Finding the arbitrary parameter L in Renormalization Group Theory

VIA fitting Monte Carlo simulations to Statistical Associating Fluid Theory

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Exploring Phase Equilibrium with Statistical non-Associating Fluid Theory:

A Generalized Renormalization Group Theory Approach.

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Abstract

Abstract goes hereeee!

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Chapter 1

Introduction

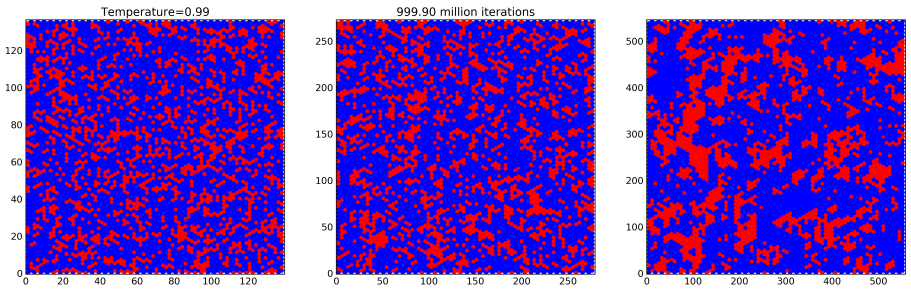
1.1 Introduction

Outline: Introduction to liquid vapor coexistence Demonstrate the problem Fix the problem what I did

The liquid-vapor phase coexistence can be found by just depositing some liquid into a sealed container. Some of the liquid will evaporate into the jar creating a vapor pressure. Provided there is enough liquid to create the necessary vapor pressure, the system will now contain both a liquid and a vapor at the same time. By sealing the liquid into a jar, we have forced the pressure of the liquid to be the same as the pressure of the gas. By allowing the atoms in the liquid to evaporate into a gas, we have also allowed the chemical potential of the liquid to be the same as the chemical potential of the gas.

Although we can find the phase coexistence by physically sealing a liquid in a jar, another method is to model the liquid using an experimentally derived model. The benefit to this method is a few observations can be used to find the parameters, and the parameters can then be used in simulations to find the rest of the coexistence curve.

To find the coexistence curve computationally, the liquid phase is usually considered to be separate from the vapor phase. This is a perfectly reasonable assumption since the surface tension normally keeps the liquid phase separate from the vapor phase. Unfortunately as the liquid approaches the critical point, the density of the liquid approaches the density of liquid. This means the surface tension decreases towards zero as the liquid approaches the critical point. This is unfortunate since the classical behavior of liquid separate from the vapor is no longer valid (see figure 1).



Although figure 1 shows an extreme example of liquid completely mixing with vapor, even under normal circumstances there exist natural fluctuations in the density of either phase. The most basic theory will deal with interactions at the shortest wavelength simply because fluctuations happen at the shortest wavelength first. The problem is that as we approach the critical point, the fluctuations grow in length scale. Fortunately there exists a method called renormalization group theory to deal with interactions on the longer length scale.

Renormalization group theory deals with the variations in density by finding the energy associated with each wavelength and each amplitude. The idea is the partition function will now sum over wavelengths and amplitudes. Forte et al. simplify the sum, but the problem is RGT contains an arbitrary initial wavelength. This initial wavelength is usually fit to the observables, but this introduces yet another free parameter since we can already change the potential used to characterize the fluid.

This project explores if it is possible fix this initial wavelength by comparing theory to Monte Carlo simulations. A Monte Carlo simulation involves putting atoms within a box and finding the density of states. The idea is that a Monte Carlo simulation at a small box size only incorporates interactions at the shortest wavelength, yet a simulation with a large box size will incorporate interactions at both short wavelengths and long wavelengths. This corresponds with how the most basic theory incorporates only short wavelength interactions, while renormalization group theory incorporates both short and long wavelength interactions. By changing the size of the box in a Monte Carlo simulation, we should be able to transition from SAFT to renormalization group theory; it is this transition that should represent the arbitrary parameter L within renormalization group theory.

Test of fancyhdr page.

Chapter 2

Methods

Outline: SAFT
liquid-vapor+run-absolute
How comparisons were made

2.1 SAFT

SW.fid+SW.fdisp+SW.fhs Explain.

2.2 Monte Carlo

Just use similar terms as SAFT, the Monte Carlo simulations are partitioned into two regimes: the excess entropy $S_{exc.\infty}$ as temperature approaches ∞, and the normalized excess free energy $F_{exc} + T \cdot S_{exc.\infty}$.

2.2.1 $S_{exc.\infty}$

The excess entropy as temperature approaches ∞ can be found by the observation that the square-well fluid is basically the same as a hard sphere model when the temperature is ∞. Which means at infinite temperature, the excess entropy of the hard sphere model should be the same as the excess entropy for the square-well fluid.

To find the excess free entropy of the hard sphere, we can make another observation that a hard sphere model at extremely low densities is basically the same as an ideal gas. The entropy of an ideal gas is well known, so we start with N atoms in an infinitely large box that also happens to be at infinite temperature. The box and all atom positions within the box are scaled to a smaller size. If the physical size of each atom were zero, then this squeezing process would be 100% successful; now the ideal gas entropy is already taken into account, so such a system would actually have no change in excess entropy. On the other hand, if there is a physical size to each atom, then such a scaling of the box would sometimes lead to failure. This failure can be thought of as being due to the reduced volume that each atom can explore, so such a scaling actually decreases the entropy relative to the ideal gas entropy. Basically the higher the failure rate, the lower the change in entropy.

The exact details regarding the process can be... **MORE**

2.2.2 Normalized Free Energy

To define the normalized free energy, we first start with the definition for free energy:
$F = U - T \cdot S$
now add zero: $F = U - T \cdot S + T \cdot S_{exc.\infty} - T \cdot S_{exc.\infty}$
rearrange: $U - T \cdot (S - S_{exc.\infty}) - T \cdot S_{exc.\infty}$
to find $S - S_{exc.\infty}$ note that: $S = -(\frac{\partial F}{\partial T})_{V,N}$

Chapter 3

GRG Theory

3.1 GRG Theory

Some more splaining.

And also a citation example [1].

And this one too [2]

Chapter 4

Data

4.1 Computation

Provide computation methods and data of what I have done so far.
This is how you can refer to fig 4.1.

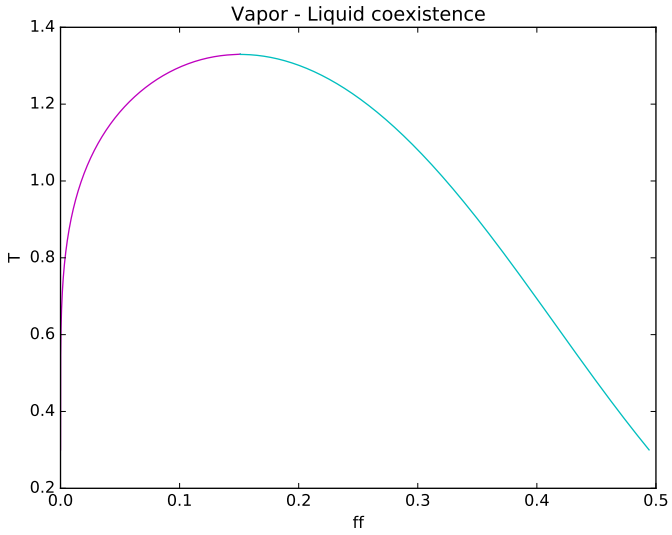
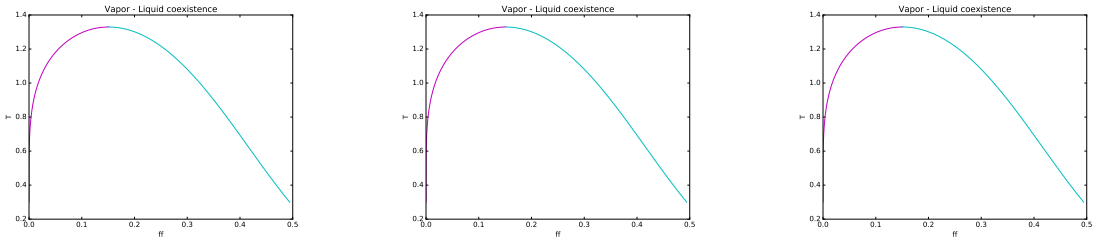


Figure 4.1: Caption for this image.



(a) Caption 01 (b) Caption 02 (c) Caption 03

Figure 4.2: Caption for all three.

Chapter 5

Conclusion

5.1 Conclusion

ta-da!