Fermi-Jagla Potential – A spherically symmetric potential mimics water

Zhiqiang Su

Advisor: H. Eugene Stanley
Collaborator: Sergey V. Buldyrev
Outline

• **Introduction**
  – Water
  – Jagla model
  – Fermi-Jagla model

• **Methods**
  – Fermi-Jagla model with Discrete Molecular Dynamics (DMD)

• **Results**
  – The Liquid Liquid Critical Point (LLCP)
  – The isobaric specific heat ($C_{lp}$) of Fermi-Jagla Liquid
  – Phase Flipping of Fermi-Jagla Liquid

• **Conclusion**
Intro: Water -- A Mysterious Liquid

Water has more than 60 anomalies (http://www.lsbu.ac.uk/water/anomalies.html)
Intro: Water -- Liquid-Liquid Phase Transition

Hypothesis
(Poole/Sciortino/Essmann/Stanley, 1992)

• Two liquids below nucleation temperature:
  – Low density liquid (LDL)
  – High density liquid (HDL)
  – Low density amorphous (LDA)
  – High density amorphous (HDA)

• Separated by liquid-liquid phase transition

• Ending in liquid-liquid critical point

Cover of JPC, volume 115, 8 Dec 2011
Intro: The Widom line of Real Water

In real water, the Widom Line has a negative slope.
Intro: Jagla Model

- $b = 1.72a$, $c = 3a$
Intro: Jagla Model -- Isochores

- Coexistence line has a positive slope, unlike real water.

Intro: The difference between Real Water and Jagla Liquid

In real water, the Widom Line has a negative slope. Xu et al. PNAS, V102, P16558 (2005)
Intro: Fermi-Jagla Model

- Can reproduce the water anomalies.
- Has LLCP
- May have Widom line with a negative slope
- Temperature of $C \downarrow \rho \uparrow$ maximum cannot be reached!!


\[
U(r) = \epsilon_0 \left[ \frac{(a/r)^n + \frac{A_0}{1 + \exp\left[\frac{A_1}{A_0}(r/a - A_2)\right]}}{1 + \exp\left[\frac{B_1}{B_0}(r/a - B_2)\right]} \right]
\]  

(1)
Method: Fermi-Jagla model in DMD

- Goals:
  - reach maximum of $C\downarrow p\uparrow$
  - Negative slope,

- Method: Fermi-Jagla model in Discrete molecular dynamics (DMD)
Result I: Isochores of Fermi-Jagla Liquid
Result II: Isotherms of Fermi-Jagla Liquid

- LLPT locates at $T_c=0.123$, $P_c=0.7481$.
- The Widom line may have a negative slope.
  We calculate the maximum temperature of $\mathcal{C}_\rho$ to verify this.
Result: $C_{\downarrow p}$ $(P>P_C)$

As the pressure increases, the temperature of maximum $C_{\downarrow p}$ shifts to a lower value, which implies that the Widom line has a negative slope.
As the pressure increases, the temperature of maximum $C_p$ shifts to a lower value, which implies that the Widom line has a negative slope.
Result: Phase flipping example

- At $P=0.75076 (> P_c)$ and $T=0.119$
Result: Phase flipping region
Conclusion

• We have found a symmetric potential that can reproduce a negative-slope of the Widom line
• We found the phase flipping phenomena in the region around the LLCP
Future Work

- Decide the phase flipping region
- Using the Fermi-Jagla potential to build a dimer model for methanol
Fitting Isochores to get Temperatures of $C_p_{\text{max}}$ and $K_{T\text{-max}}$