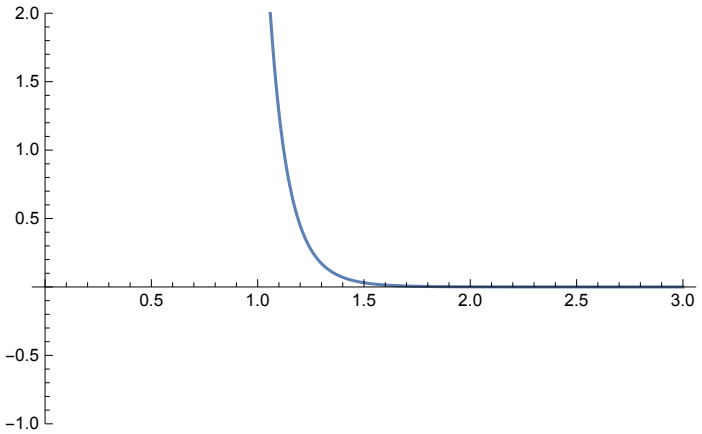
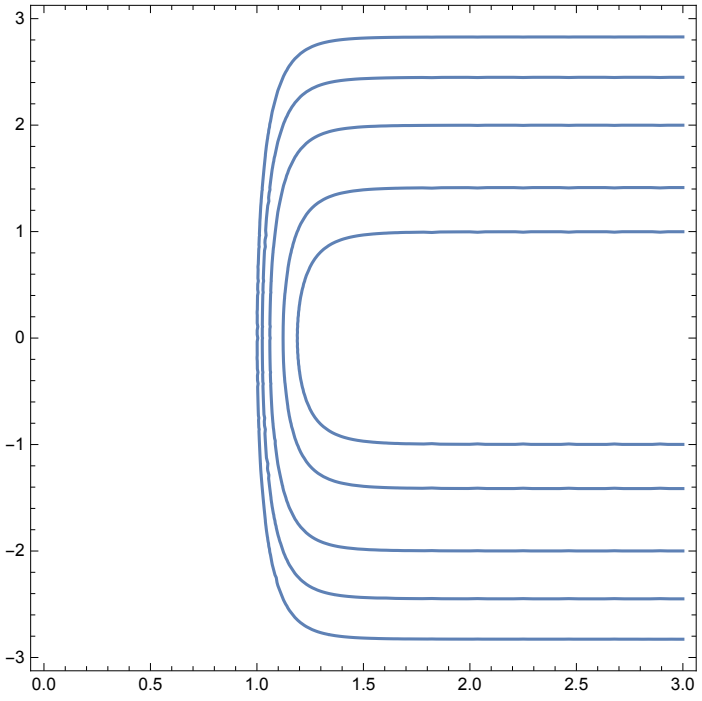
```
(* Lennard-Jones potential with a centrifugal term *)
a = 1.0; (* Depth of LJ well *)
l = 1.0; (* Angular momentum *)
v12[r_] = 4 * a / r^12; (* Repulsive hard-core potential *)
v6[r_] = -4 * a / r^6; (* Van der Waals potential *)
vCentr[r_] = 0.5 * l^2 / r^2; (* Centrifugal potential *)
t[p_] = 0.5 * p^2; (* Kinetic energy *)
vLJ[r_] = v12[r] + v6[r]; (* Lennard-Jones potential *)
v[r_] = vLJ[r] + vCentr[r]; (* Effective potential *)
f[r_] = -D[v[r], r]; (* Force *)
h[r_] = -D[f[r], r]; (* Hessian *)
rMin = r /. NSolve[{f[r] == 0, h[r] > 0, r > 0}, r, Reals][[1]]
rMax = r /. NSolve[{f[r] == 0, h[r] < 0, r > 0}, r, Reals][[1]]
vMin = v[rMin];
vMax = v[rMax];
```

```
1.136
```

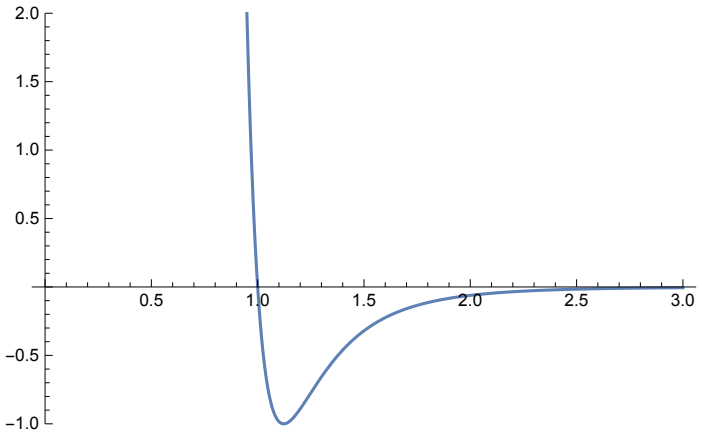
```
2.20364
```

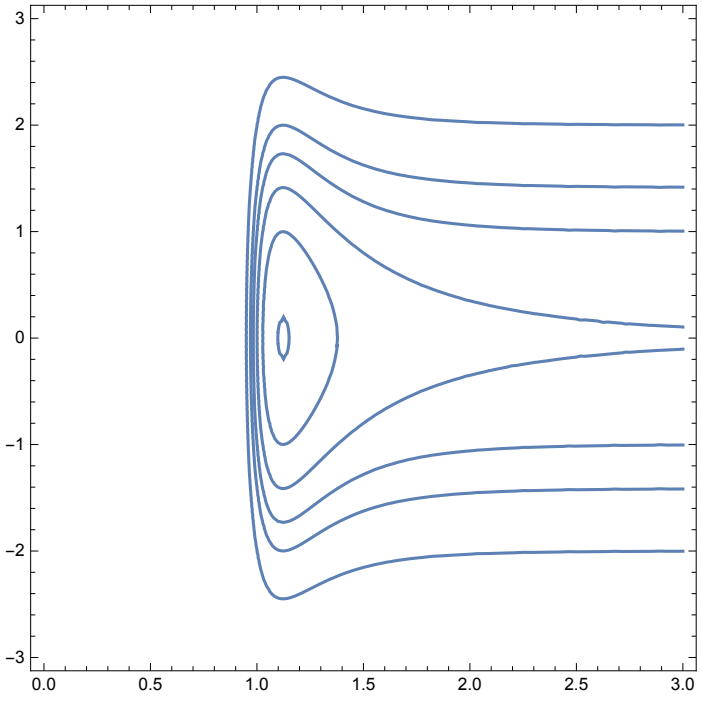
```
(* Purely repulsive r12 potential *)
Plot[v12[r], {r, 0, 3}, PlotRange → {-a, 2}]
h[r_, p_] = t[p] + v12[r];
ContourPlot[h[r, p] == {0.5, 1., 2., 3., 4.}, {r, 0, 3}, {p, -3, 3}]
```





```
(* Lennard-Jones potential *)
Plot[vLJ[r], {r, 0, 3}, PlotRange → {-a, 2}]
h[r_, p_] = t[p] + vLJ[r];
ContourPlot[h[r, p] == {-0.98, -0.5 , 0.0, 0.5 , 1. , 2.} * a, {r, 0, 3}, {p, -3, 3}]
```





```
(* Lennard-Jones with centrifugal repulsion *)
h[r_, p_] = t[p] + v[r];
Plot[v[r], {r, 0, 1.55 * rMax}, PlotRange → {-a, 2}]
ContourPlot[h[r, p] == {0.98 * vMin, 0.5 * vMin, 0.0, 0.8 * vMax, vMax * 1.01, 0.4, 1., 2.},
 {r, 0, 1.5 * rMax}, {p, -3, 3}]
```