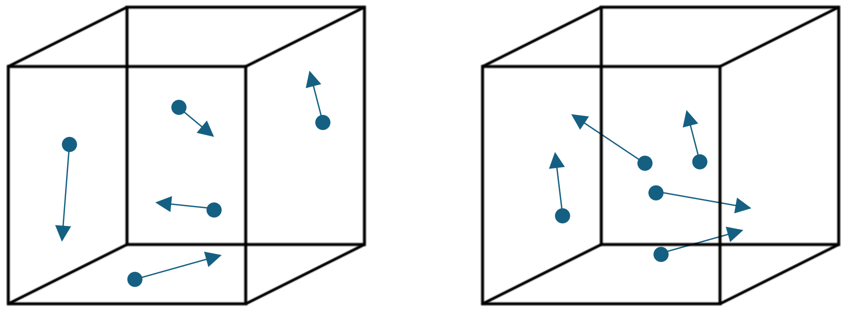
# Ensembles

- Defined by fixing some macroscopic variables (e.g., N, V, T)



N = 5
V = cube volume
T = ambient

- Observe the microstates many, many times



- Probability $P(\boldsymbol{v})$ or $P(\boldsymbol{p},\boldsymbol{q})$
- Ensemble average:

$$\langle O\rangle = \int O(\boldsymbol{p},\boldsymbol{q})\, P(\boldsymbol{p},\boldsymbol{q})\, d\boldsymbol{p}\, d\boldsymbol{q}$$

$$\langle O\rangle = \sum_{\boldsymbol{v}} \langle \boldsymbol{v}|\hat{O}|\boldsymbol{v}\rangle\, P(\boldsymbol{v})$$

# The NVE (microcanonical) ensemble

- N, V, E are fixed
- Probability $P(\boldsymbol{\nu})$ is the same for all observable microstates $\boldsymbol{\nu}$
- Only their number matters: $\Omega$
- Statistical definition of entropy: $S = k_B \ln \Omega$

# The NVE ensemble recipe

- Calculate $\Omega(N, V, E)$, nearly always by using combinatorics
- Find $S(N, V, E) = k_B \ln \Omega(N, V, E)$ and simplify with Stirling's approximation $\ln N! \approx N \ln N - N$
- If asked about the temperature, remember $\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{N,V}$