

# **Finding the arbitrary parameter $L$ in Renormalization Group Theory**

VIA fitting Monte Carlo simulations to Statistical  
Associating Fluid Theory

**Billy Edward Geerhart III**

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Department of Physics  
Oregon State University  
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# **Exploring Phase Equilibrium with Statistical non-Associating Fluid Theory:**

A Generalized Renormalization Group Theory Approach.

**Ryan M. Scheirer**

## **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 arbitrary L+outline rest of paper

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 vapor at the same time. A typical thermodynamics problem will first find the free energy of the liquid by itself, then find the free energy of the vapor by itself, and finally minimize the total free energy while keeping the total number of atoms between the liquid and solid at a constant  $N$ . By keeping the atoms in a sealed box we are enforcing the  $Pressure_{liquid} = Pressure_{vapor}$ , and by allowing the atoms to move between liquid and vapor state we are enforcing that  $Mu_{liquid} = Mu_{vapor}$ .

The typical thermodynamic analysis of treating each phase as a separate entity is usually fine under normal conditions, but a problem occurs as the liquid approaches the critical point. The critical point occurs as the temperature of the liquid is raised; this causes thermal vibrations in the liquid to reduce the liquid density, and it also causes a denser vapor as the atoms are able to escape the surface of the liquid easier. Basically this causes the density of the liquid to approach the density of the gas as the system reaches the critical point.

\*expand using 2d liquid and vapor graphs near critical point\*

Near the critical point the liquid and vapor states start to mix, which means the typical thermodynamic analysis of treating each phase separately no longer works. One method to get around this problem is called renormalization group theory (RGT). RGT recognizes that oscillations in the density occur at all temperatures rather than just at the critical point. These oscillations should naturally have an energy associated with them, so RGT starts with the first approximation of treating a liquid/vapor as a single phase, but then applies thermodynamics to the oscillations.

\*\*ADD MORE\*\*

Within RGT, the oscillations are found by starting at a particular box size called  $L$ . The oscillations within a box of length  $L$  can't have oscillations longer than the size  $L$  simply because of the periodic boundary conditions. The calculations usually start at a small box of length  $L$  to find the short wavelength oscillations, then double the box size to find even longer wave length oscillations. The problem is this

box length  $L$  is usually an arbitrary parameter that needs to be fit to either the experimental data or to large Monte-Carlo simulations. An alternative approach is to realize the base theory that RGT revolves around already contains the smallest scale oscillations. The alternative approach exploits this by trying to fit Monte-Carlo simulations to SAFT. To do this the box size is varied until the Monte-Carlo simulations can recreate the thermodynamics of SAFT. \*add more\*

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  $\infty$ , 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  $\infty$  can be found by the observation that the square-well fluid is basically the same as a hard sphere model when the temperature is  $\infty$ . 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  $S_{exc.\infty}$  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.

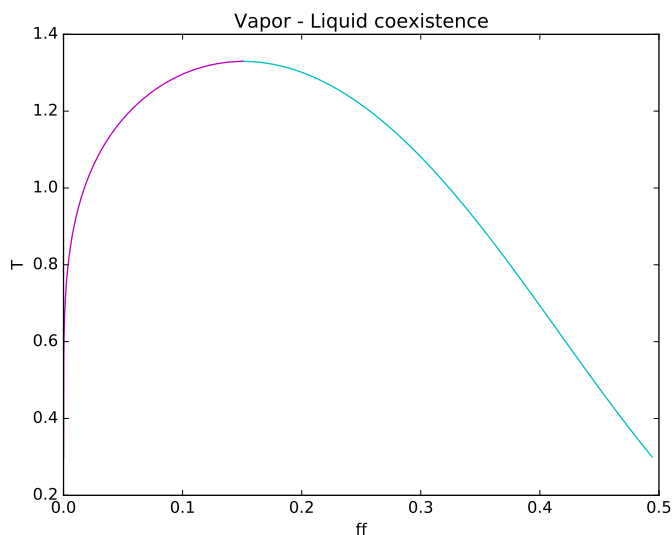
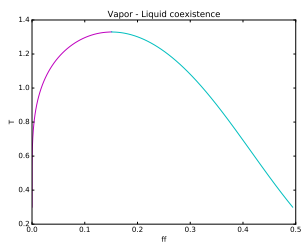
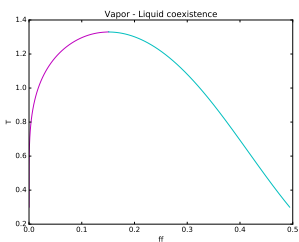


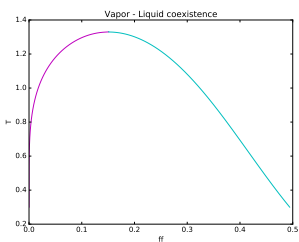
Figure 4.1: Caption for this image.



(a) Caption 01



(b) Caption 02



(c) Caption 03

Figure 4.2: Caption for all three.

# Chapter 5

## Conclusion

### 5.1 Conclusion

ta-da!