Liquid-solid transitions in the three-body hard-core model

(T. Comparin, S. Kapfer, W. Krauth, EPL 2015)

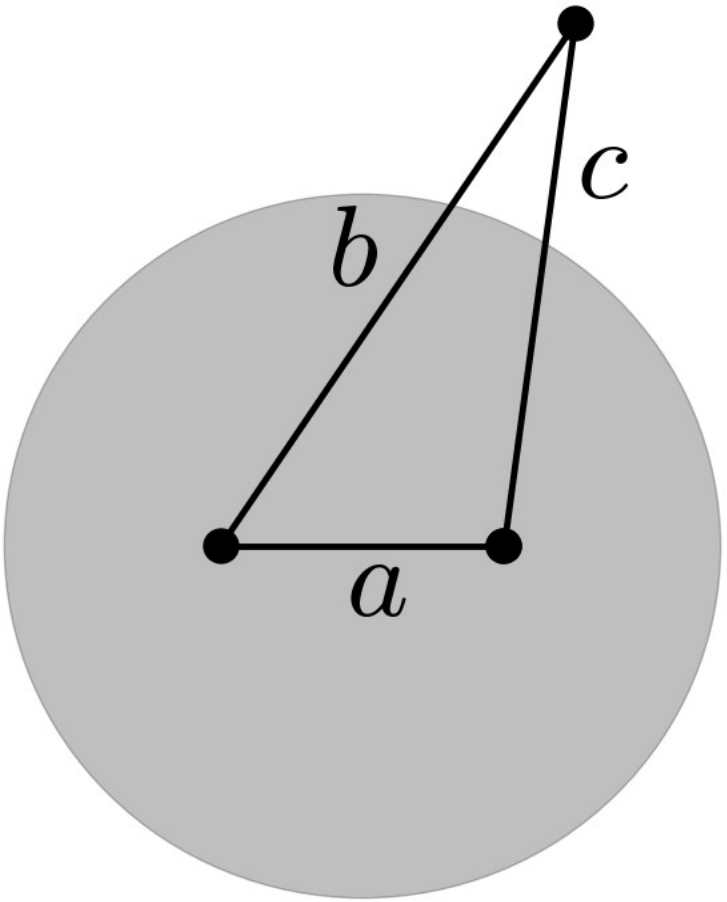
- Two-body hard-core (rods, disks, spheres):

$$\text{dist} > \text{diameter}$$

- Three-body hard-core:

$$a^2 + b^2 + c^2 > 3R_0^2$$

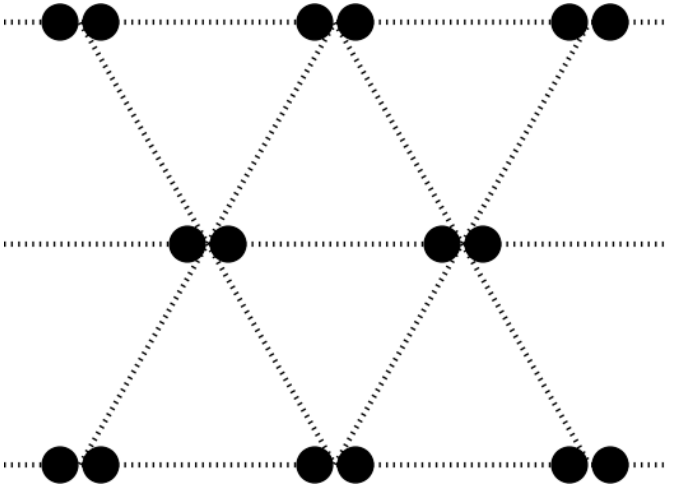
(two fixed positions generate an excluded circle for the third one)



Close-packed structures?

(enumeration + simulated annealing)

Lattice of single particles
vs
lattice of dimers

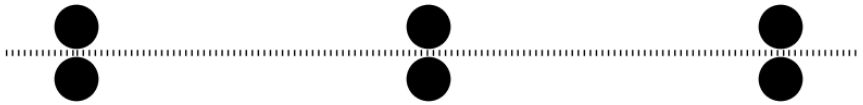


2D

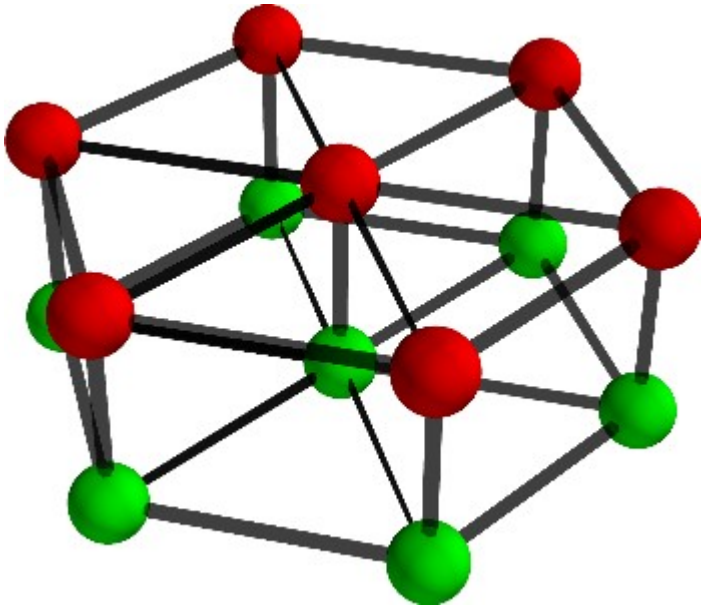
1D

monomers: $\rho R_0 \simeq 1.414$

dimers: $\rho R_0 \simeq 1.633$

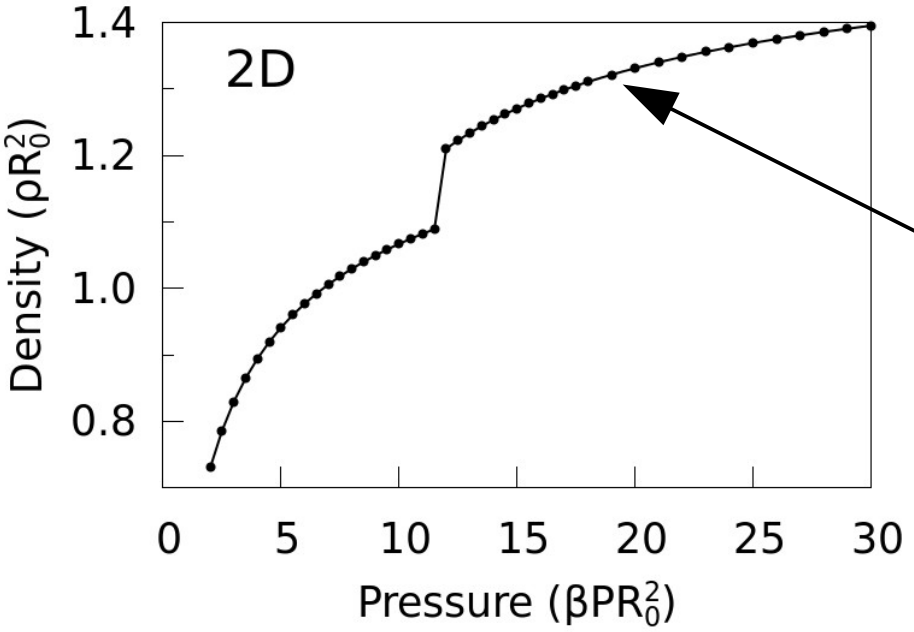


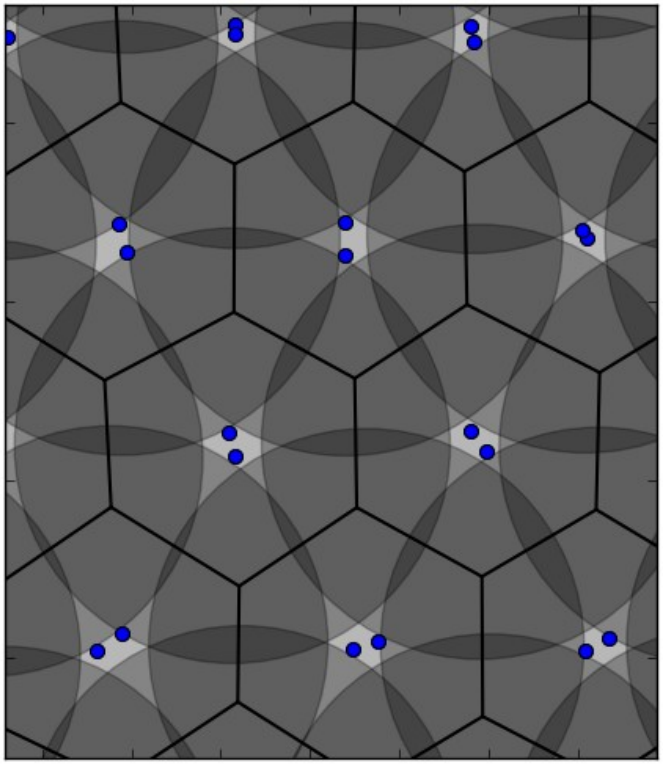
3D



Finite pressure?

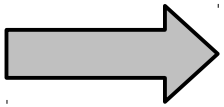
(NPT Monte Carlo)





2D: effective spin model
for dimer orientations

Frustrated (effective)
interactions



No finite magnetization