

The Phase Diagram of Supercooled Water

Kevin Stokely

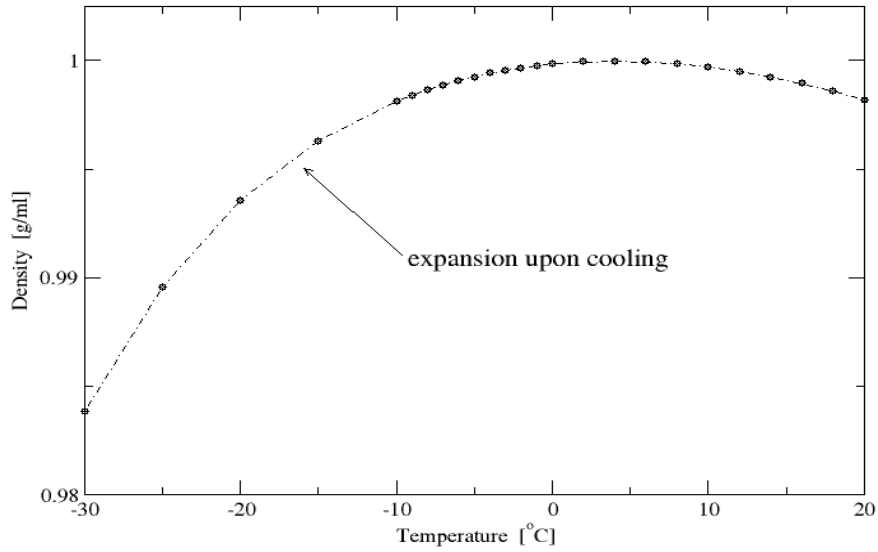
G. Franzese, H. E. Stanley

February 29, 2012
APS Meeting



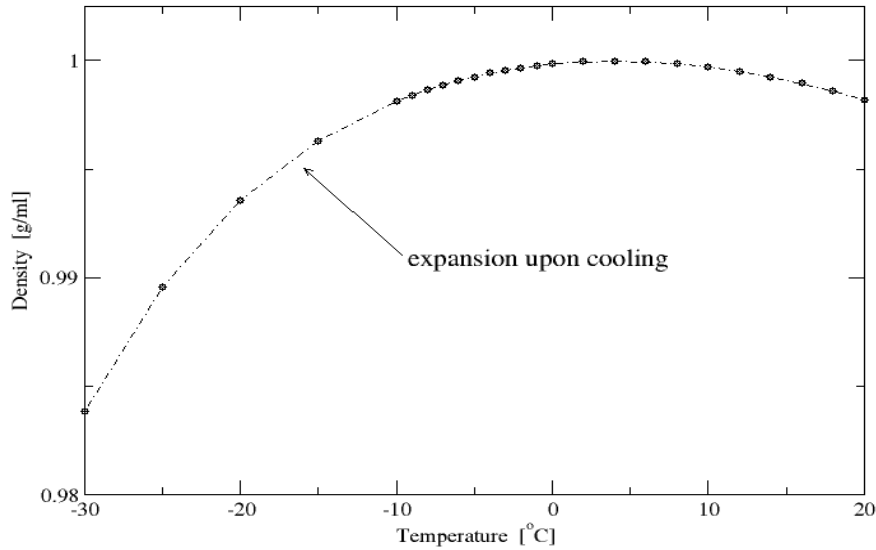
Liquid water has some unusual properties

Density Anomaly

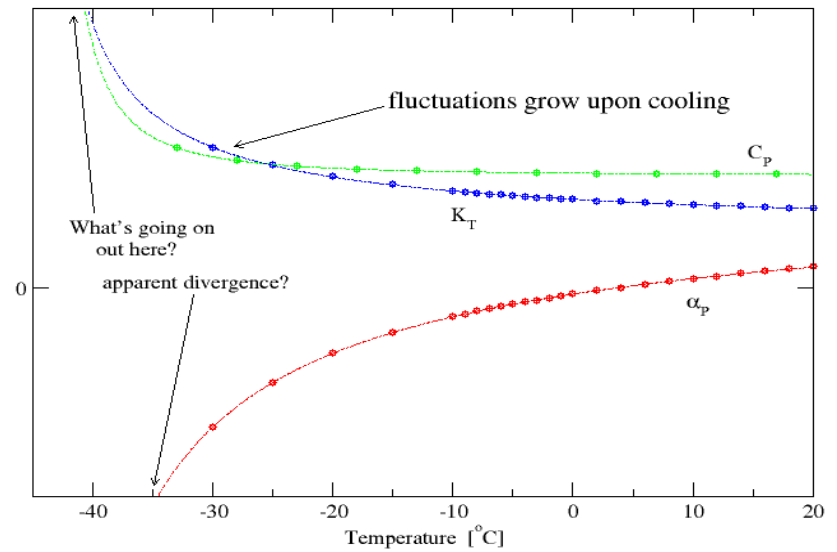


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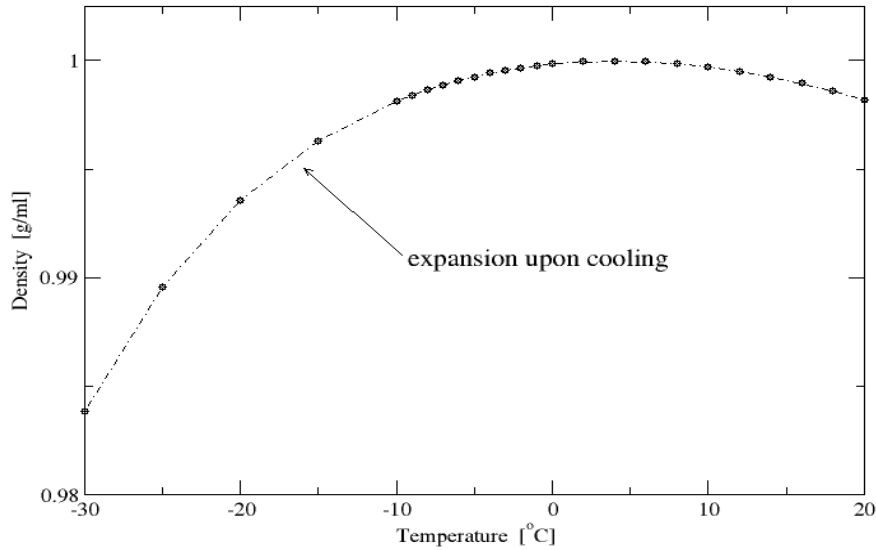


Thermodynamic Anomalies

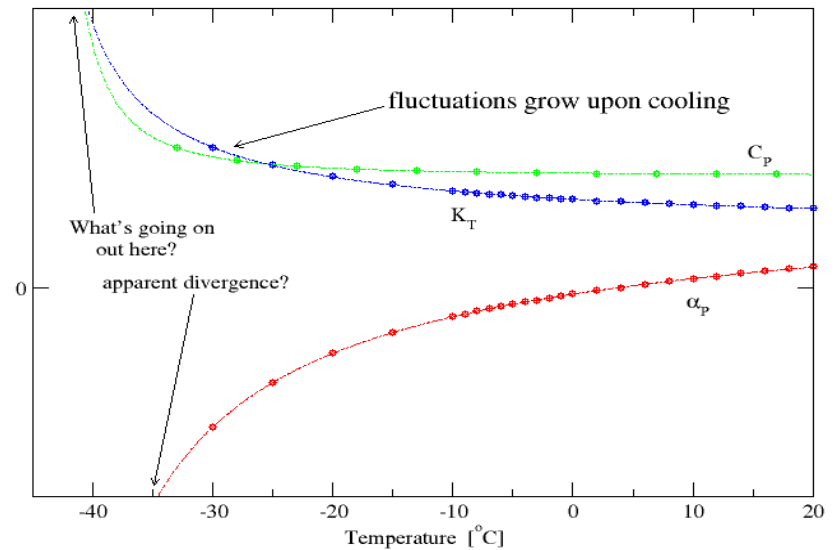


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Density Anomaly

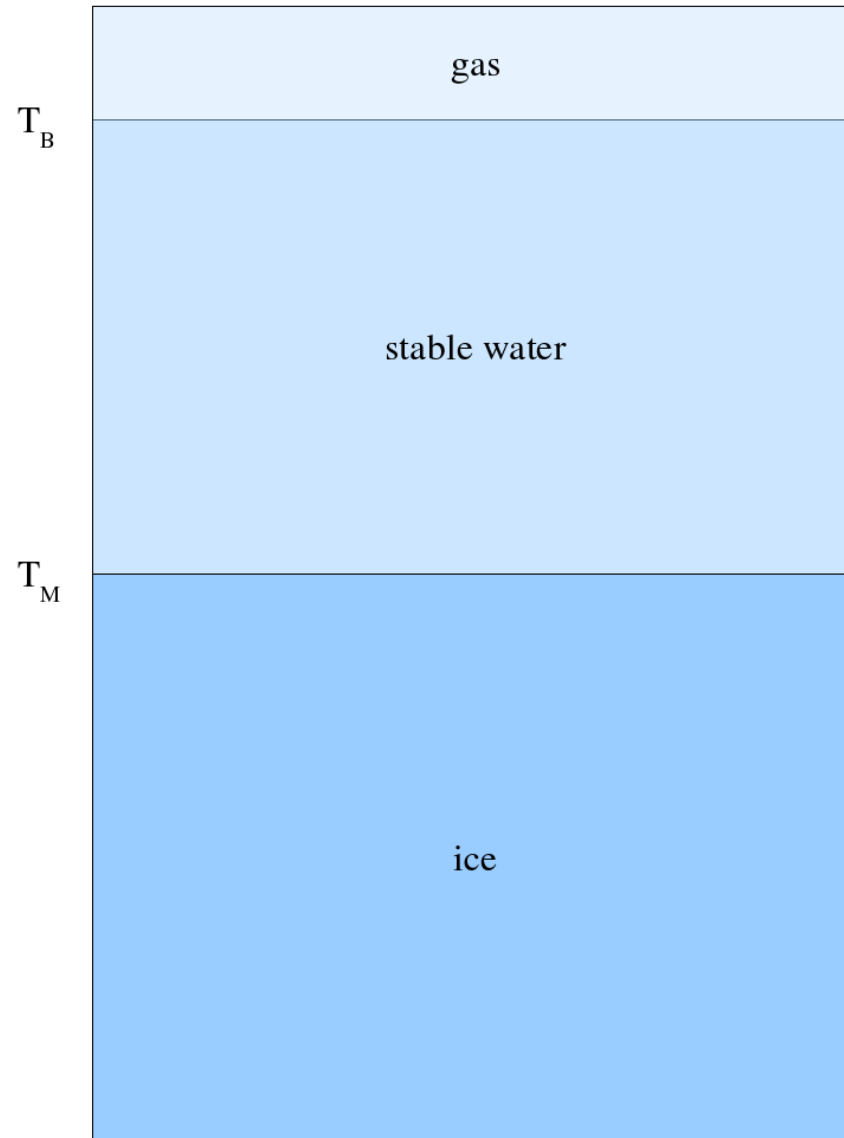


Thermodynamic Anomalies

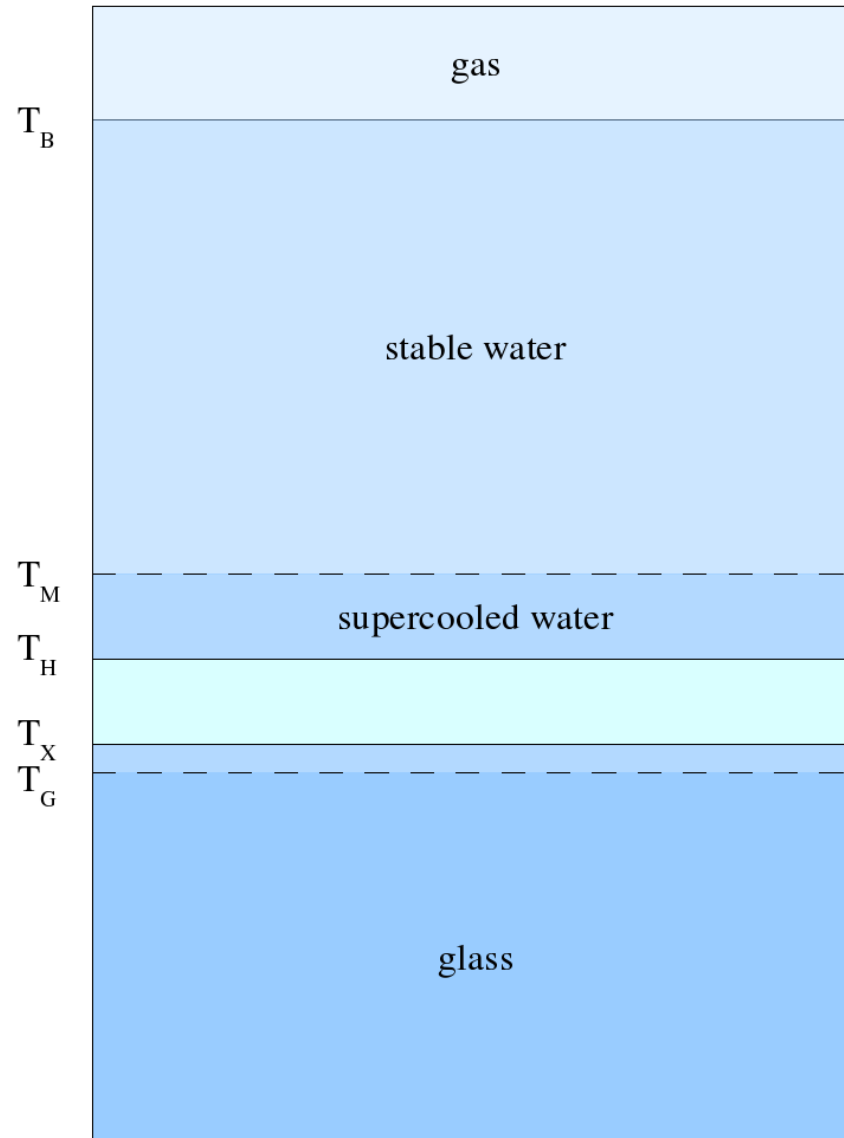


It would be nice to know the phase diagram.

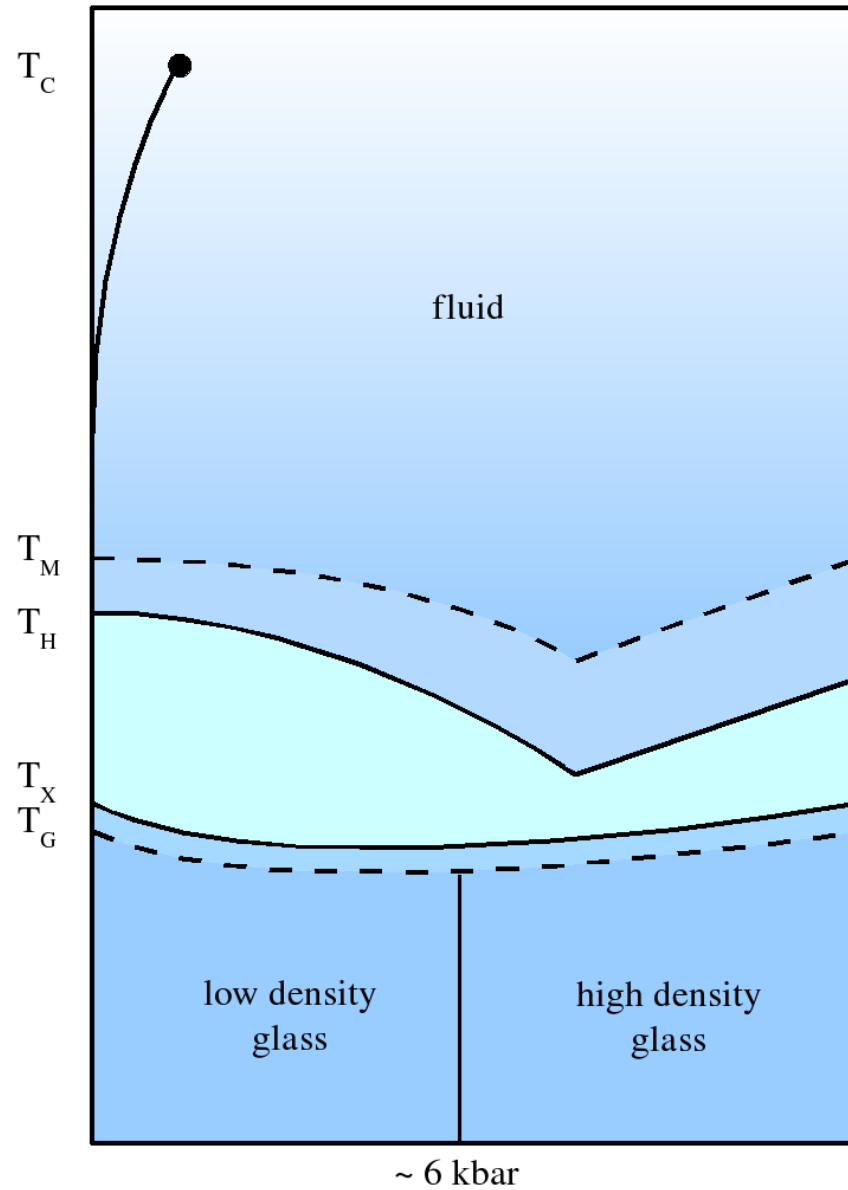
The phase diagram of water

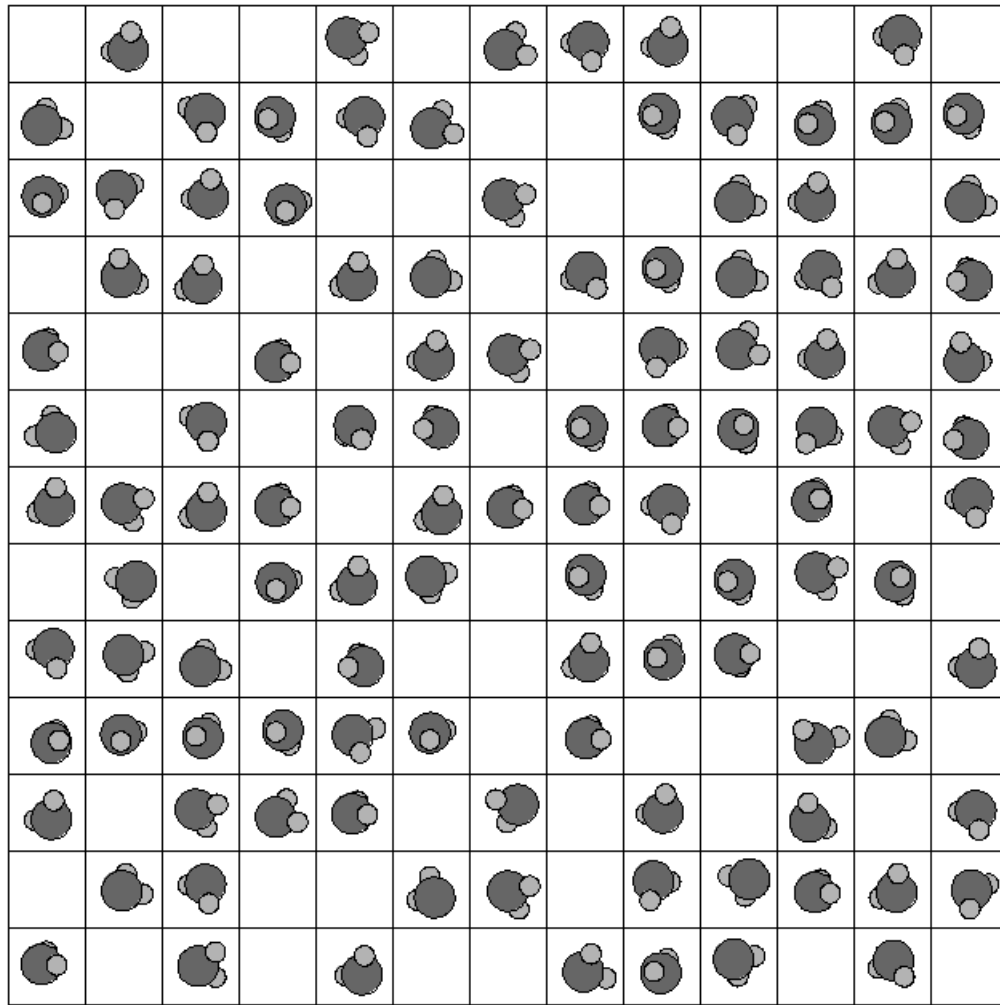


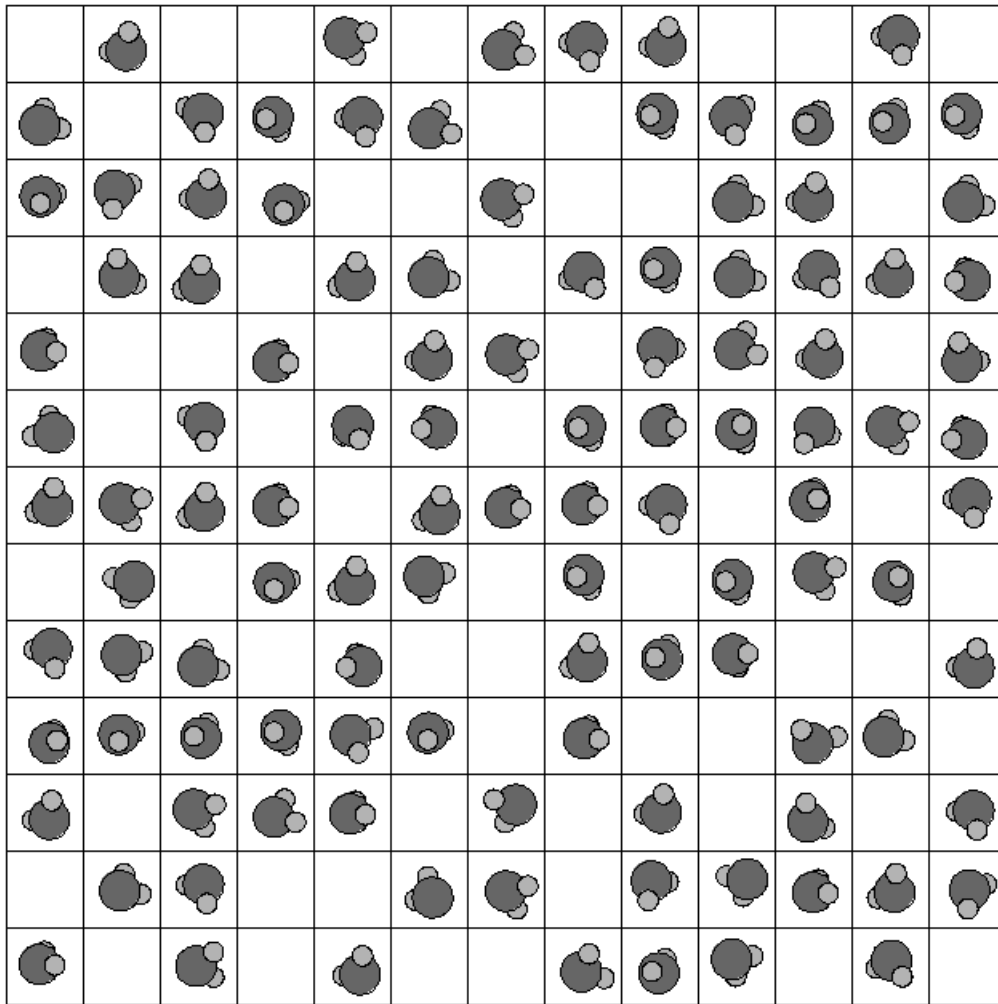
The phase diagram of fluid water



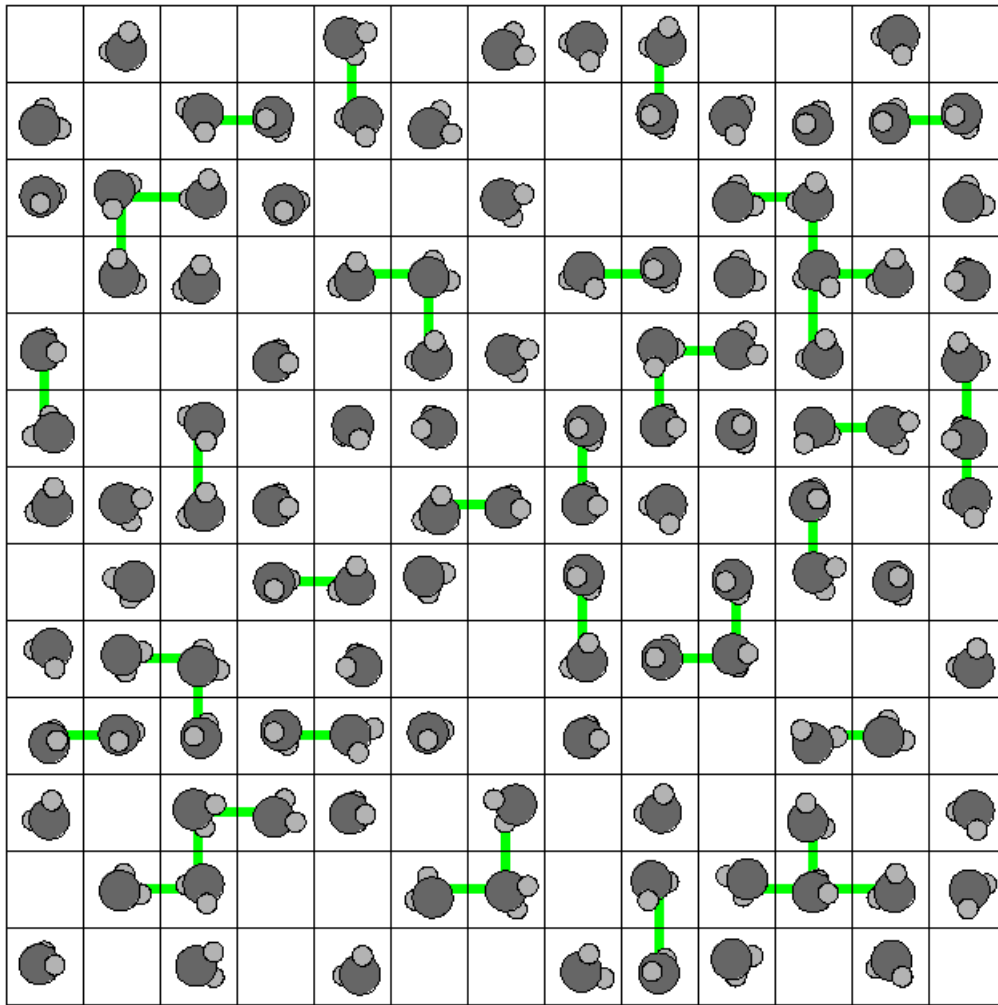
The phase diagram of fluid water



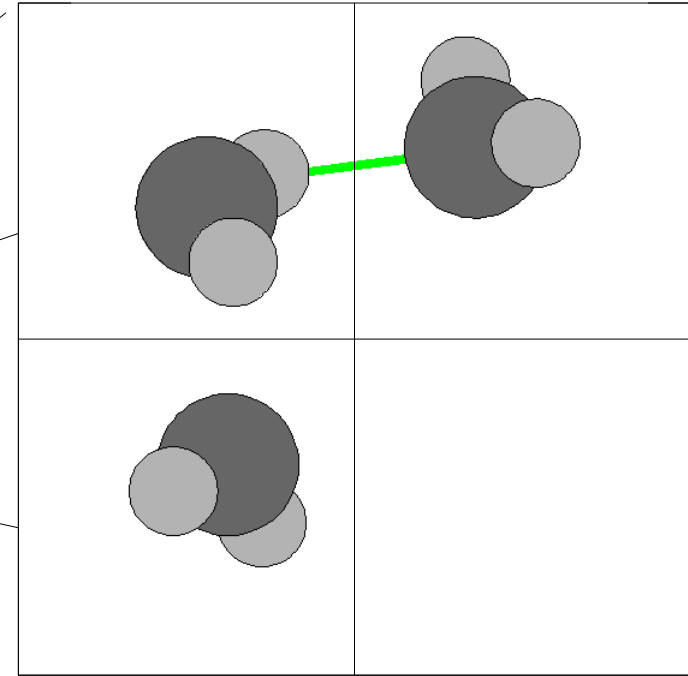
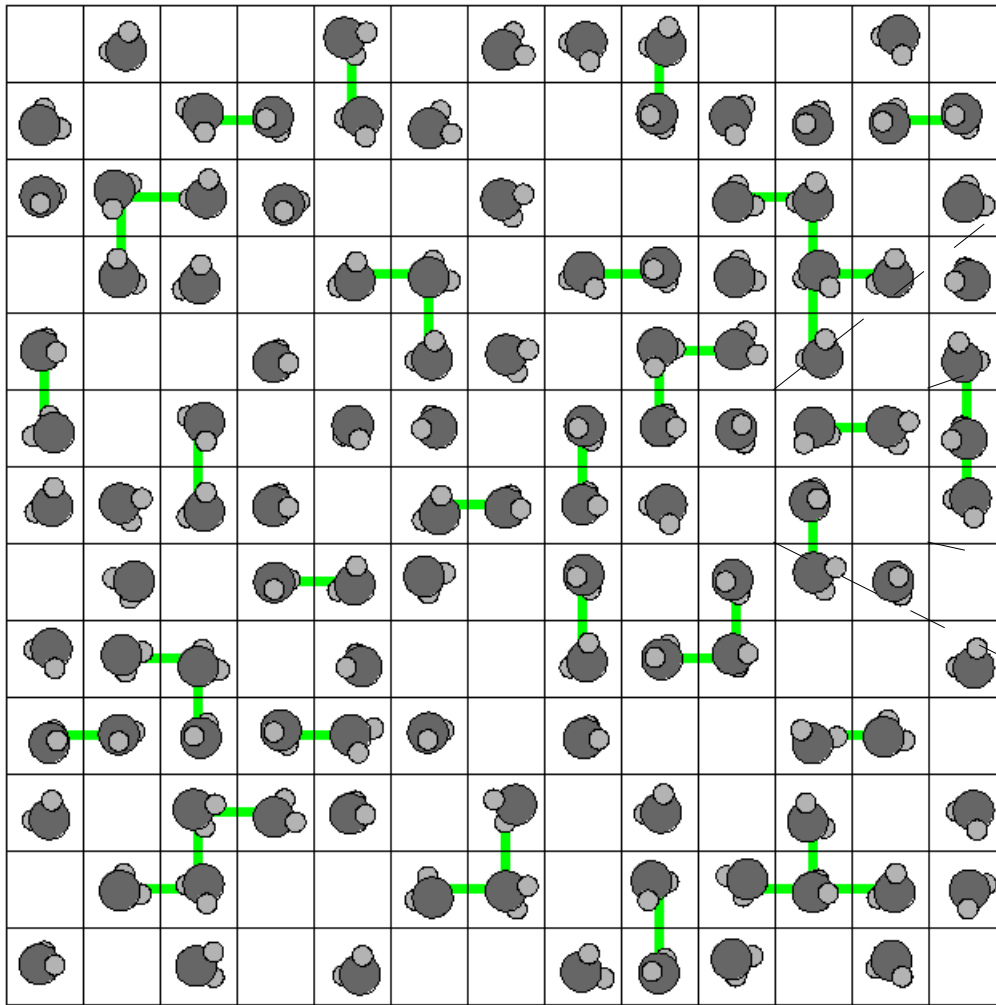




Model = Lattice Gas

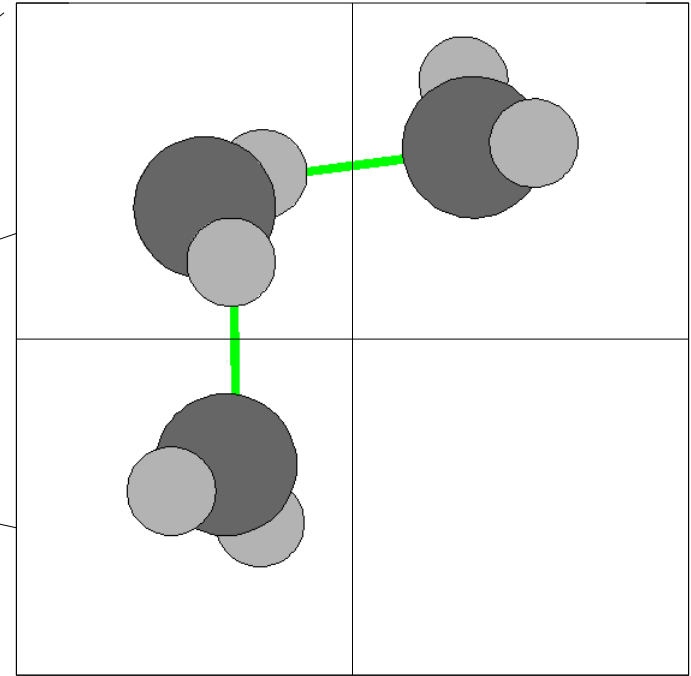
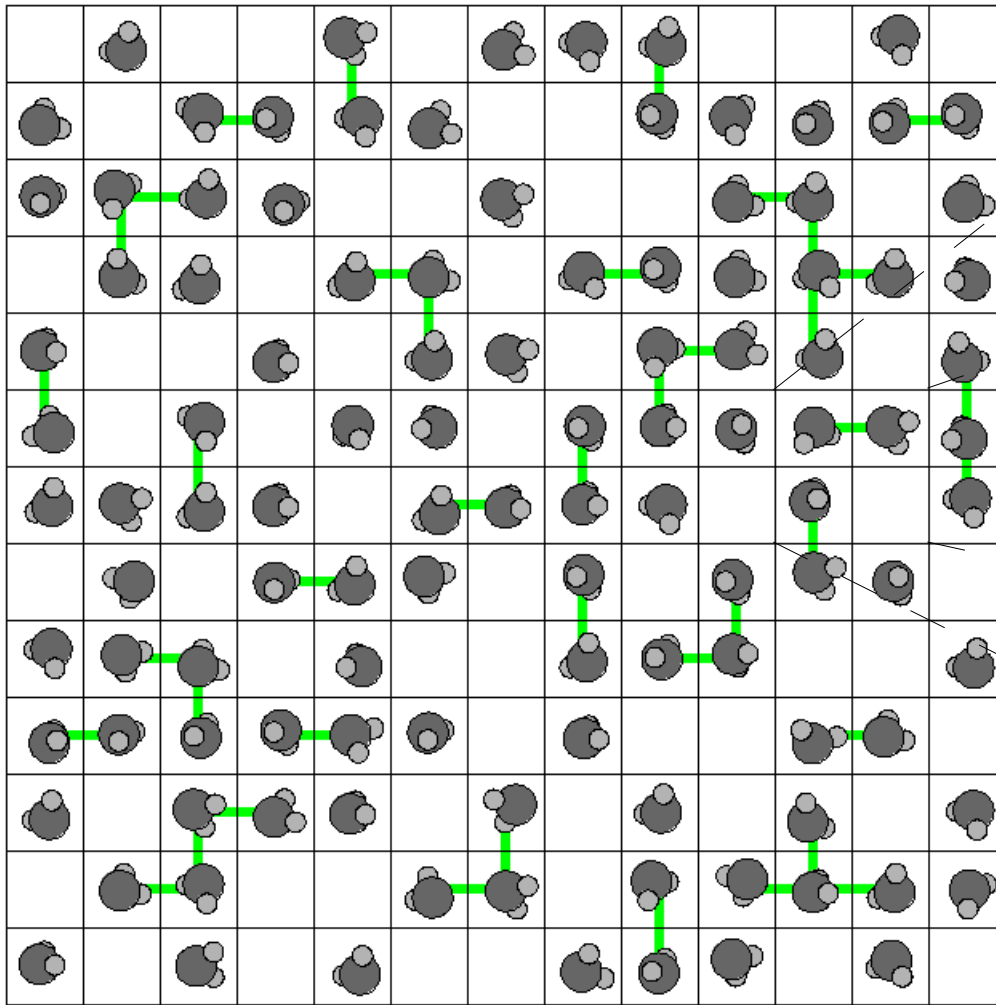


Model = Lattice Gas + Hydrogen Bonds



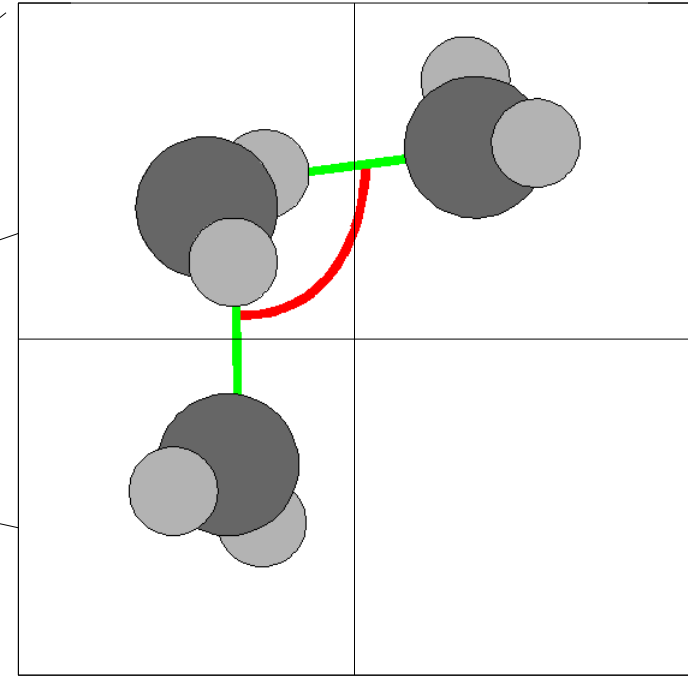
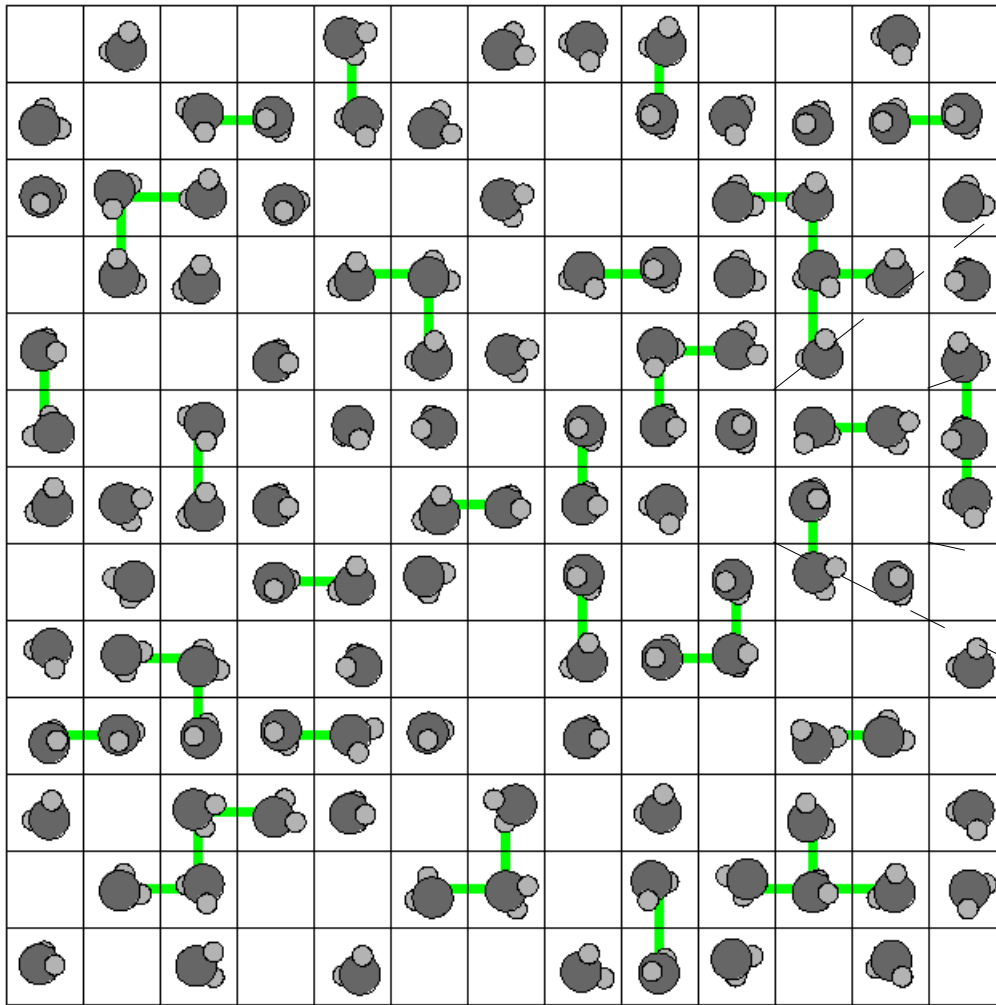
Model = Lattice Gas + Hydrogen Bonds

Pair Energy: **J**
 Volume Increase



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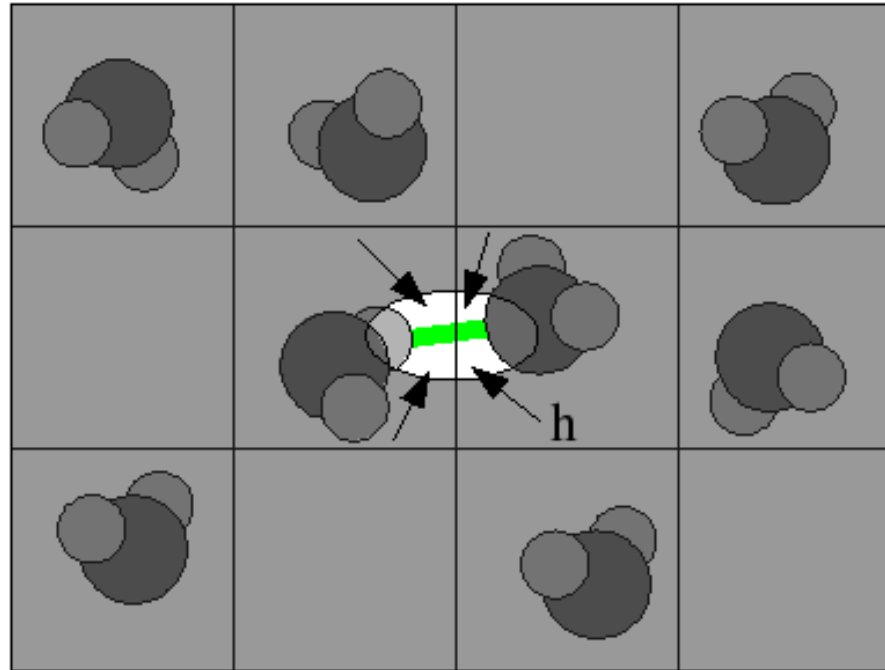


Model = Lattice Gas + Hydrogen Bonds

Pair Energy: J
Volume Increase

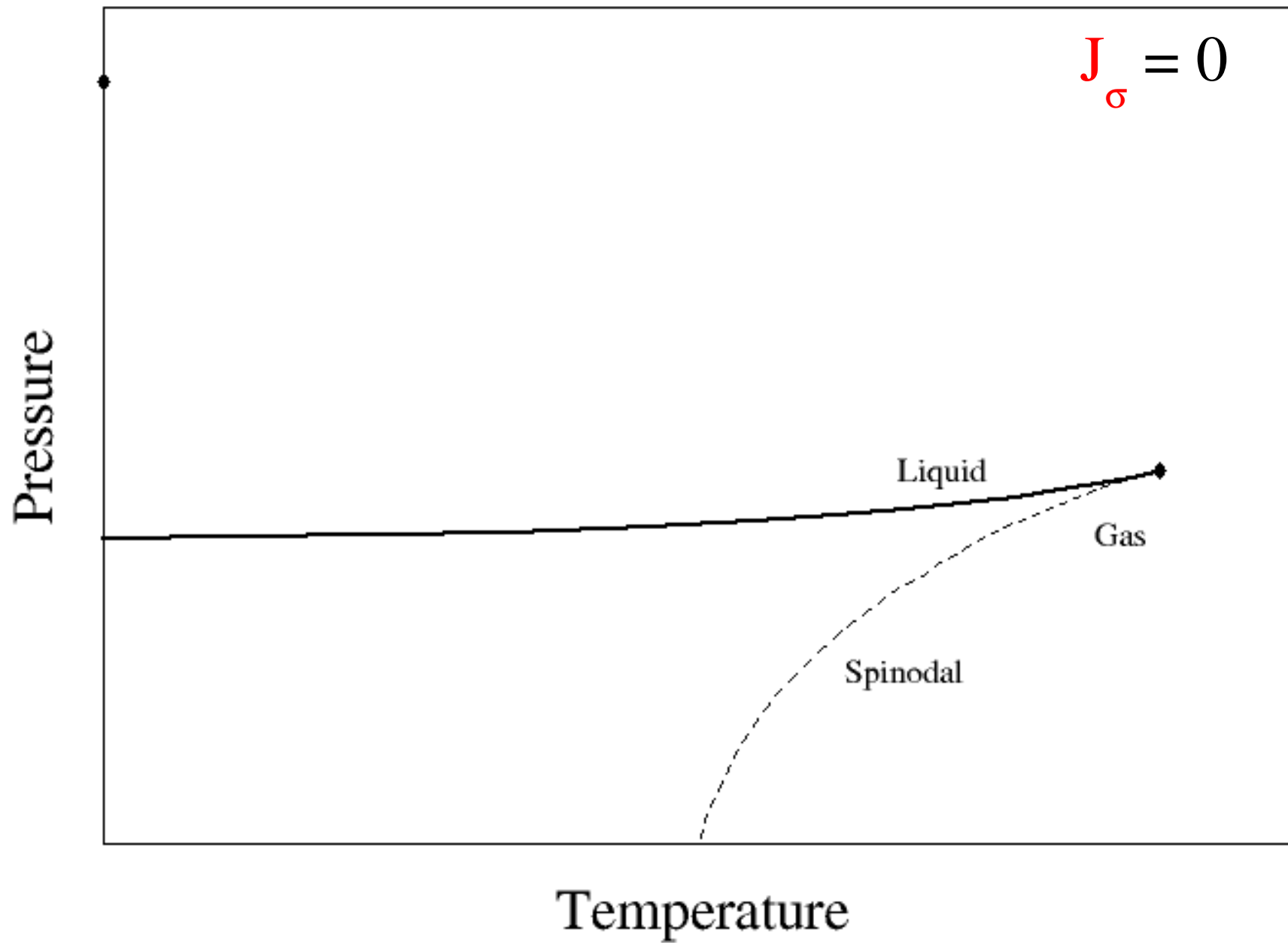
Many-body Energy: J_σ

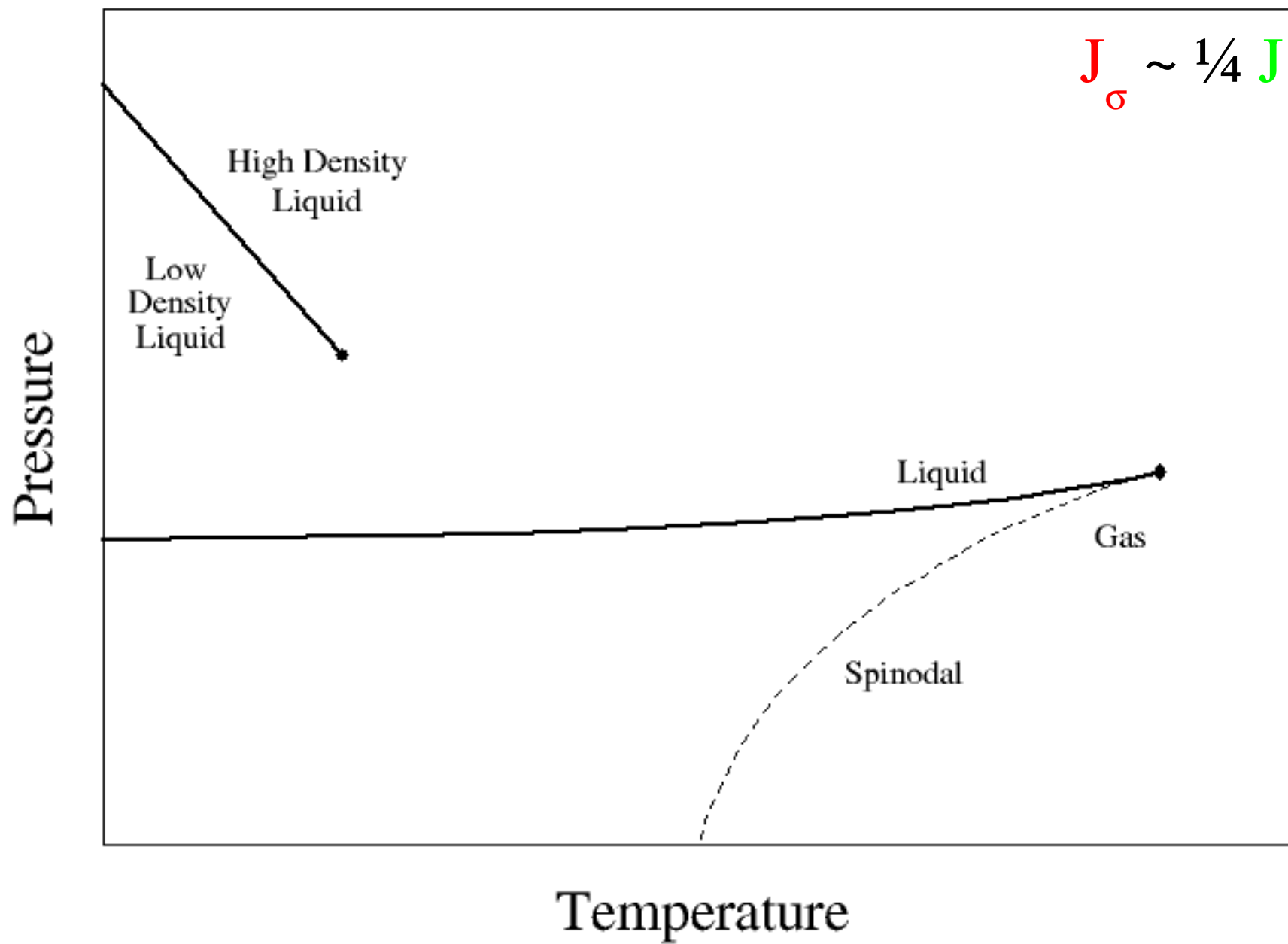
The model may be solved
within a cavity approximation.

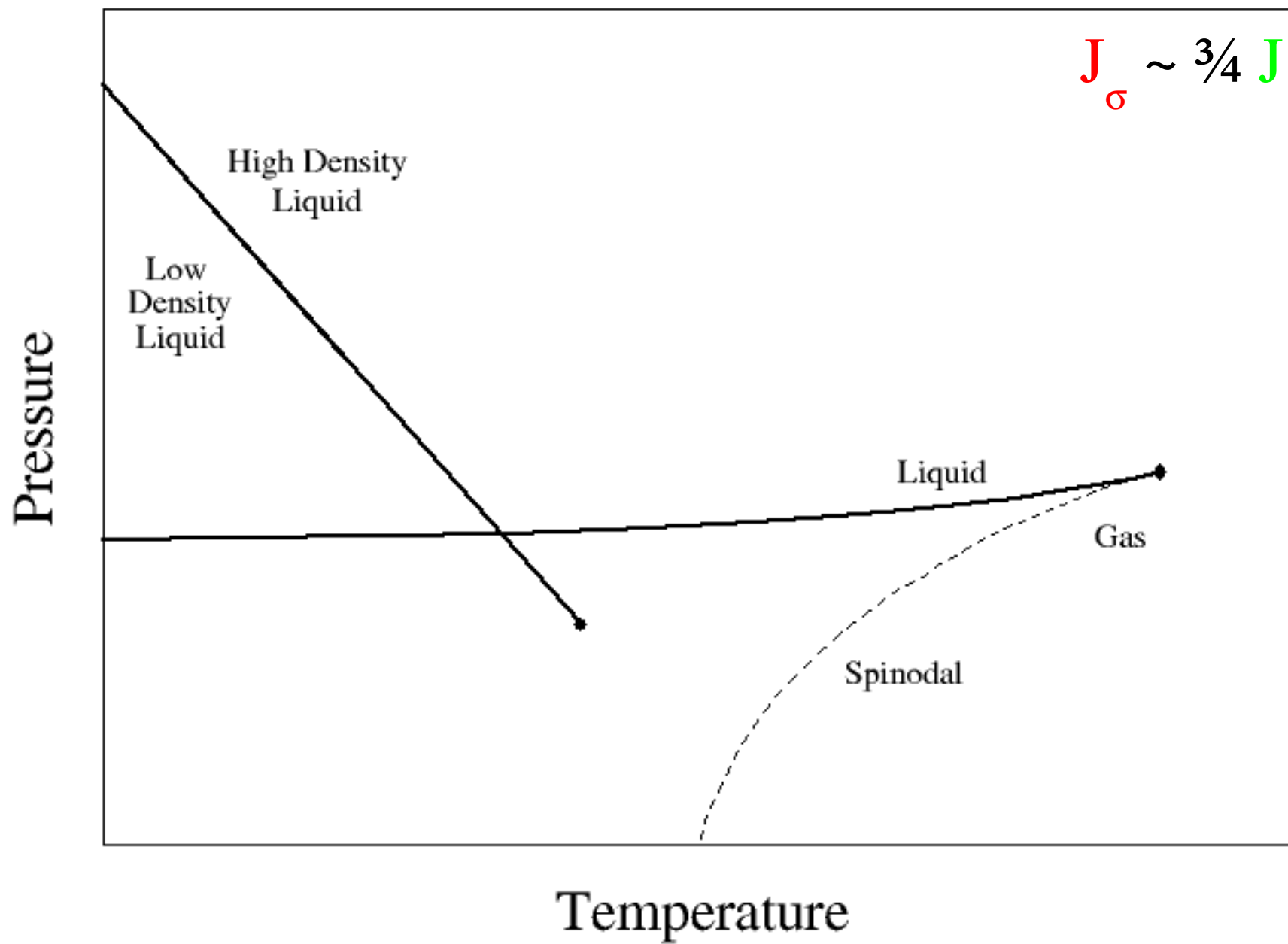


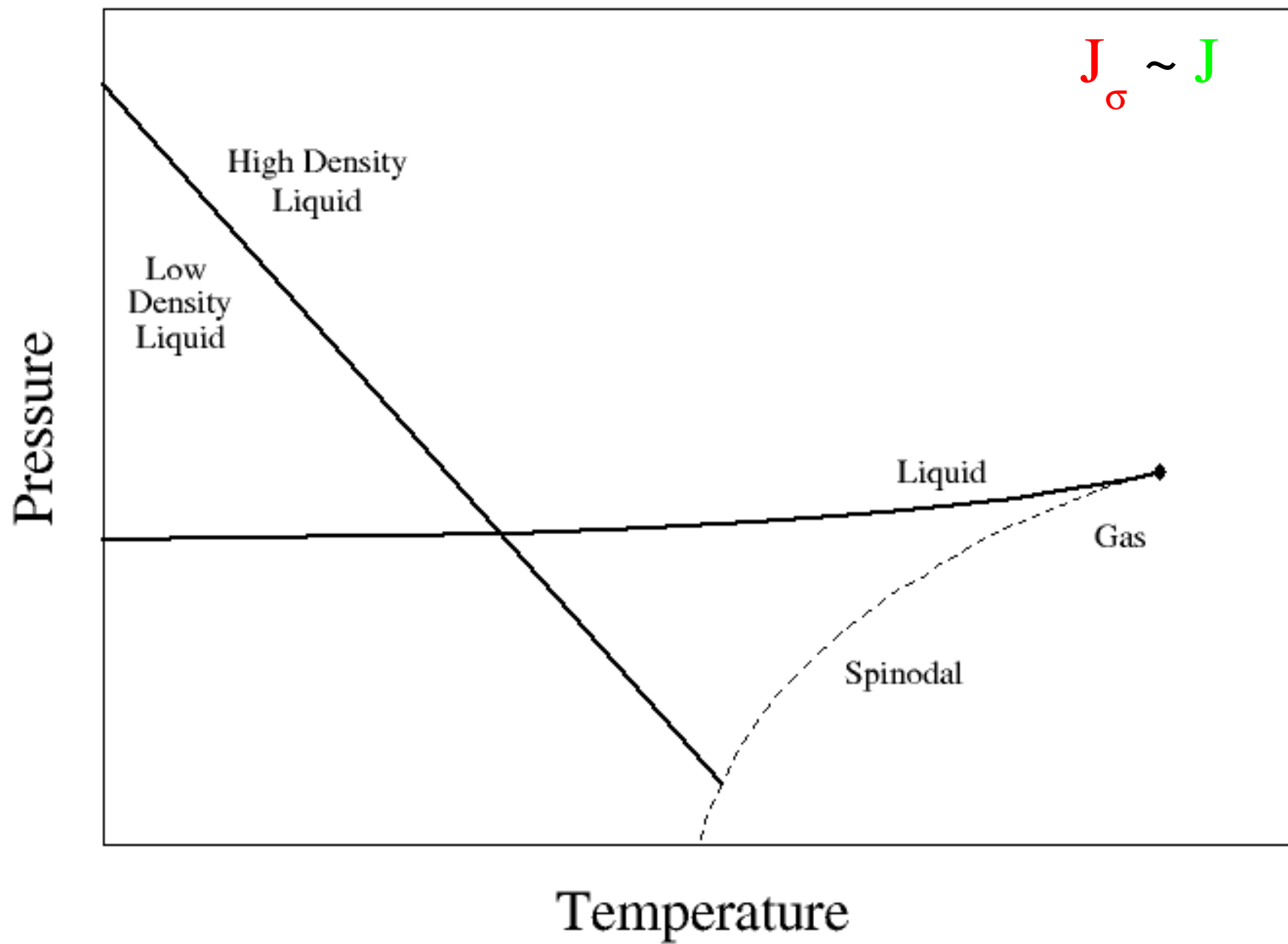
G. Franzese, M. I. Marques, and H. E. Stanley
"Intramolecular Coupling as a Mechanism for a Liquid-Liquid Phase Transition"
Phys. Rev. E 67, 011103 (2003)

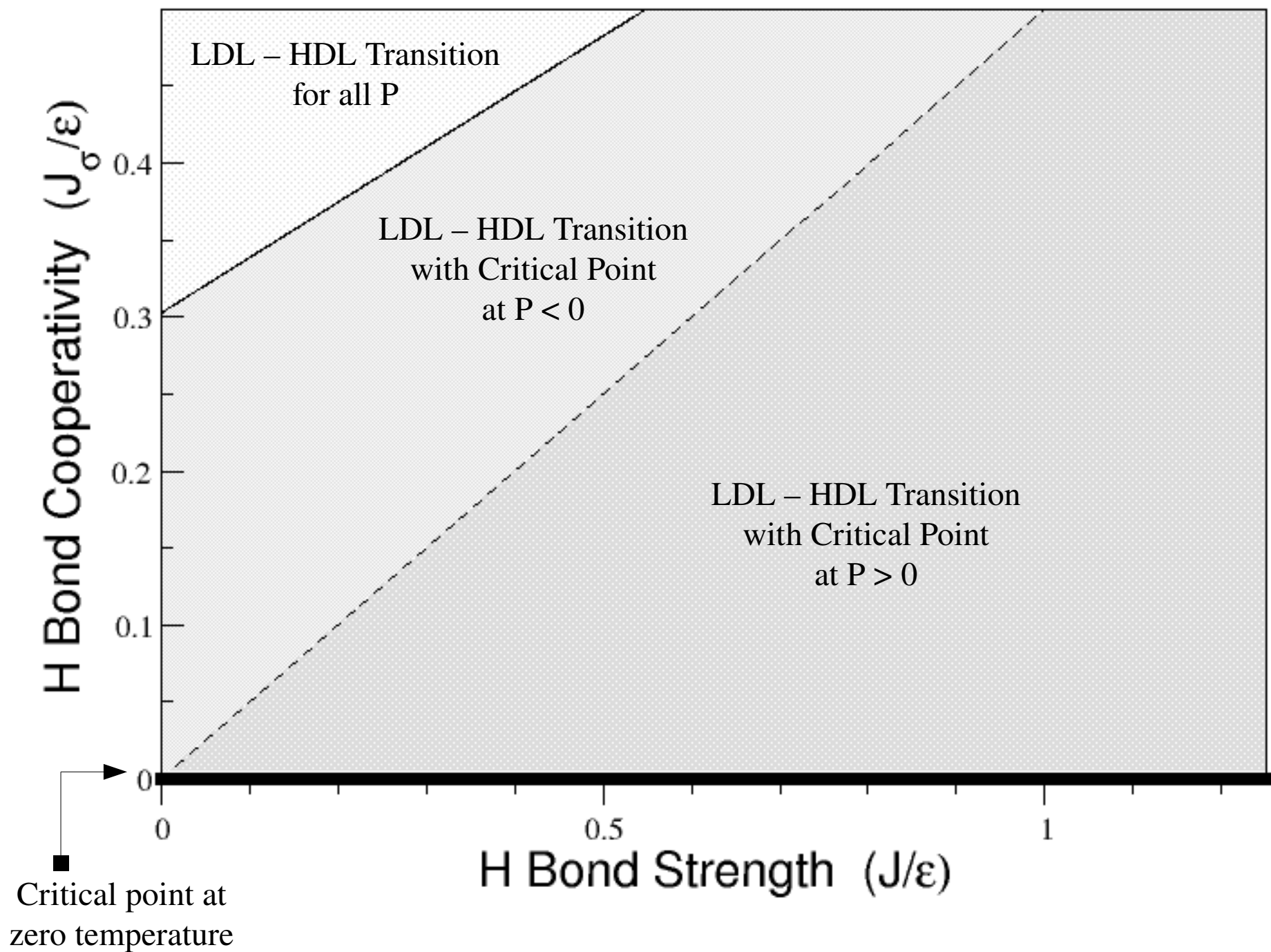
K. Stokely, M. G. Mazza, H. E. Stanley, and G. Franzese
"Effect of Hydrogen Bond Cooperativity on the Behavior of Water"
Proc. Natl. Acad. Sci. USA 107, 1301 (2010)











Take Home Message:

Model = Lattice Gas + Hydrogen Bonds

Several low temperature phase behaviors arise,
depending on the relative strength of the
pair and many-body H bond energies.

K. Stokely, M. G. Mazza, H. E. Stanley, and G. Franzese
Proc. Natl. Acad. Sci. USA 107, 1301 (2011).

