

N. R. Bernardino^{1,2} and M. M. Telo da Gama^{1,2}

¹ Centro de Física Teórica e Computacional, Avenida Professor Gama Pinto 2, P-1649-003 Lisboa, Portugal

² Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, P-1749-016 Lisboa, Portugal

nelsonrb@cii.fc.ul.pt

1. Abstract

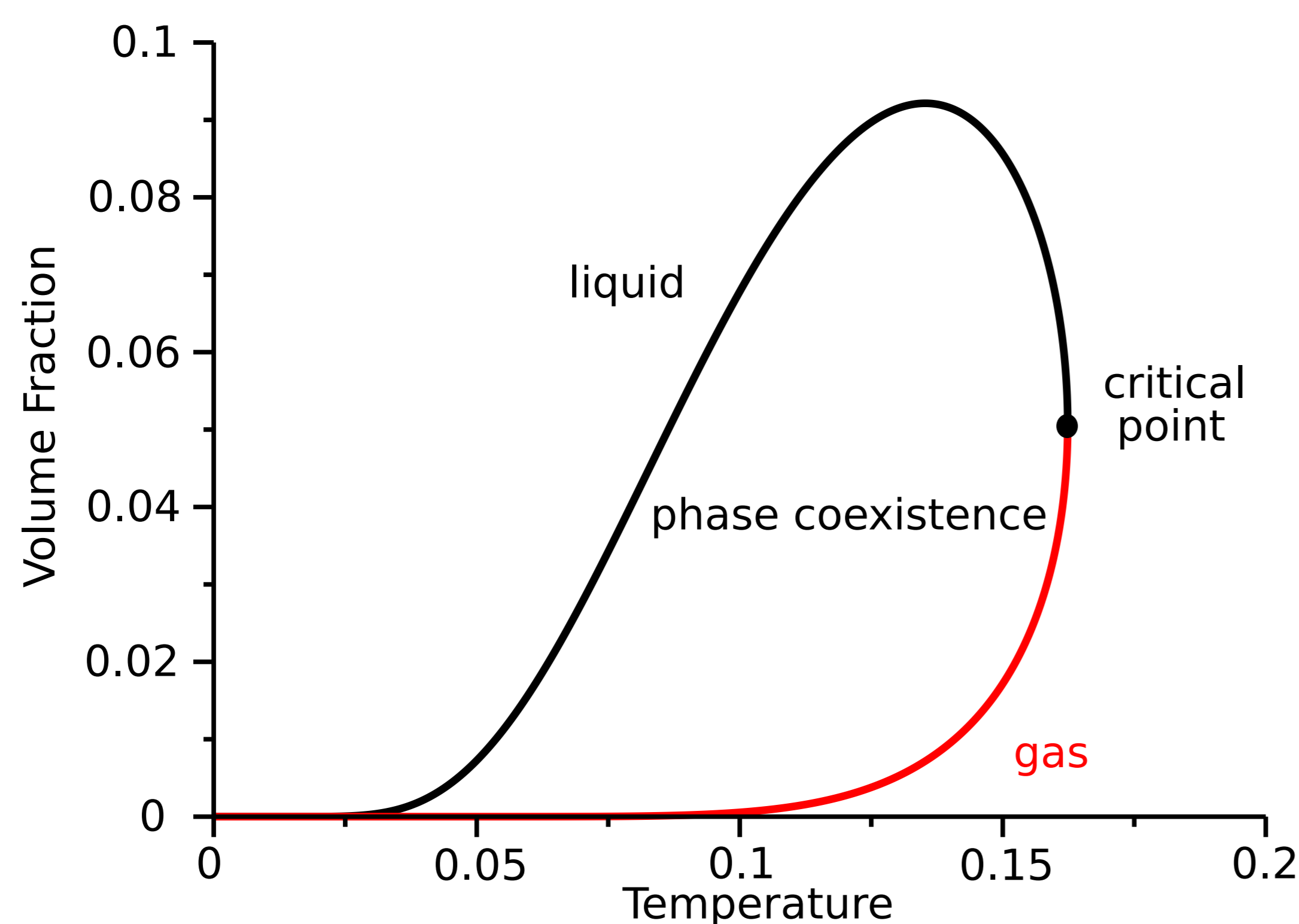
- ◆ We study the wetting properties of associating fluids.
- ◆ Associating fluids (such as patchy colloids or micro-emulsions) can have a re-entrant phase diagram.
- ◆ The re-entrance in the phase diagram leads to “funny” wetting properties.
- ◆ All the properties can be calculated with a very simple model.

2. Introduction: Associating Fluids

- ◆ Several important soft materials fall under the category of *associating fluids*.
- ◆ These associating fluids are fluids whose components can *aggregate* in larger components, such as chains. Examples include *dipolar fluids*, *micro-emulsions*, *patchy colloids*, etc [1,2].
- ◆ There is a certain *universality* of the thermodynamic behaviour of these fluids, because the thermodynamics is dominated by *chaining* and *branching* of the components.
- ◆ This universality is well captured by a simple Landau-Safran [1] free energy density:

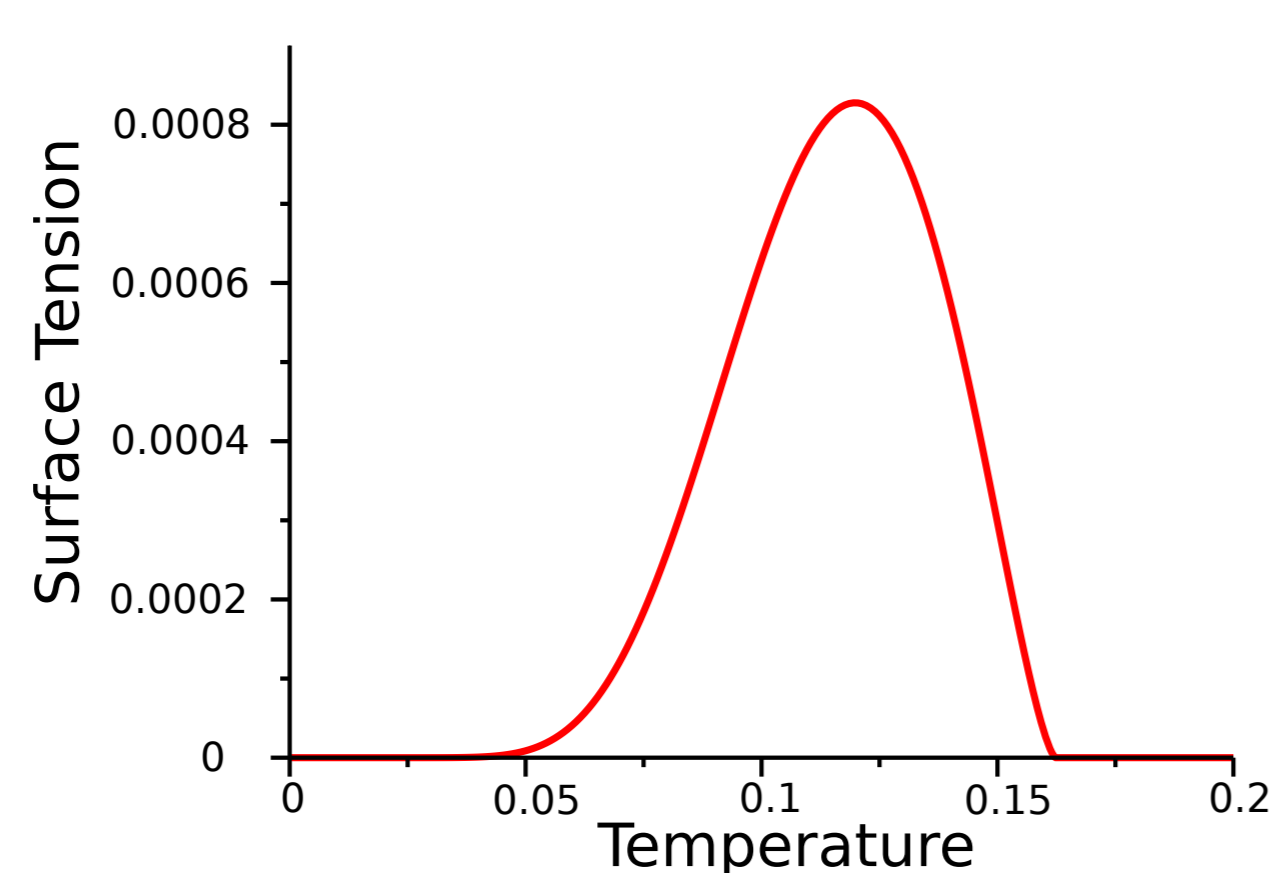
$$f = -(2\phi)^{1/2}e^{-\varepsilon_1/T} - 1/3(2\phi)^{3/2}e^{-\varepsilon_2/T} + 1/2\phi^2$$

- ◆ This free-energy leads to the re-entrant phase diagram below:

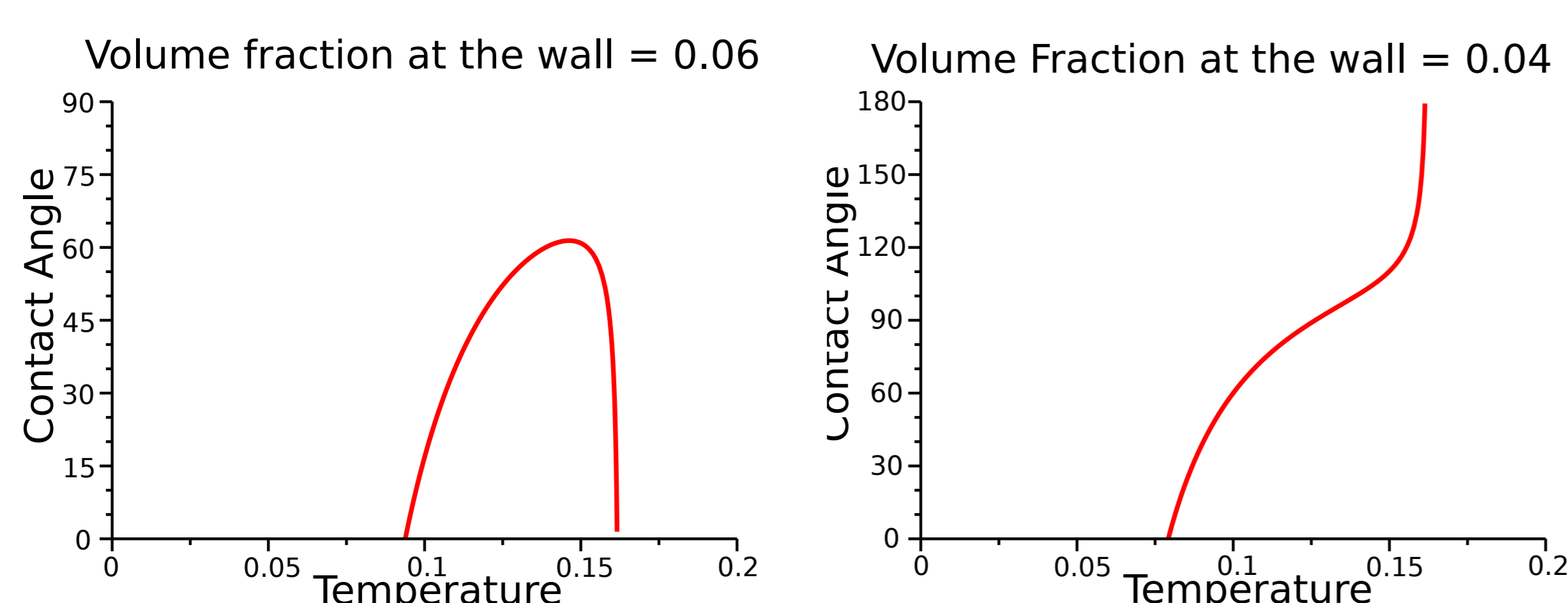


3. Surface Tension and Contact Angle

- ◆ Liquid-gas surface tension:

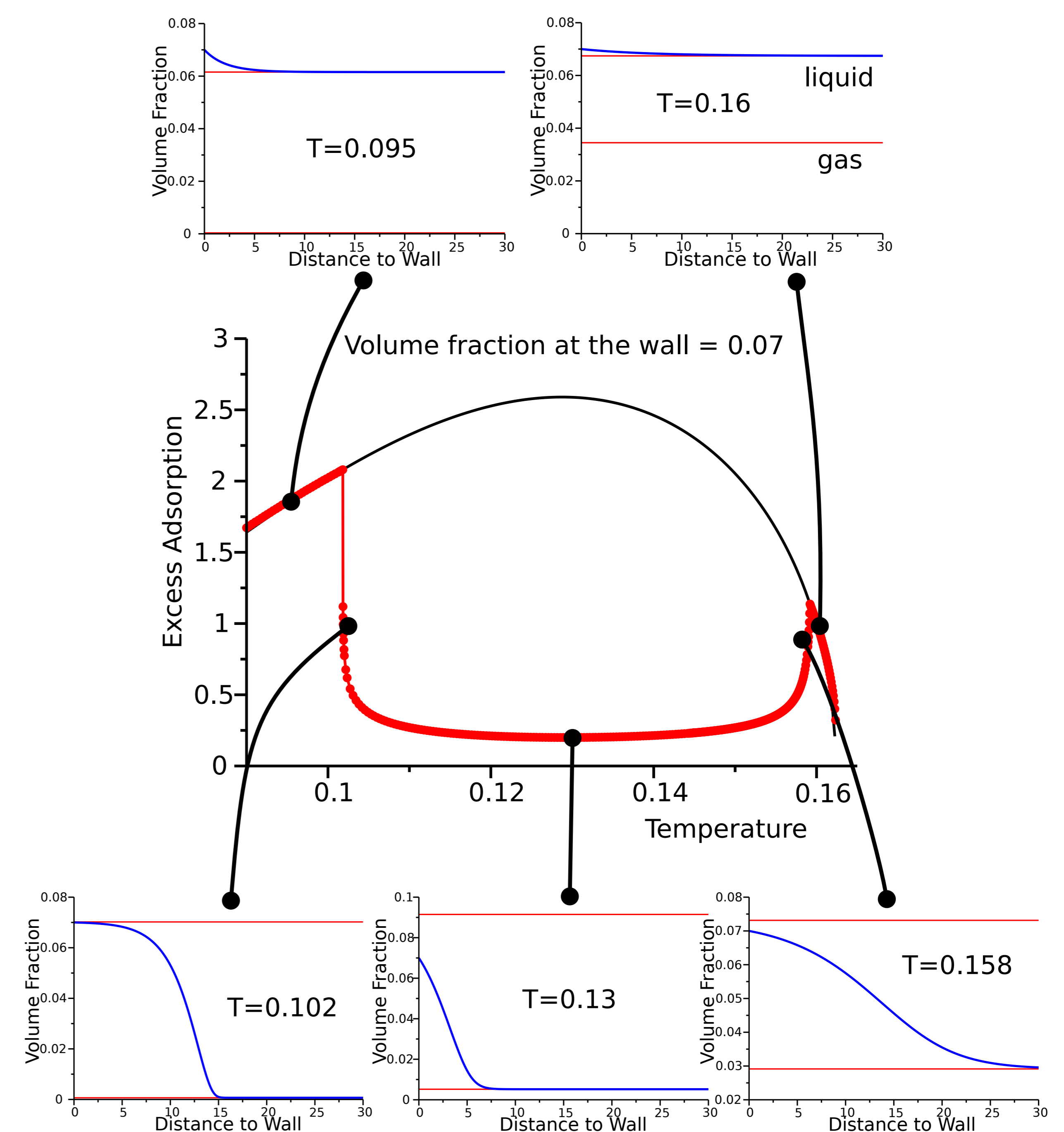


- ◆ Contact angle:



4. Adsorption and Wetting Transitions

- ◆ Two “colliding” wetting transitions:



5. Simple Minded Calculations

- ◆ All these features are captured by the World’s Simplest DFT: Double-Parabola Landau Theory:

$$\Omega = \text{Min}[1/2(\phi - \phi_{\text{gas}})^2, 1/2(\phi - \phi_{\text{liquid}})^2]$$

with $\phi_{\text{gas}} = 1$ and $\phi_{\text{liquid}} = 2(1 - (T - 1)^2)$.

- ◆ With this simple model we can calculate everything, at mean-field level, including surface tensions, contact angles, density profiles, and properties of the wetting transitions.

- ◆ It is a clean, pedagogical, example to learn wetting phenomena.

6. Conclusions

- ◆ Interesting interfacial properties of associating fluids due to re-entrance in the phase diagram, also observed in [3].
- ◆ Re-entrant wetting, with the “collision” of two wetting transitions.
- ◆ We can calculate all the interesting properties with the World’s Simplest DFT: Double-Parabola Landau Theory.

7. References & Acknowledgements

- [1] T Tlusty and SA Safran, *Science*, **290**, 1328 (2000).
 [2] JM Tavares, PIC Teixeira, and MM Telo da Gama, *Mol Phys*, **107**, 453 (2009).
 [3] C Pérez, P Roquero, and V Talanquer, *J Chem Phys*, **100**, 5913 (1994);
 CM Chen, MC Yeh, and LJ Chen, *J Phys Chem B* **110**, 3294 (2006).

We acknowledge financial support from the Portuguese Foundation for Science and Technology (SFRH/BPD/63183/2009 and PEst-OE/FIS/UI0618/2011) and helpful insights from José Maria Tavares.