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The van der Waals Fluid's liquid vapor coexistence locus, using Maxima/Gnuplot

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1 Abstract

The Maxima/Gnuplot code for plotting the van der Waals locus of liquid and vapor molar volumes as a function of pressure and temperature (all reduced) is presented. [2].

2 Introduction

The Sage equations from reference 2 which are used to plot the coexistence curve of liquid and vapor pressures and temperatures are re-interpreted here using Maxima (and Gnuplot).

Using Maxima, one can essentially employ Gnuplot to plot the same function as the original Sage material presented in papers 96 & 97 but employing more sophisticated annotations (among other things). The code (we actually use wxMaxima, not Maxima itself) is:

```
reset;
vg(x) := -1/6*(4*x*exp(2*x) - exp(4*x) + 1)*exp(x)/(x*exp(3*x) +
x*exp(x) - exp(3*x) + exp(x)) + 1/3 $

vl(x)  := -1/6*(4*x*exp(2*x) - exp(4*x) + 1)*exp(-x)/(x*exp(3*x) + x*exp(x) -
exp(3*x) + exp(x)) + 1/3$

T(d) :=
```

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[2]David, Carl W., "The van der Waals Fluid's liquid vapor coexistence locus" (2018). Chemistry Education Materials. 96 & 97. https://opencommons.uconn.edu/chem_educ/96&97

```
-27/4*((4*d*exp(2*d) - exp(4*d) + 1)*((4*d*exp(2*d) - exp(4*d) + 1)*exp(-d)
 /(d*exp(3*d) + d*exp(d) - exp(3*d) + exp(d)) - 2)^2*exp(d)/(d*exp(3*d) + d*exp(d) -
 exp(3*d) + exp(d)) + (((4*d*exp(2*d) - exp(4*d) + 1)*exp(d)/(d*exp(3*d) + d*exp(d) -
 exp(3*d) + exp(d)) - 2)^2 + 4*(4*d*exp(2*d) - exp(4*d) + 1)*exp(d)/(d*exp(3*d) +
 d*exp(d) - exp(3*d) + exp(d)) - 4)*((4*d*exp(2*d) - exp(4*d) + 1)*exp(-d)/
 (d*exp(3*d) + d*exp(d) - exp(3*d) +
 exp(d)) - 2) + 2*((4*d*exp(2*d) - exp(4*d) + 1)*exp(d)/
 (d*exp(3*d) +
 d*exp(d) - exp(3*d) + exp(d)) - 2)^2 +
 4*(4*d*exp(2*d) - exp(4*d) + 1)*exp(d)/(d*exp(3*d) + d*exp(d) - exp(3*d) +
 exp(d)) - 8)/(((4*d*exp(2*d) - exp(4*d) +
 1)*exp(-d)/(d*exp(3*d) + d*exp(d) - exp(3*d) + exp(d)) - 2)^2*((4*d*exp(2*d) -
 exp(4*d) + 1)*exp(d)/(d*exp(3*d) + d*exp(d) - exp(3*d) + exp(d)) - 2)^2);

  p(d) := 8*T(d)/(3*vg(d)-1)-3/vg(d)^2$
```

These last four equations were cut from the Sage output and pasted into the Maxima code; then a major editing was done to get exponentiation into Maxima acceptable form.

```
wxplot2d([vg(x),vl(x)],[x,0.1,1]);
wxplot2d(T(x),[x,0.1,1]);
wxplot2d(p(x),[x,0.1,1]);
s1:parametric(T(d),vg(d),p(d),d,0.0,0.9)$
s2:parametric(T(d),vl(d),p(d),d,0.0,0.9)$
draw3d(nticks=21,line_width=2,color=red,key="gas",s1,
  line_width=2,color=blue,key="liquid",s2,
  zlabel="p",xlabel="T",ylabel="v");
    /*wxdraw3 draws here; else draws in rotatable gnuplot window*/
draw_file(terminal =  'png, file_name = "~/Desktop/vdw5_out");
```

The results are shown in Figure 1 (below). Note that the default view was used.

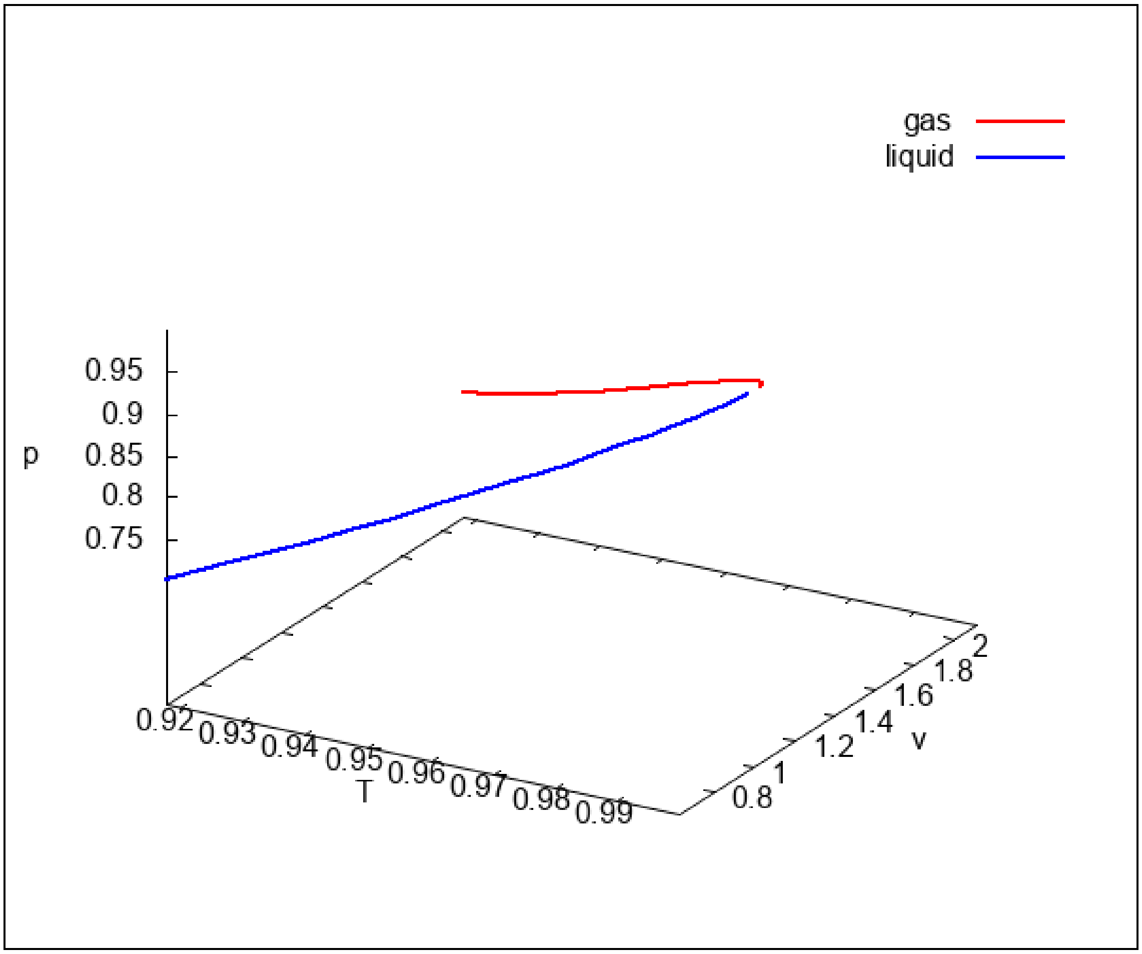

Figure 1: The full “3D” plot done using Maxima. The code shown does not work on a Windows 10 machine, only an Ubuntu equipped device. The non-closure of the two loci at (1,1,1) remains a mystery. (We remind the reader that these are reduced variables notwithstanding the labels show.) When running this code as actually shown, the plot shows up in a separate window, which allows the user to re-orient the plot using the mouse. The drawing shown here was generated by the last line of code.