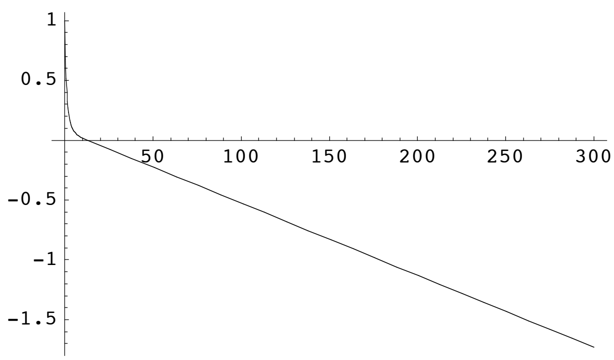
Thomas-Fermi for Al^+

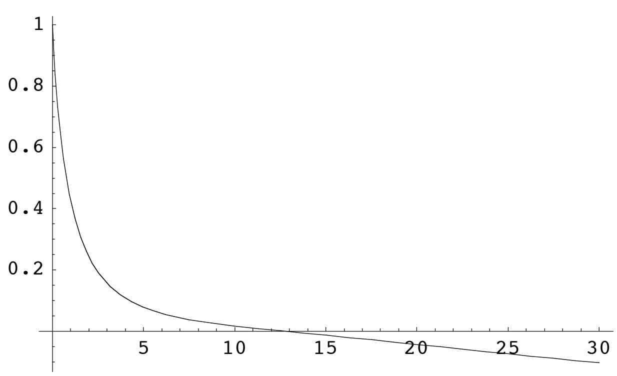
Following the discusions on the positive ions in the lecture notes, we need to find $\chi'(0)$ so that $x_0\ \chi'(x_0) = -(Z-N)/Z = -1/13$ for Al^+. After some trial-and-error, I find $\chi'(0) = -1.5881063075$ works:

In[1]:=
```
chisol = NDSolve[
  {(1 + 4/3 x^(3/2)) y''[x] + 4 x^(1/2) y'[x] + If[x == 0, 0, y[x]/x^(1/2) (1 - (1 + 4/3 x^(3/2))^(3/2) Max[y[x], 0]^(1/2))] ==
    0, y[0] == 1, y'[0] == -1.5881063075}, y, {x, 0, 300}];
χ[x_] := (1 + 4/3*x^(3/2)) y[x]; Plot[χ[x] /. chisol, {x, 0, 300}]
```



Out[1]= - Graphics -

In[2]:=
```
Plot[χ[x] /. chisol, {x, 0, 30}]
```



Out[2]= - Graphics -

Look for where $\chi(x_0) = 0$,

In[3]:=
```
x0 = x /. FindRoot[χ[x] /. chisol, {x, 0, 100}]
```

Out[3]= 12.7649

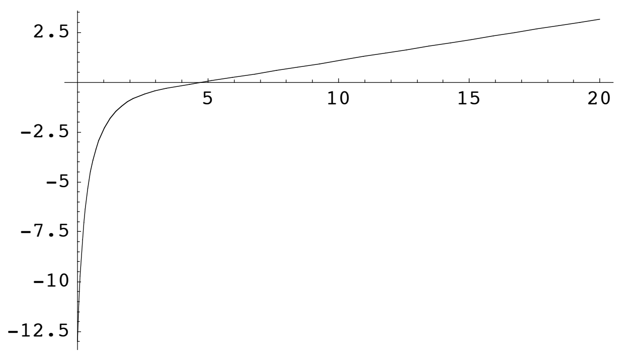
Now make sure $x_0\ \chi'(x_0) = -1/13$, *In[4]:=* $\mathbf{Z\,x\,\chi'[x]\ /.\ chisol\ /.\ \{x \to x_0\}\ /.\ \{Z \to 13\}}$

Out[4]= {-1.}

Using the definition $e\,\Phi(r) = \frac{Z\,e}{r}\,\chi(r)$ and variables $r = Z^{-1/3}\,b\,x$, $b = \frac{1}{2}\,(\frac{3\,\pi}{4})^{2/3}\,\frac{\hbar^2}{m\,e^2}$, we define (in the atomic unit $e = m = \hbar = 1$)

In[5]:= $\mathbf{\Phi[r\_] := -\frac{Z}{r}\,\chi\left[\left(Z^{-1/3}\,\frac{1}{2}\,\left(\frac{3\,\pi}{4}\right)^{2/3}\right)^{-1} r\right]\ /.\ \left\{r_0 \to Z^{-1/3}\,\frac{1}{2}\,\left(\frac{3\,\pi}{4}\right)^{2/3} x_0\right\}\ /.\ chisol[[1]]\ /.\ \{Z \to 13\}}$

In[6]:= **Plot[r Φ[r], {r, 0, 20}]**



Out[6]= - Graphics -

The Fermi energy is just $\epsilon_F = \frac{-e}{r_0}$, where $r_0 = Z^{-1/3}\,b\,x_0 = Z^{-1/3}\,\frac{1}{2}\,(\frac{3\,\pi}{4})^{2/3}\,x_0$ in the atomic unit.

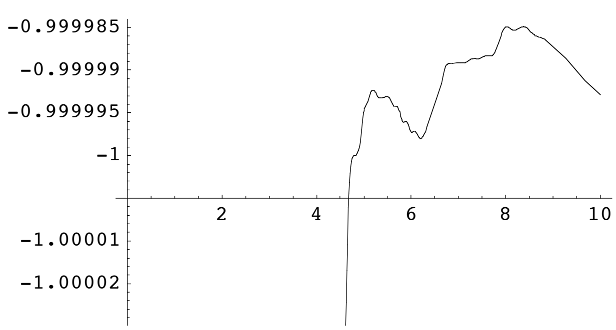
In[7]:= $\mathbf{\phi[r\_] :=}$

$\mathbf{-\frac{Z}{r}\,\chi\left[\left(Z^{-1/3}\,\frac{1}{2}\,\left(\frac{3\,\pi}{4}\right)^{2/3}\right)^{-1} r\right] - \frac{1}{r_0}\ /.\ \left\{r_0 \text{ -> } Z^{-1/3}\,\frac{1}{2}\,\left(\frac{3\,\pi}{4}\right)^{2/3} x_0\right\}\ /.\ chisol[[1]]\ /.\ \{Z \to 13\}}$

In[8]:= $\mathbf{Z^{-1/3}\,\frac{1}{2}\,\left(\frac{3\,\pi}{4}\right)^{2/3} x_0\ /.\ \{Z \to 13\}}$

Out[8]= 4.80635

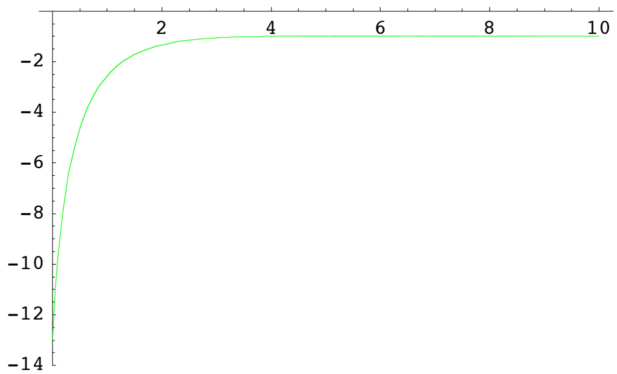
In[9]:= **Plot[r ϕ[r], {r, 0, 10}]**



Out[9]= - Graphics -

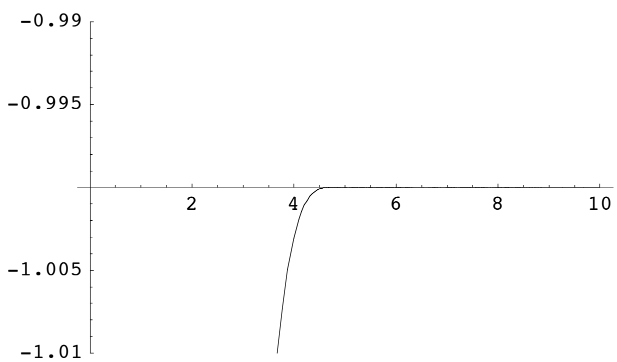
Indeed, $\phi(r)$ becomes $(-1)\,\frac{e^2}{r}$ due to the overall positive charge beyond $r > r_0$ where the electron number density vanishes. The coefficient is consistent with -1 within the tiny numerical errors. To make this point clear, let us plot it on bigger scales,

```
In[10]:= Plot[r ϕ[r], {r, 0, 10}, PlotRange → {-14, 0}, PlotStyle → RGBColor[0, 1, 0]]
```




```
Out[10]= - Graphics -
```

```
In[11]:= Plot[r ϕ[r], {r, 0, 10}, PlotRange → {-1.01, -0.99}]
```

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Out[11]= - Graphics -
```