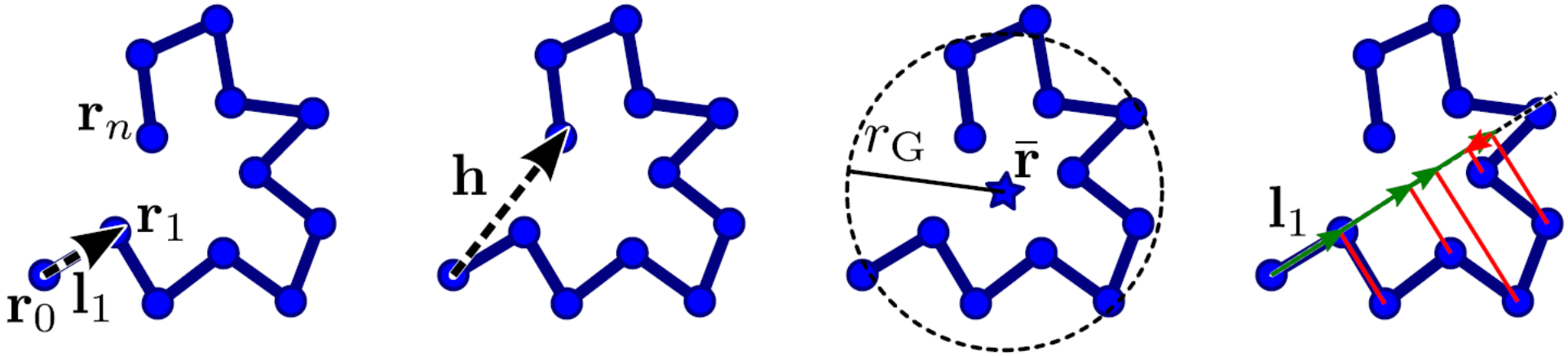
Lab 5: Polymers

MSE421-Statistical Mechanics

Size of polymers

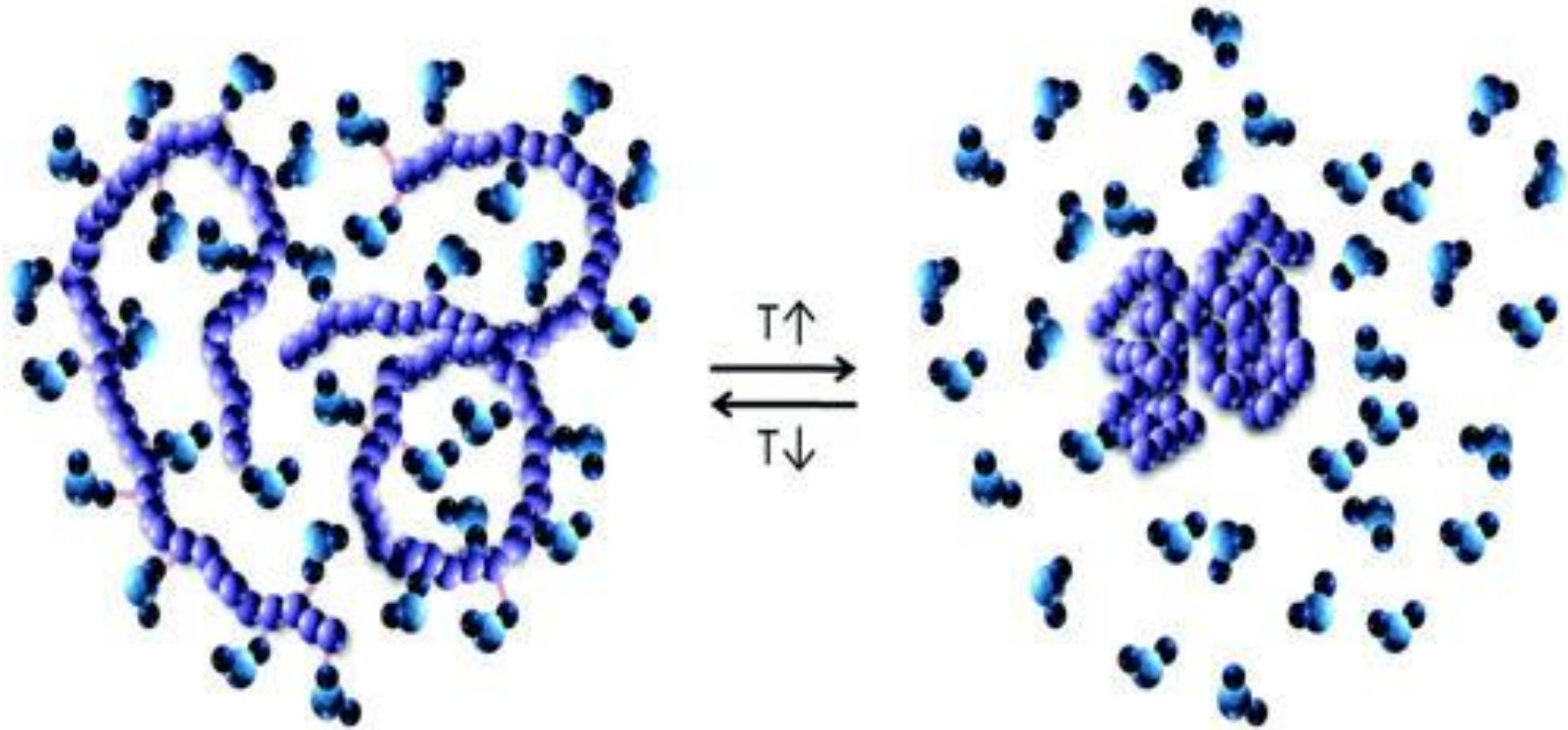
Different ways to measure the size of a polymer



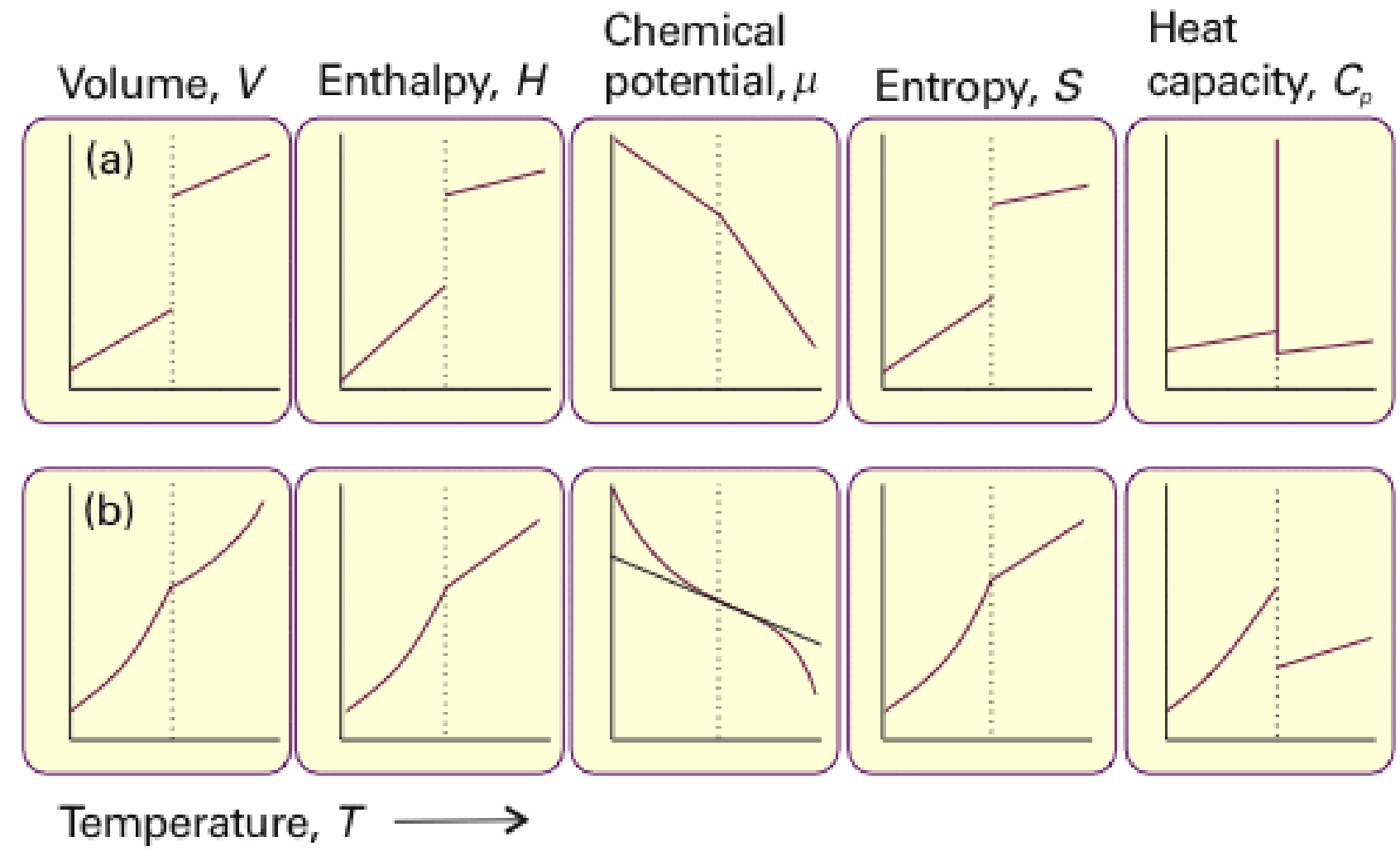
Measure of size

- Ideal Chain $\sqrt{\langle \boldsymbol{h}^2 \rangle} \propto \sqrt{N}$
- Rigid Rods $\sqrt{\langle \boldsymbol{h}^2 \rangle} \propto N$
- Real Polymers $\sqrt{\langle \boldsymbol{h}^2 \rangle} \propto N^{\nu}$

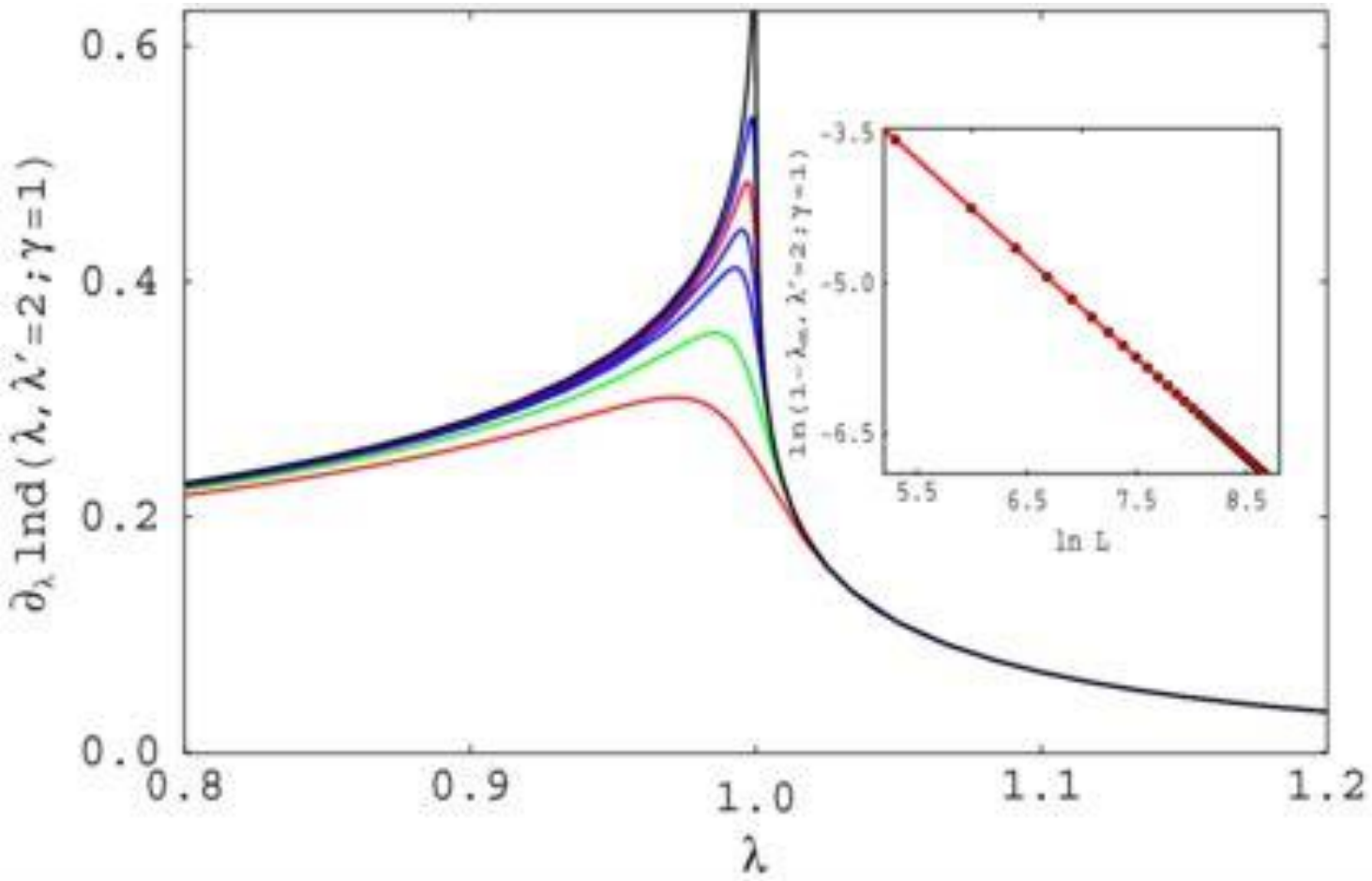
Coil Globule Transition



Phase Transitions



Finite size scaling



How to compute distances between atoms

In the main window, choose:

- Mouse → Label → Bonds

Now, clicking with the mouse on two atoms will display the distance between them.

- Graphics → Labels

In the box on the top left, select “bonds” and select the bond from the list that appears below. You can then export this by clicking on “Graph” and then “save”.