Solution to Schrödinger equation for a Na atom

Formal solution for the radial component of the electron wavefunction f(r; n, l).
r: radial distance from nucleus
n: main quantum number; l: angular momentum quantum number
LaguerreL: generalized Laguerre polynomials.
Z: nuclear electric charge. a: fine structure constant

In[•]:=
```
f[r_, n_, l_] :=
```
$$\sqrt{\left(\frac{2\,Z}{n\,a}\right)^3 \frac{(n-l-1)\,!}{2\,n\,(n+l)\,!}}\ \text{Exp}\left[\frac{-Z\,r}{n\,a}\right]\left(\frac{2\,Z\,r}{n\,a}\right)^l\ \text{LaguerreL}\left[n-l-1,\ 2\,l+1,\ \frac{2\,Z\,r}{n\,a}\right]$$

In[•]:=
```
Z = 11;
a = 1 / 137;
```

Let us write it in terms of the reduced radius r -> $\rho = \frac{Z r}{a} \frac{1}{b}$, where b is the Bohr radius. The variable ρ defines the scale, i.e. how many times the Bohr radius is contained in the radial length r:

In[•]:=
$$R[\rho\_,\ n\_,\ l\_] := \sqrt{\left(\frac{2\,Z}{n\,a}\right)^3 \frac{(n-l-1)\,!}{2\,n\,(n+l)\,!}}\ \text{Exp}\left[\frac{-\rho}{n}\right]\left(\frac{2\,\rho}{n}\right)^l\ \text{LaguerreL}\left[n-l-1,\ 2\,l+1,\ \frac{2\,\rho}{n}\right]$$

Atomic radius of Na: ; ionic radius: 154 pm
Metallic sodium: bcc crystal, interatomic distance d=370 pm; ionic radius r0=186 pm
Bohr radius: b = 53 pm

d=370/53 a0= ~7 b
r0= 190/53 a0= 3.6 b
Let’s put these values as reference for the future plots as vertical lines

In[•]:=
```
radius =
  ListPlot[{{3.6, -10}, {3.6, 10}}, Joined → True, PlotStyle → {Gray, Dashed}];
distance = ListPlot[{{7, -10}, {7, 10}}, Joined → True, PlotStyle → Gray];
```

Probability of finding an electron at distance r from the nucleus: radial integral of the square modulus.
The probability requires that the wavefunction is normalized. Normalization is performed by integration over r in the (0,∞) interval:

$$I0010 = \text{Integrate}\left[r^2\ (R[r,\ 1,\ 0])^2,\ \{r,\ 0,\ \infty\}\right];$$
$$I0020 = \text{Integrate}\left[r^2\ (R[r,\ 2,\ 0])^2,\ \{r,\ 0,\ \infty\}\right];$$
$$I0030 = \text{Integrate}\left[r^2\ (R[r,\ 3,\ 0])^2,\ \{r,\ 0,\ \infty\}\right];$$
$$I0021 = \text{Integrate}\left[r^2\ (R[r,\ 2,\ 1])^2,\ \{r,\ 0,\ \infty\}\right];$$

We can now plot the radial probability distribution for the following orbitals:
1s (n=1, l=0)
2s (n=2, l=0)
3s (n=3, l=0)

2p (n=2, l=1)

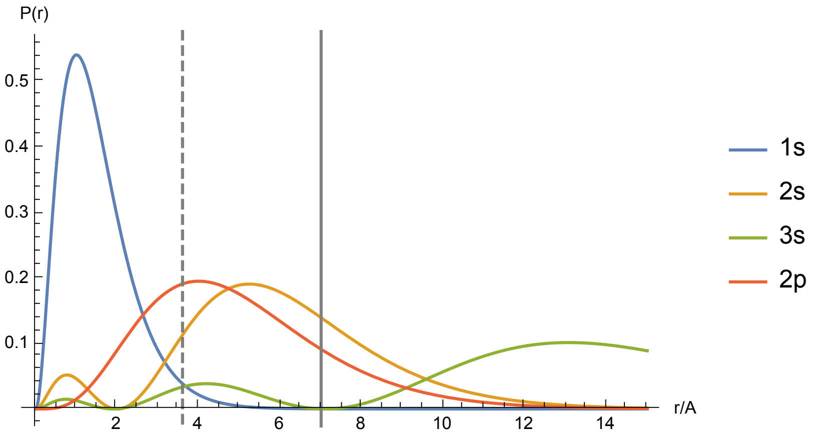
In[∘]:=
```
orbitals = Plot[{r^2 (R[r, 1, 0])^2 / I0010, r^2 (R[r, 2, 0])^2 / I0020,
    r^2 (R[r, 3, 0])^2 / I0030, r^2 (R[r, 2, 1])^2 / I0021}, {r, 0, 15},
   PlotRange → Full, PlotLegends → {"1s", "2s", "3s", "2p"}];
```

Dashed gray line: atomic radius

Continuous line: interatomic distance

In[∘]:=
```
Show[orbitals, radius, distance, AxesLabel → {"r/A", "P(r)"}]
```

Out[∘]=



What is the probability to find the electron within a radial distance x from the nucleus? I calculate the integral of the square modulus of R(x) between 0 and x:

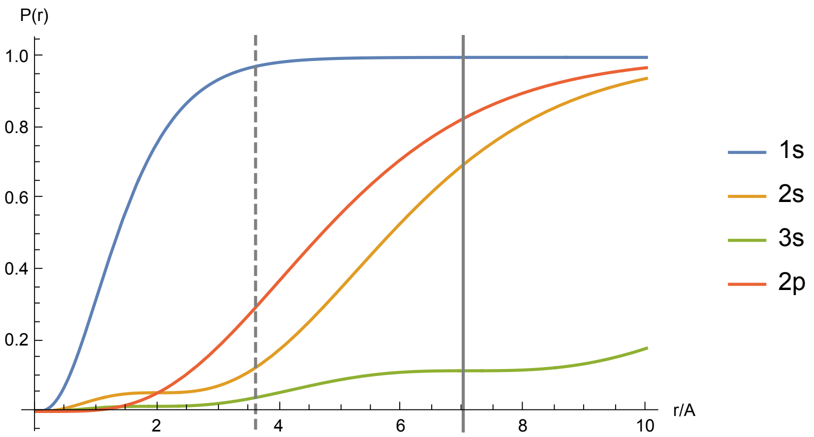
```
CDF10 = Plot[Integrate[r^2 (R[r, 1, 0])^2, {r, 0, x}] / I0010, {x, 0, 10}];
CDF20 = Plot[Integrate[r^2 (R[r, 2, 0])^2, {r, 0, x}] / I0020, {x, 0, 10}];
CDF30 = Plot[Integrate[r^2 (R[r, 3, 0])^2, {r, 0, x}] / I0030, {x, 0, 10}];
CDF21 = Plot[Integrate[r^2 (R[r, 2, 1])^2, {r, 0, x}] / I0021, {x, 0, 10}];
```

Plot of such probability:

In[∘]:=
```
CDForbitals = Plot[
   {
    Integrate[r^2 (R[r, 1, 0])^2, {r, 0, x}] / I0010,
    Integrate[r^2 (R[r, 2, 0])^2, {r, 0, x}] / I0020,
    Integrate[r^2 (R[r, 3, 0])^2, {r, 0, x}] / I0030,
    Integrate[r^2 (R[r, 2, 1])^2, {r, 0, x}] / I0021},
   {x, 0, 10}, PlotLegends → {"1s", "2s", "3s", "2p"}];
```

```
In[•]:= Show[CDForbitals, radius, distance,
          PlotLegends → {"1s", "2s", "3s", "2p"}, AxesLabel → {"r/A", "P(r)"}]
```

OptionValue: Unknown option PlotLegends for Graphics.

Out[•]=


To summarize, probability for

1s: almost 1 within the atomic radius

2s: 0.1 within the atomic radius, 0.7 within the interatomic distance: it overlaps more with the nearest neighbour atom than with the binding atom!!!

3s: 0.05 within the atomic radius, 0.1 within the interatomic distance: same overlap between the binding atom and the nearest neighbour!!

2p: 0.3 within the atomic radius, 0.8 within the interatomic distance: it overlaps more with the nearest neighbour atom than with the binding atom!!!

Note: this is a partial picture: angular distribution is not taken into account.

For completeness: table of radial distributions vs Bohr atom for the first 6 orbitals of a hydrogen-like atom: