Projects

van der Waals EOS

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JUST

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projects

1. Chaos theory
2. Linear Algebra
3. Multiple Integration
4. Schrodinger Equation
5. Monte-Carlo Integration
6. van der Waals EOS (equilibrium points)

Equation of State

van der Waals EOS

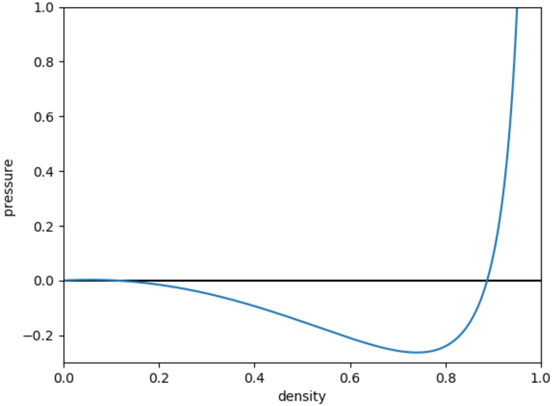
$$P = \frac{NRT}{V - Nb} - \frac{aN^2}{V^2}$$

$$P(n) = \frac{nT}{1 - n} - n^2$$

parameters

P : Pressure n : density (0,1)
T : Temperature (0,1)

Equation of State



Method one

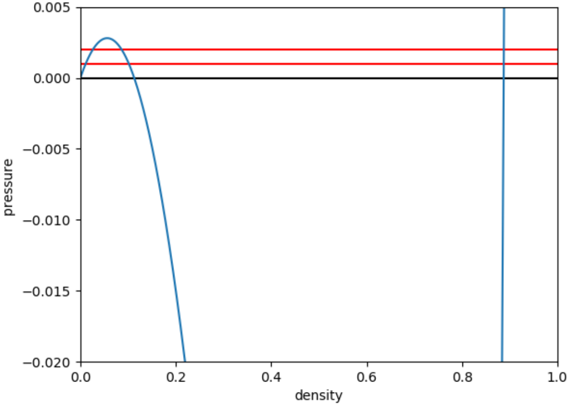
Equilibrium points of van der Waals EOS

Maxwell construction.

Algorithm

vary P slowly,
if the area above the curve equals the area under the curve,
stop
the end points are vapor and liquid densities,respectively.

Equation of State



Method two

at equilibrium

$$P(n_g) = P(n_l)$$

$$\mu(n_g) = \mu(n_l)$$

chemical potential

$$\mu(n) = -Tln(\frac{1}{n} - 1) + \frac{T}{1-n} - 2n$$

Algorithm

Newton-Raphson method for nonlinear system.

Method two

For more information about the algorithm, see the link below with example

link

https://link.springer.com/content/pdf/bbm%3A978-3-319-69407-8%2F1.pdf