Gráficas del fluido de van der Waals

Este es un archivo para el programa *Mathematica* por lo que se dejan indicadas las instrucciones.

La energía libre de Helmholtz (molar) de van der Waals es

$$f = -RT\left[\ln\frac{v-b}{N_0\lambda^3}+1\right]-\frac{a}{v} \quad \text{con} \quad \lambda=\frac{h}{\sqrt{2\pi mkT}}$$

Siempre que se tenga que realizar un cálculo numérico, primero hay que adimensionalizar. Para hacerlo, se necesitan tres cantidades para formar con ellas las unidades de masa, tiempo y longitud. Esto es equivalente a dar valores arbitrarios a tres constantes. Las demás cantidades quedan entonces expresadas en términos de ellas. Escogemos entonces,

$$R = 1, \; b = 1, \; a = 10.$$

Como tenemos la libertad de escoger la masa del átomo en cuestión, usamos

$$N_0\left(\frac{h}{\sqrt{2\pi mk}}\right)^3 = 1$$

Por lo tanto, la energía libre de Helmholtz adimensionalizada es

$$f = -t\left[\ln(v-1)+\frac{3}{2}\ln(t)+1\right]-\frac{10}{v}$$

con t y v la temperatura y volumen adimensionalizados.

La presión es

$$p = \frac{t}{v-1}-\frac{10}{v^2}$$

El potencial químico es

$$\mu = f + p\,v$$

El punto crítico es

$$p_c = \frac{10}{27} \quad v_c = 3 \quad T_c = \frac{80}{27}$$

Definiciones

In[117]:=
```
p[v_, t_] = t / (v - 1) - 10 / v^2;
```

In[118]:=
```
f[v_, t_] = - t (Log[v - 1] + 1.5 * Log[t] + 1) - 10 / v;
```

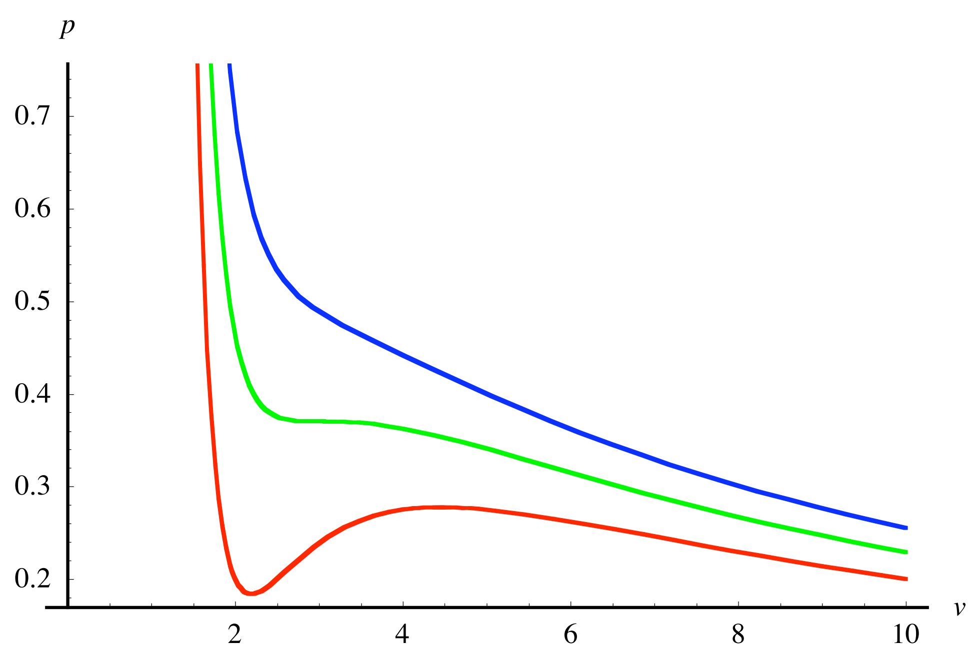
In[119]:=
```
g[v_, t_, p_] = f[v, t] + p * v;
```

In[167]:=
```
tc = 80 / 27;
pc = 10 / 27;
```

Figura 1

Isotermas de van der Waals para $T > T_c$(AZUL), $T = T_c$ (VERDE) y $T < T_c$(ROJO)

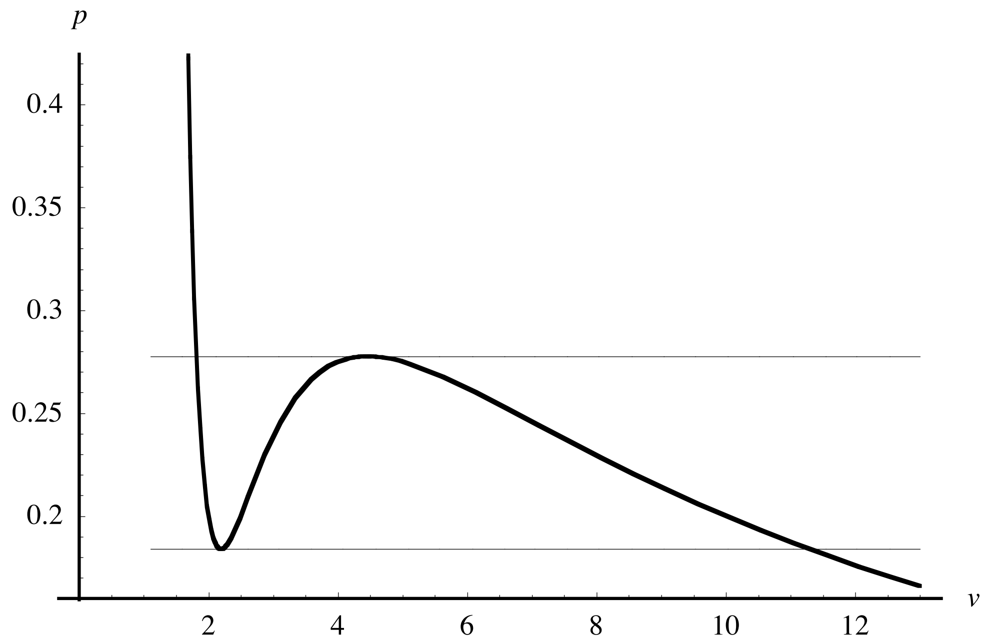
In[123]:=
```
Plot[{p[v, 2.7], p[v, tc], p[v, 3.2]}, {v, 1.5, 10},
 AxesOrigin → {0.0, 0.17}, TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, p}, PlotStyle →
  {{RGBColor[1, 0, 0], Thickness[0.005]}, {RGBColor[0, 1, 0], Thickness[0.005]},
   {RGBColor[0, 0, 1], Thickness[0.005]}}, AxesStyle → Thickness[0.004]]
```



Out[123]=
```
- Graphics -
```

Figura 2

Isoterma de van der Waals para $T < T_c$ (temperatura, t = 2.7)
Cálculo de (p_{max}, v_{max}) y (p_{min}, v_{min}) $\left(\frac{\partial p}{\partial v}\right)_T = 0$

In[125]:=
```
Solve[D[p[v, 2.7], v] == 0, v]
```
Out[125]=
```
{{v → 0.757678}, {v → 2.19426}, {v → 4.45547}}
```
In[144]:=
```
vmin = 2.19426;
vmax = 4.45547;
```
In[146]:=
```
pmax = p[vmax, 2.7];
pmin = p[vmin, 2.7];
```
In[159]:=
```
Plot[{p[v, 2.7], pmax, pmin}, {v, 1.1, 13}, AxesOrigin → {0., 0.16},
 TextStyle → {FontFamily → "Times", FontSize → 14}, AxesLabel → TraditionalForm /@ {v, p},
 PlotStyle → { Thickness[0.005], Thickness[0.001], Thickness[0.001]}
 , AxesStyle → Thickness[0.004]]
```


Out[159]=
```
- Graphics -
```

Figura 3

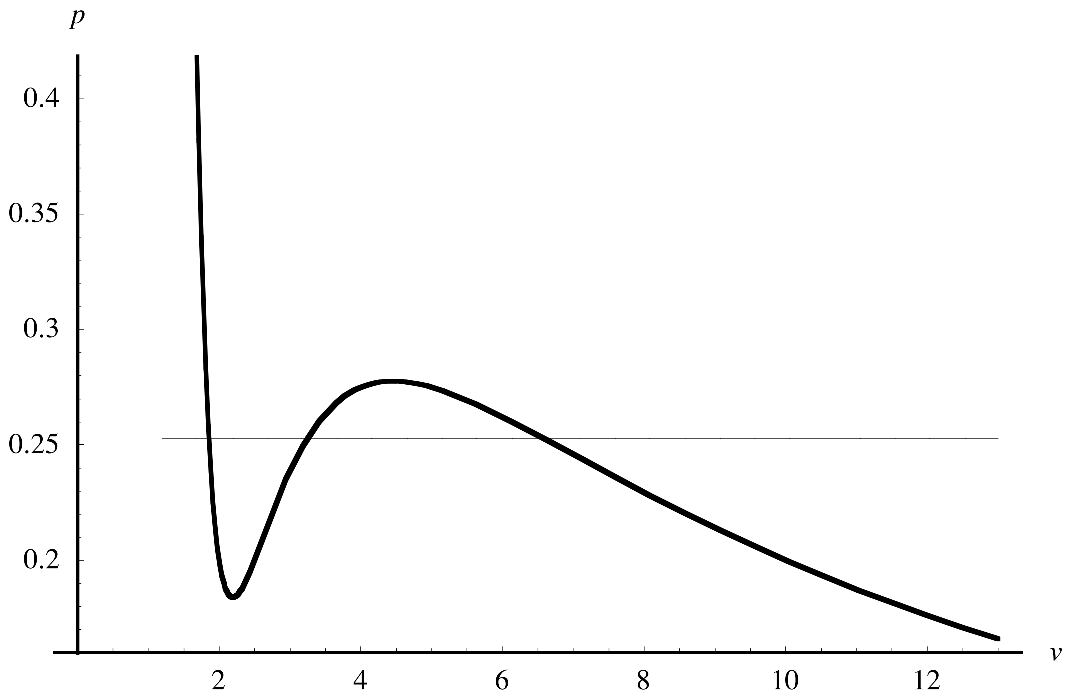
Isoterma de van der Waals para $T < T_c$ (temperatura, t = 2.7)
Cálculo de p_{coex}, v_l y v_g .Tales cantidades corresponde a la construcción de Maxwell de áreas iguales. Sin embargo, esto es equivalente a resolver simultánemante,
$p(v_l, T) = p(v_g, T)$ y $\mu(v_l, T) = \mu(v_g, T)$

In[149]:=
```
FindRoot[{f[x, 2.7] + p[x, 2.7] * x - f[y, 2.7] - p[y, 2.7] * y == 0, p[x, 2.7] - p[y, 2.7] == 0},
 {x, 1.8}, {y, 8}]
```
Out[149]=
```
{x → 1.85349, y → 6.59637}
```
In[150]:=
```
vl = 1.85349;
vg = 6.59637;
```
checando ...

In[154]:=
```
p[vg, 2.7]
```
Out[154]=
```
0.252634
```
In[155]:=
```
p[vl, 2.7]
```
Out[155]=
```
0.252634
```
In[156]:=
```
pcoex = p[vg, 2.7];
```

In[160]:=

```
Plot[{p[v, 2.7], pcoex}, {v, 1.2, 13}, AxesOrigin → {0., 0.16},
 TextStyle → {FontFamily → "Times", FontSize → 14}, AxesLabel → TraditionalForm /@ {v, p},
 PlotStyle → { Thickness[0.005], Thickness[0.001]}
 , AxesStyle → Thickness[0.004]]
```



Out[160]=

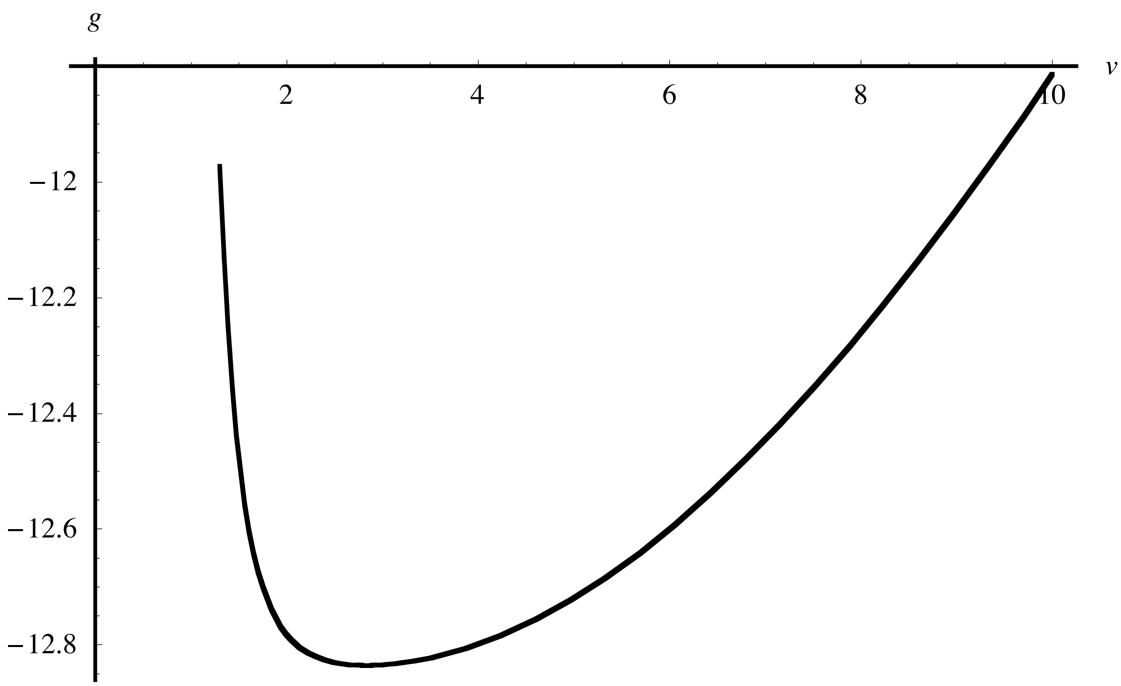
- Graphics -

Figura 4

$g(v; T, p) = f(v, T) + p\,v$ para $T > T_c$ (temperatura t = 3.2, presión p = 0.5)

In[161]:=

```
Plot[g[v, 3.2, 0.5], {v, 1.3, 10}, AxesOrigin → {0., -11.8},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



Out[161]=

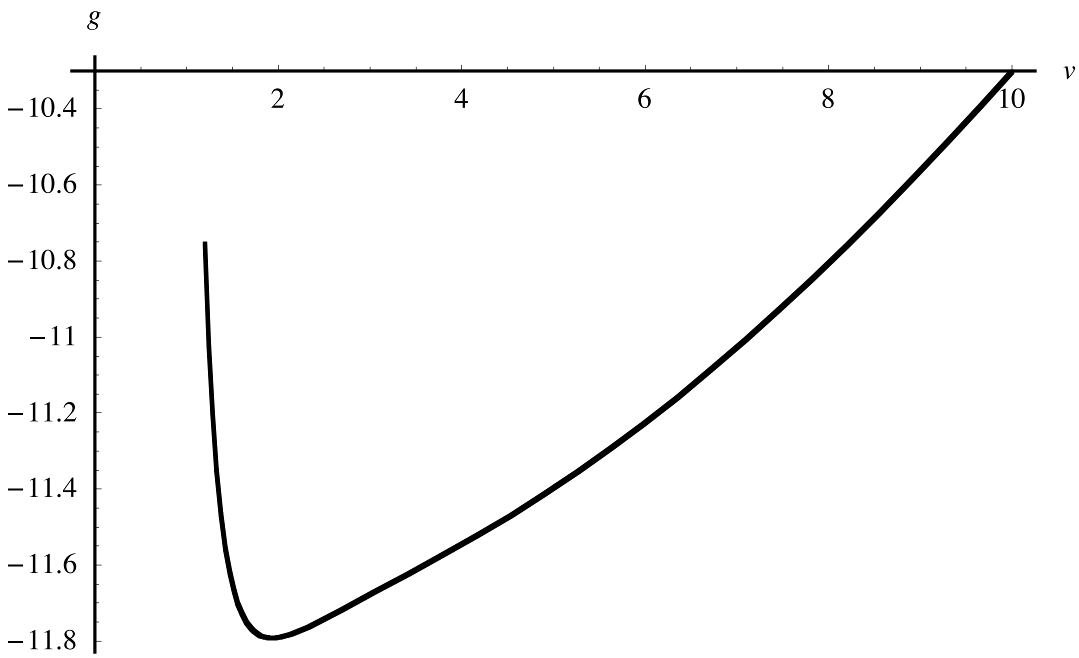
```
- Graphics -
```

Figura 5 (tres figuras)

$g(v; T, p) = f(v, T) + p\,v$ para $T = T_c$ y $p > p_c$ (temperatura tc = 80/27, presión p = 0.5)

In[170]:=

```
Plot[g[v, tc, 0.5], {v, 1.2, 10}, AxesOrigin → {0., -10.3},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



Out[170]=

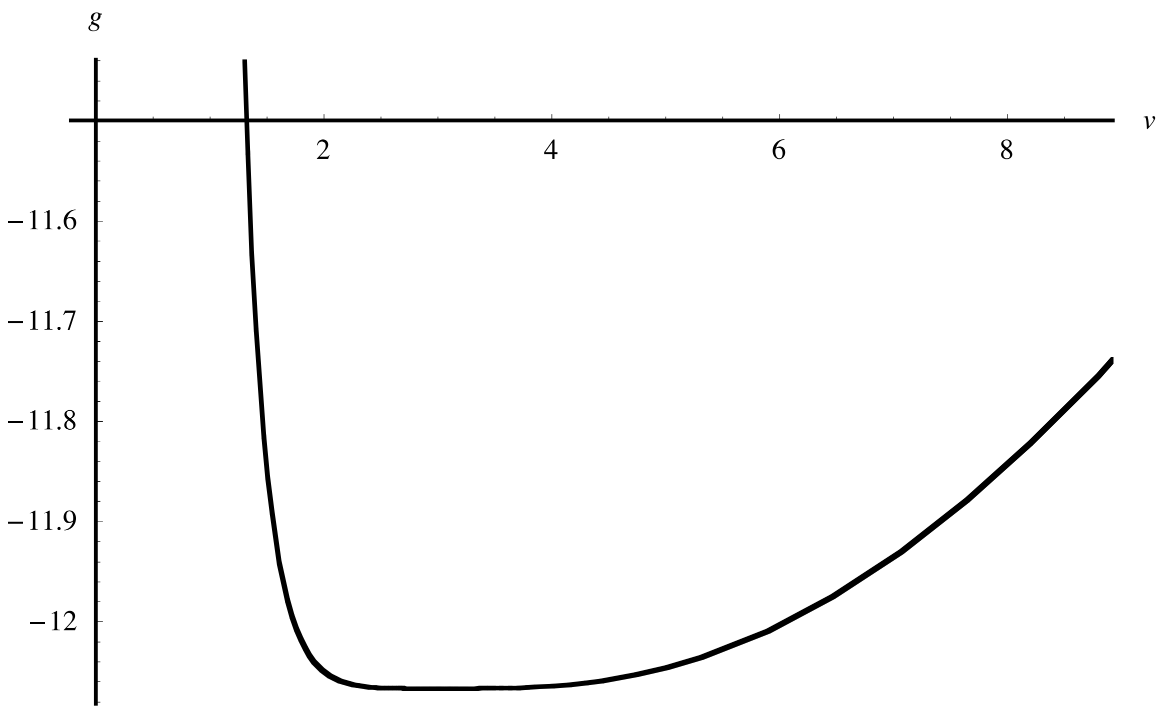
- Graphics -

$g(v; T, p) = f(v, T) + p\,v$ para $T = T_c$ y $p = p_c$ (temperatura tc = 80/27, presión pc = 10/27)

Note que el mínimo ocurre en vc = 3

In[169]:=

```
Plot[g[v, tc, pc], {v, 1.2, 15}, AxesOrigin → {0., -11.5},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```

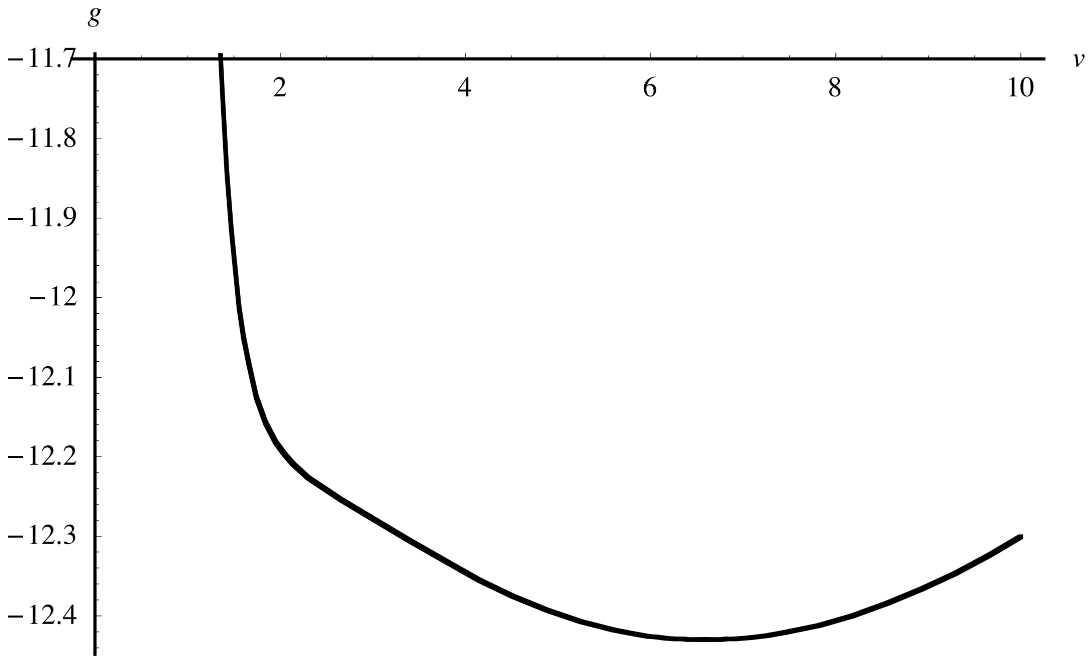


Out[169]=

- Graphics -

$g(v; T, p) = f(v, T) + p\,v$ para $T = T_c$ y $p < p_c$ (temperatura tc = 80/27, presión p = 0.3)

In[172]:=
```
Plot[g[v, tc, 0.3], {v, 1.2, 10}, AxesOrigin → {0., -11.7},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



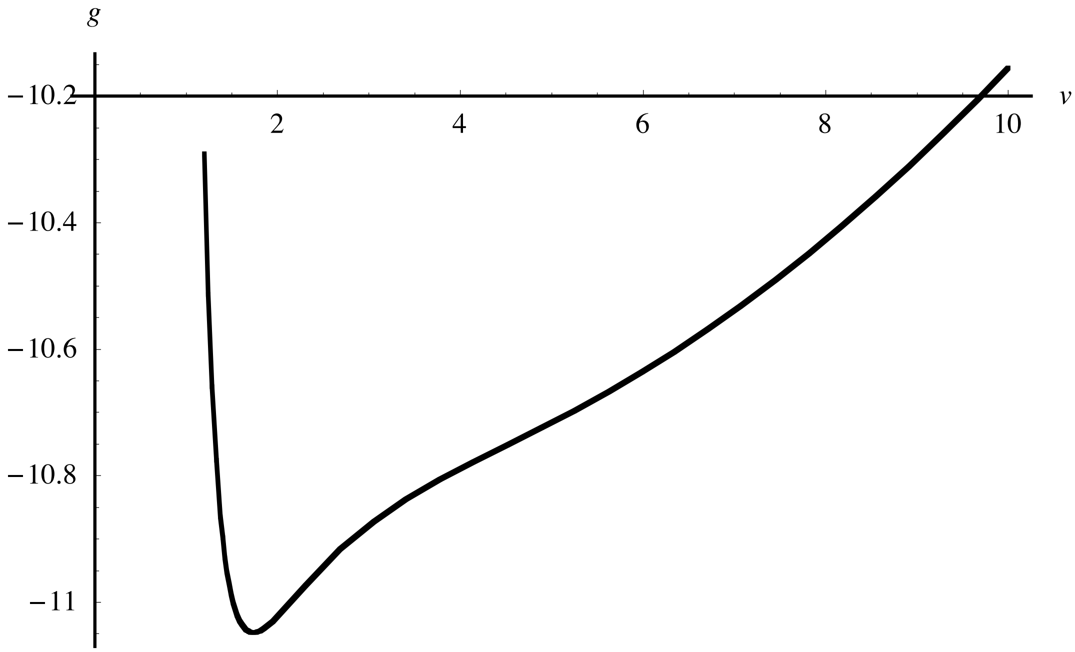
Out[172]=
```
- Graphics -
```

Figura 6 (seis figuras)

$g(v; T, p) = f(v, T) + p\,v$ para $T < T_c$ y $p > p_{max}$ (temperatura t =2.7, presión p = 0.35)

In[174]:=

```
Plot[g[v, 2.7, 0.35], {v, 1.2, 10}, AxesOrigin → {0., -10.2},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



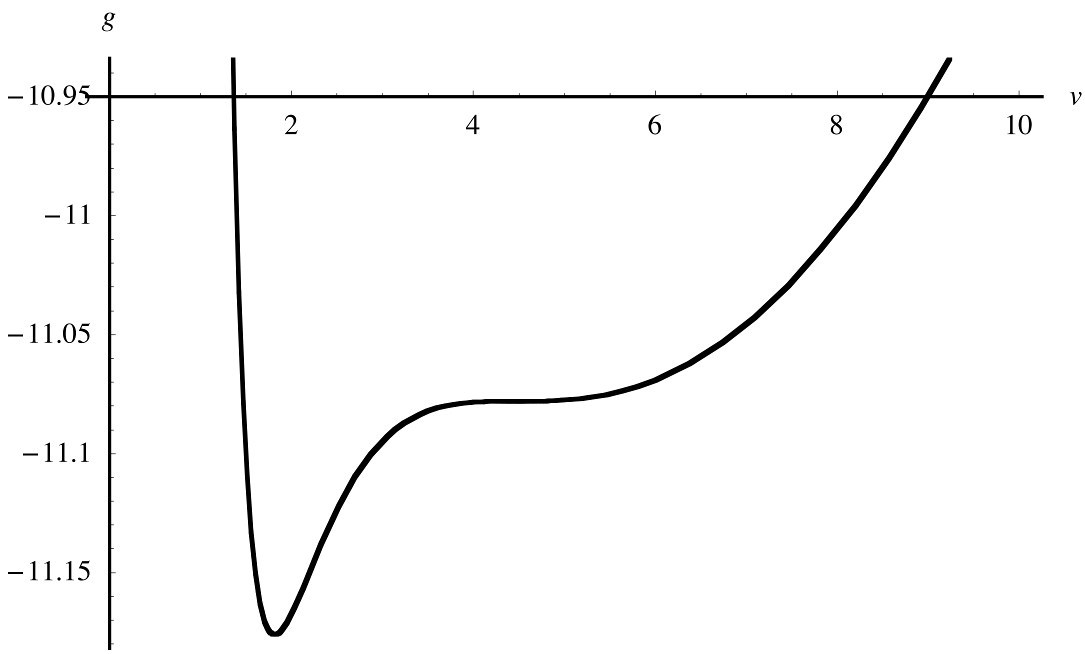
Out[174]=

```
- Graphics -
```

$g(v; T, p) = f(v, T) + p\,v$ para $T < T_c$ y $p = p_{max}$ (temperatura t =2.7, presión p = pmax)

In[177]:=

```
Plot[g[v, 2.7, pmax], {v, 1.2, 10}, AxesOrigin → {0., -10.95},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



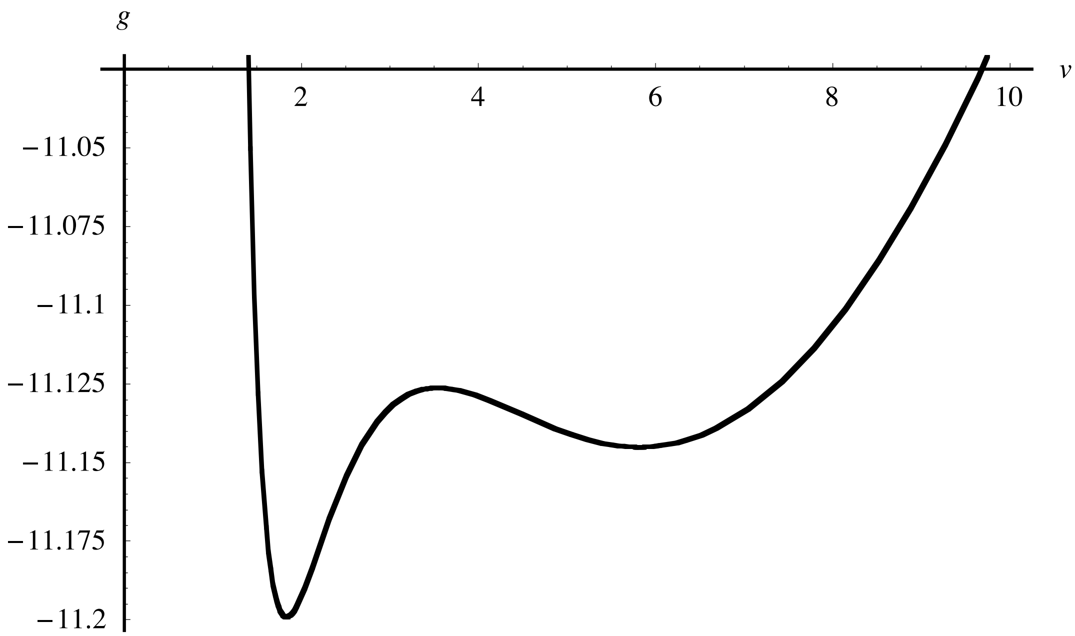
Out[177]=

- Graphics -

$g(v; T, p) = f(v, T) + p\,v$ para $T < T_c$ y $p_{max} > p > p_{coex}$ (temperatura t =2.7, presión p = 0.265)

In[179]:=

```
Plot[g[v, 2.7, 0.265], {v, 1.2, 10}, AxesOrigin → {0., -11.025},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



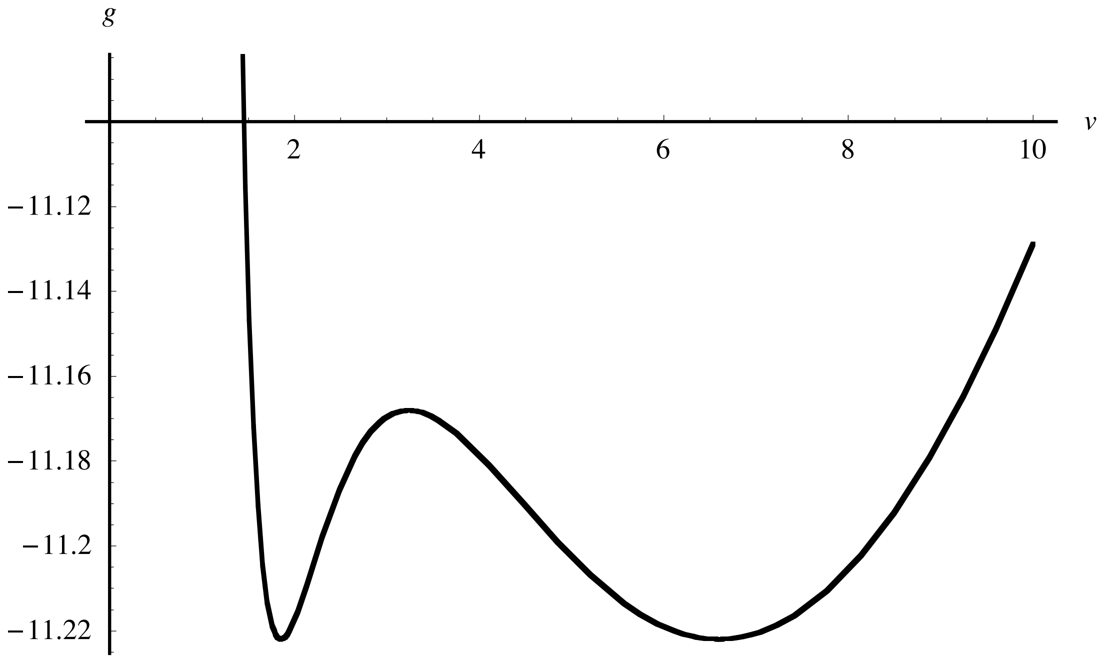
Out[179]=

```
- Graphics -
```

$g(v; T, p) = f(v, T) + p\,v$ para $T < T_c$ y $p = p_{\text{coex}}$ (temperatura t =2.7, presión p = pcoex)

In[181]:=

```
Plot[g[v, 2.7, pcoex], {v, 1.2, 10}, AxesOrigin → {0., -11.1},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



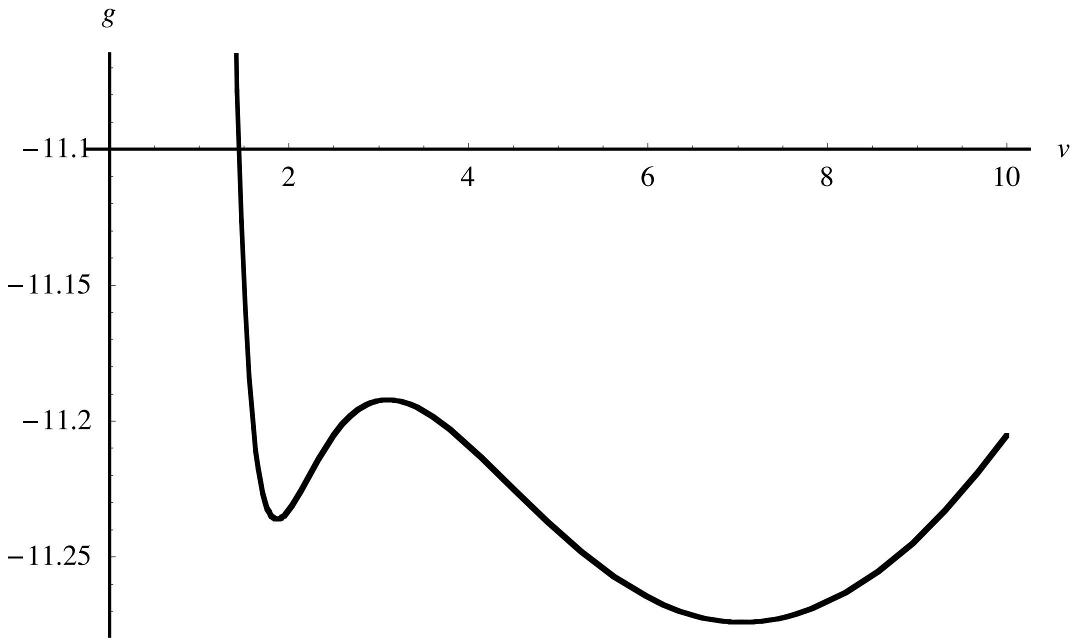
Out[181]=

- Graphics -

In[182]:=

$g(v; T, p) = f(v, T) + p\,v$ para $T < T_c$ y $p_{coex} > p > p_{min}$ (temperatura t =2.7, presión p = 0.245)

In[182]:=
```
Plot[g[v, 2.7, 0.245], {v, 1.2, 10}, AxesOrigin → {0., -11.1},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



Out[182]=
```
- Graphics -
```

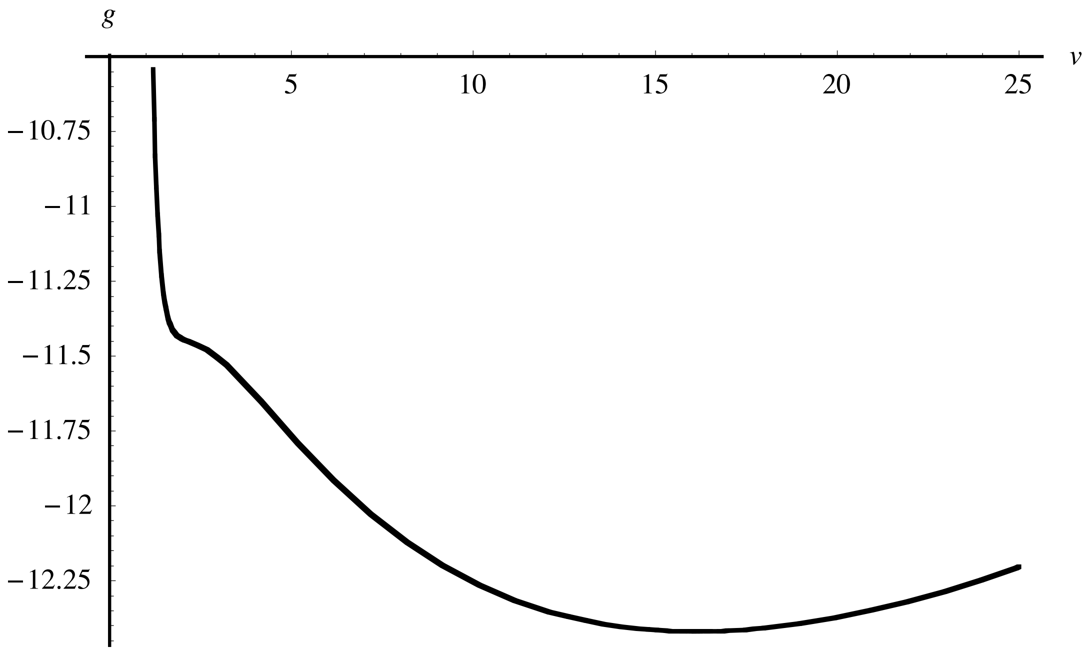
In[50]:= `p[2.194261904476178, 2.7]`

Out[50]= `0.183875`

$g(v; T, p) = f(v, T) + p\,v$ para $T < T_c$ y $p_{\min} > p$ (temperatura t =2.7, presión p = 0.14)

In[184]:=

```
Plot[g[v, 2.7, 0.14], {v, 1.2, 25}, AxesOrigin → {0., -10.5},
 TextStyle → {FontFamily → "Times", FontSize → 14},
 AxesLabel → TraditionalForm /@ {v, g}, PlotStyle → { Thickness[0.005]}
 , AxesStyle → Thickness[0.004]]
```



Out[184]=

```
- Graphics -
```

In[82]:=

```
Plot[{p[v, 2.9], p[v, 2.85], p[v, 2.8], p[v, 2.93], p[v, 80 / 27], p[v, 2.75]},
 {v, 1.7, 7}, AxesOrigin → {1.5, 0.21}, AxesLabel → None, Ticks → None, PlotStyle →
  {{RGBColor[1, 0, 0]} , {RGBColor[0, 1, 0]}, {RGBColor[0, 0, 1]}, {CMYKColor[0, 0, 1, 0]},
   {CMYKColor[0, 0, 0, 1]}, {CMYKColor[0, 1, 0, 0]}}, AxesStyle → Thickness[0.004]]
```