Basis Sets

Hydrogen Orbitals

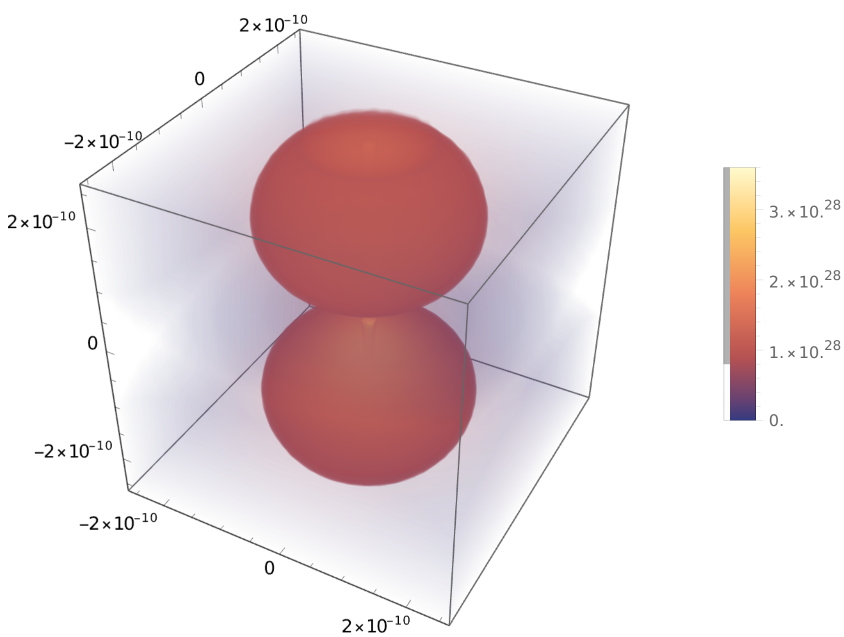
In[◦]:=
```
a0 = Quantity["BohrRadius"] / Quantity["Meters"]
```

Out[◦]= $5.29177211 \times 10^{-11}$

In[◦]:=
```
ψ[{n_, l_, m_}, {r_, θ_, ϕ_}] :=
  With[{ρ = 2 r / (n a0)}, Sqrt[(2 / (n a0))^3 (n - l - 1)! / (2 n (n + l)!)] Exp[-ρ / 2]
    ρ^l LaguerreL[n - l - 1, 2 l + 1, ρ] SphericalHarmonicY[l, m, θ, ϕ]]
```

In[◦]:=
```
DensityPlot3D[
  (Abs@ψ[{2, 1, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^2,
  {x, -5 a0, 5 a0}, {y, -5 a0, 5 a0}, {z, -5 a0, 5 a0}, PlotLegends → Automatic]
```

Out[◦]=



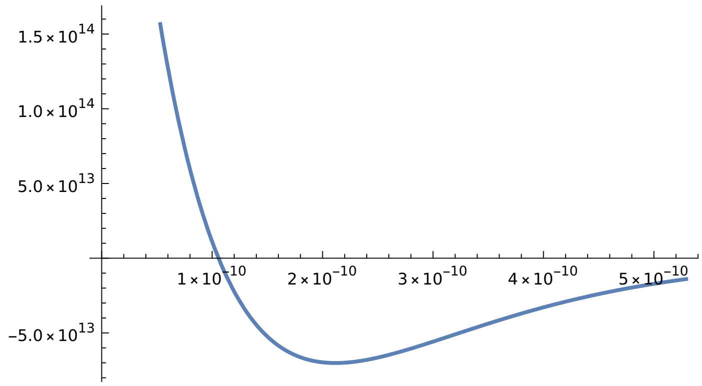
Radial Part

In[◦]:=
```
ψ[{2, 0, 0}, {r, θ, ϕ}]
```

Out[◦]= $2.59088642 \times 10^{14}\, e^{-9.44863062\times10^{9}\, r} \left(2.000000000 - 1.889726125 \times 10^{10}\, r\right)$

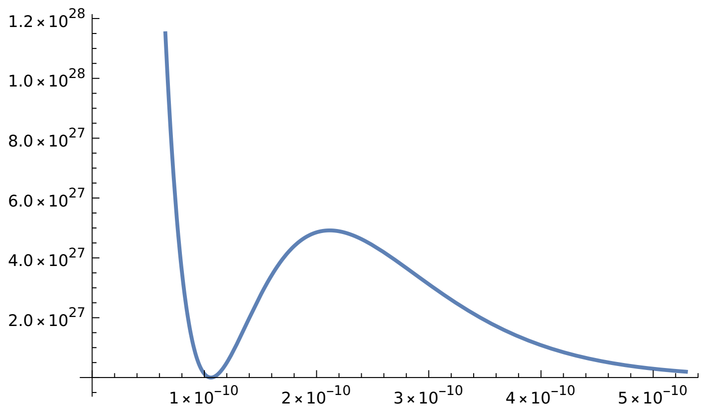
In[∘]:= `Plot[ψ[{2, 0, 0}, {r, θ, ϕ}], {r, 0, 10 a0}]`

Out[∘]=



In[∘]:= `Plot[(Abs@ψ[{2, 0, 0}, {r, θ, ϕ}])^2, {r, 0, 10 a0}]`

Out[∘]=



In[∘]:= `ψ[{2, 0, 0}, {r, θ, ϕ}]`

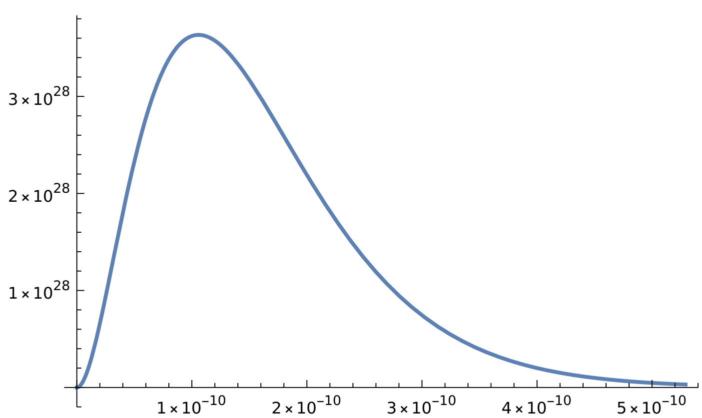
Out[∘]= $2.59088642 \times 10^{14}\, e^{-9.44863062\times 10^{9}\, r} \left(2.000000000 - 1.889726125 \times 10^{10}\, r\right)$

In[∘]:= `ψ[{2, 1, 0}, {r, θ, ϕ}]`

Out[∘]= $4.89606576 \times 10^{24}\, e^{-9.44863062\times 10^{9}\, r}\, r \operatorname{Cos}[\theta]$

In[∘]:= `Plot[(Abs@ψ[{2, 1, 0}, {r, 0, ϕ}])^2, {r, 0, 10 a0}]`

Out[∘]=

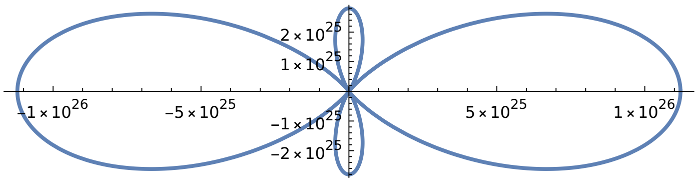


Angular Part

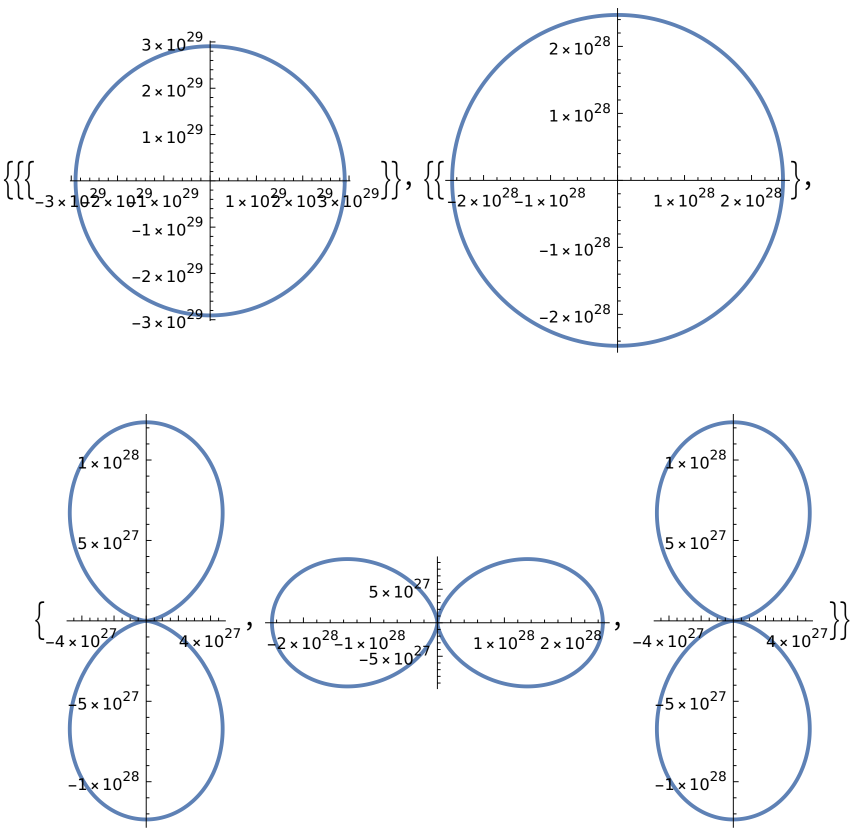
In[∘]:=
```
ψ[{2, 1, 0}, {a0, θ, ϕ}]
```

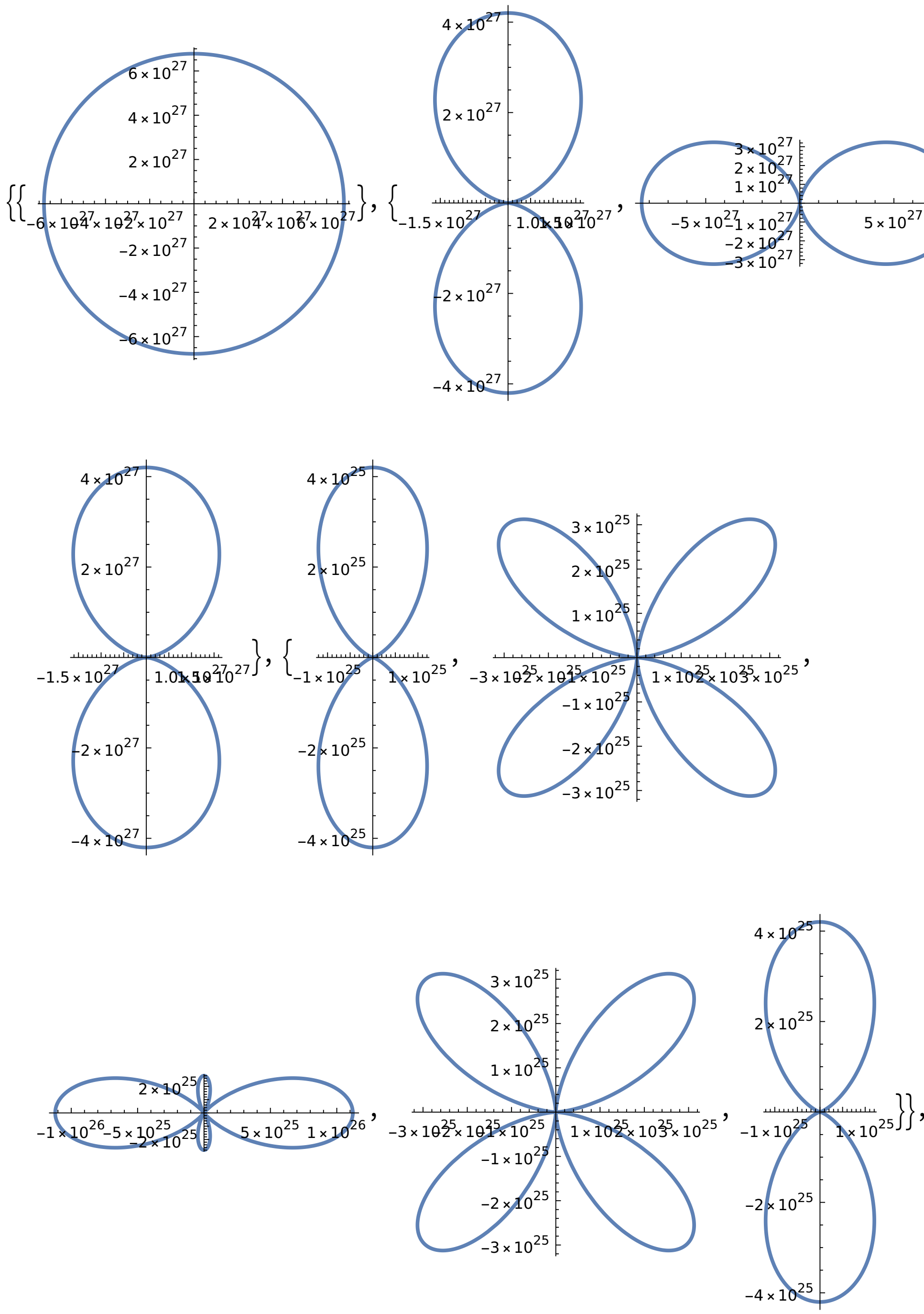
Out[∘]= $1.57145205 \times 10^{14}\ \mathrm{Cos}[\theta]$

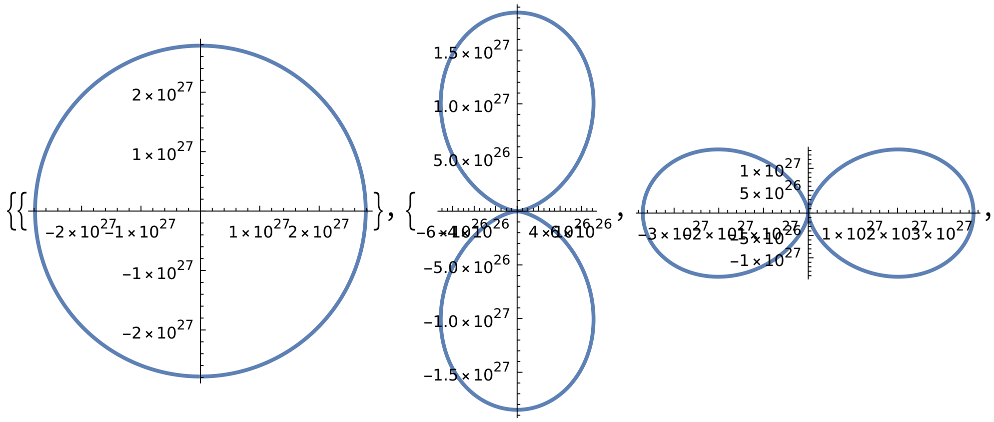
In[∘]:=
```
PolarPlot[(Abs@ψ[{3, 2, 0}, {a0, θ, ϕ}])^2, {θ, 0, 2 Pi}]
```

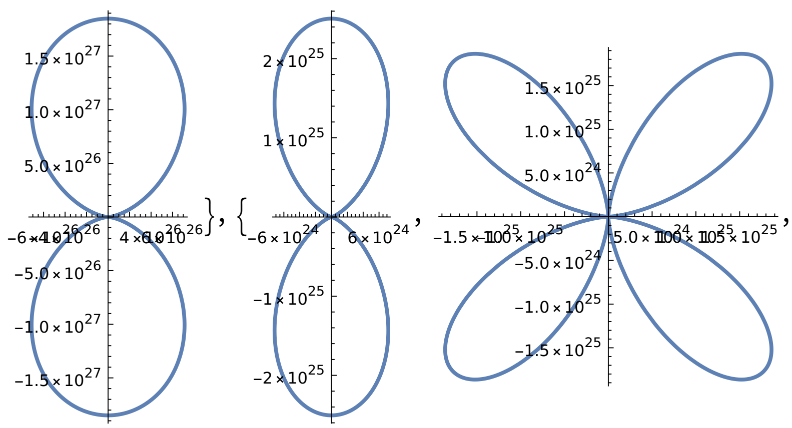
Out[∘]=


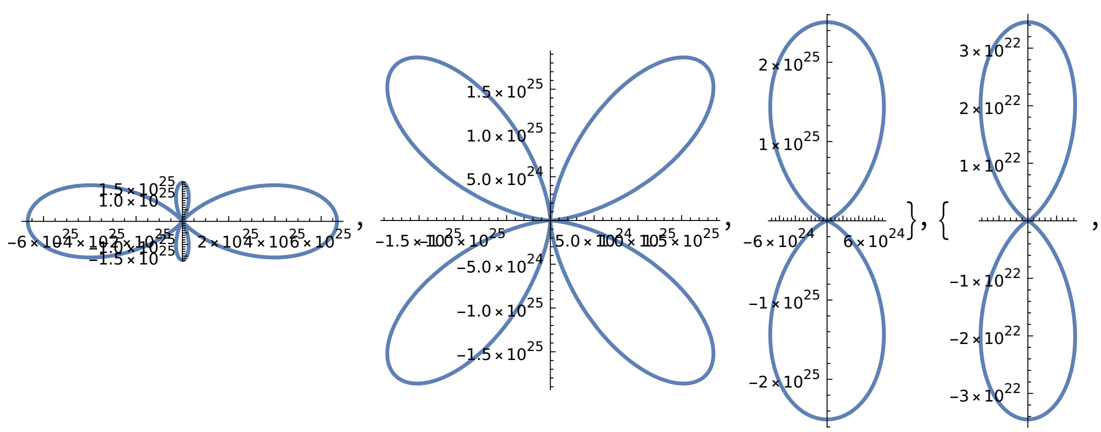
In[∘]:=
```
Table[PolarPlot[Simplify[(Abs@ψ[{n, l, m}, {a0, θ, ϕ}])^2, Assumptions → ϕ > 0], {θ, 0, 2 Pi}],
 {n, 1, 4}, {l, 0, n - 1}, {m, -l, l}]
```

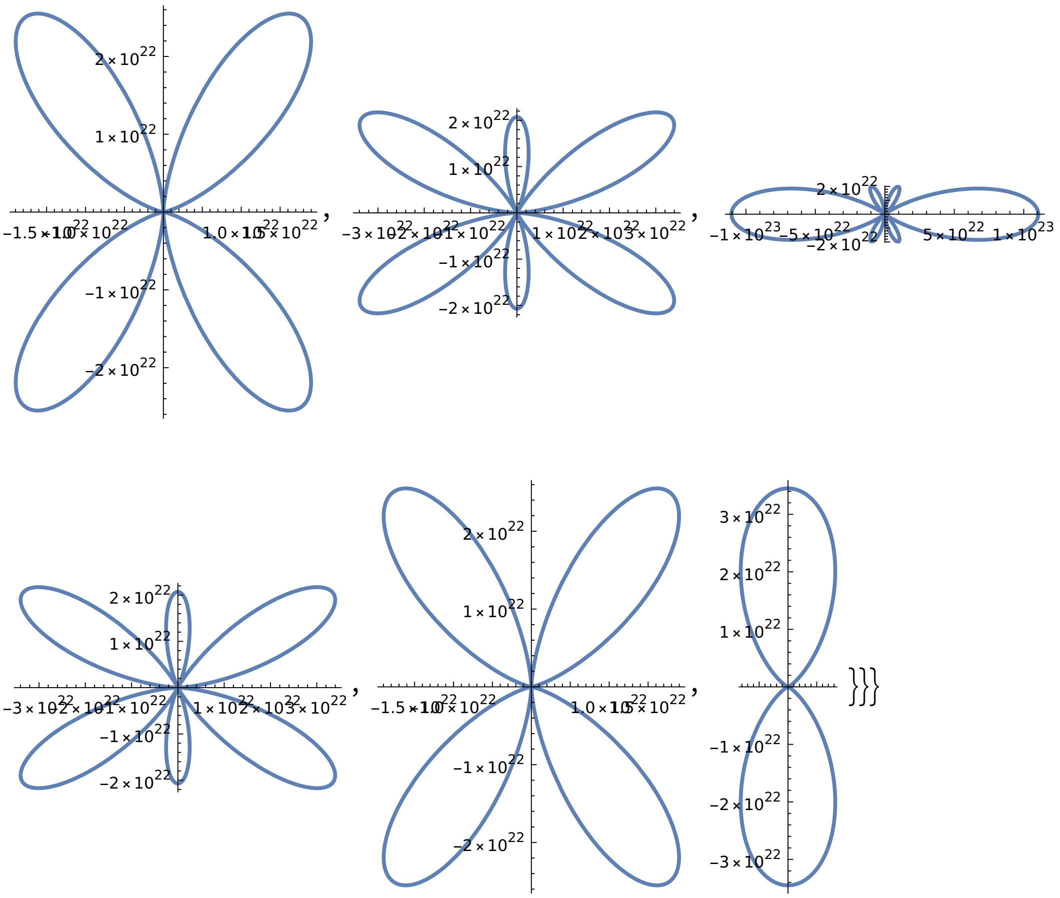
Out[∘]=



6 × 10^27
4 × 10^27
2 × 10^27
−2 × 10^27
−4 × 10^27
−6 × 10^27
−1.5 × 10^27
5 × 10^27
−5 × 10^27
3 × 10^27
1 × 10^27
−1 × 10^27
−3 × 10^27
4 × 10^25
2 × 10^25
−2 × 10^25
−4 × 10^25
3 × 10^25
1 × 10^25
−1 × 10^25
−3 × 10^25
−1 × 10^26
1 × 10^26
5 × 10^25
−5 × 10^25









Slater Orbitals (STOs)

In[∘]:= `a0 = a`

Out[∘]= a

In[∘]:= `ψ[{1, 0, 0}, {r, θ, ϕ}]`

Out[∘]=
$$\frac{\sqrt{\frac{1}{a^3}}\ e^{-\frac{r}{a}}}{\sqrt{\pi}}$$

In[◦]:= `Table[ψ[{n, 0, 0}, {r, θ, ϕ}], {n, 1, 5}]`

Out[◦]=
$$\left\{\frac{\sqrt{\frac{1}{a^3}}\, e^{-\frac{r}{a}}}{\sqrt{\pi}}, \frac{\sqrt{\frac{1}{a^3}}\, e^{-\frac{r}{2a}}\left(2-\frac{r}{a}\right)}{4\sqrt{2\pi}}, \left(\sqrt{\frac{1}{a^3}}\, e^{-\frac{r}{3a}}\left(27a^2-18ar+2r^2\right)\right)\Big/\left(81a^2\sqrt{3\pi}\right),\right.$$
$$\left(\left(\frac{1}{a^3}\right)^{3/2} e^{-\frac{r}{4a}}\left(192a^3-144a^2r+24ar^2-r^3\right)\right)\Big/\left(1536\sqrt{\pi}\right),$$
$$\left.\left(\sqrt{\frac{1}{a^3}}\, e^{-\frac{r}{5a}}\left(9375a^4-7500a^3r+1500a^2r^2-100ar^3+2r^4\right)\right)\Big/\left(46\,875\,a^4\sqrt{5\pi}\right)\right\}$$

In[◦]:= `ψ[{1, 0, 0}, {r, θ, ϕ}]`

When the nuclei has a charge Z

$$\frac{\sqrt{\frac{Z\wedge 3}{a^3}}\, e^{-Z\frac{r}{a}}}{\sqrt{\pi}}$$

In[◦]:= `a = 1`

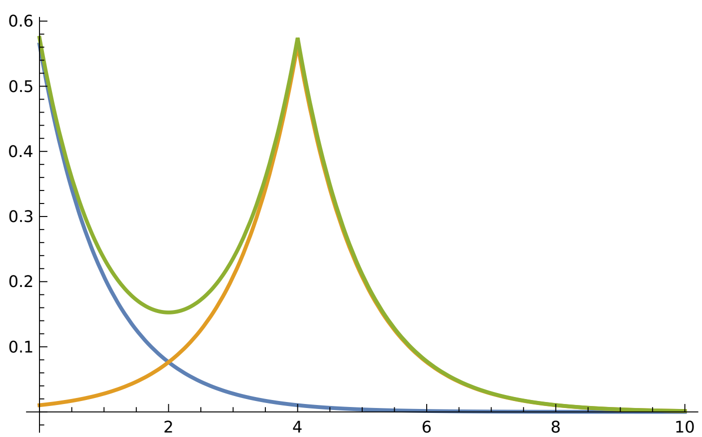
Out[◦]= 1

In[◦]:= `ψ[{1, 0, 0}, {r, θ, ϕ}] // InputForm`

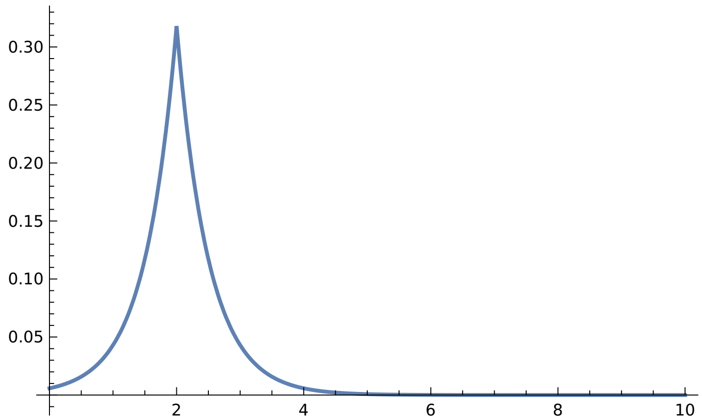
Out[◦]//InputForm=
`1/(E^r*Sqrt[Pi])`

In[◦]:= `SimplifiedSTO[r_, R_] := 1 / (E^(Abs@(r - R)) * Sqrt[Pi])`

In[◦]:= `Plot[{SimplifiedSTO[r, 0], SimplifiedSTO[r, 4], SimplifiedSTO[r, 0] + SimplifiedSTO[r, 4]}, {r, 0, 10}, PlotRange → All]`

Out[◦]=


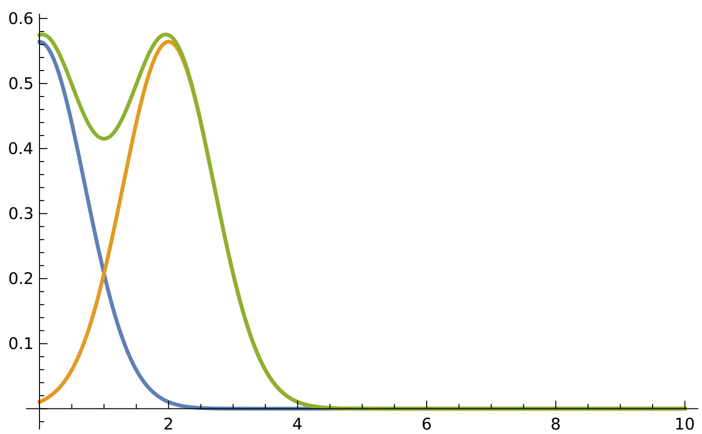
In[∘]:=
```
Plot[(Abs@SimplifiedSTO[r, 2])^2, {r, 0, 10}, PlotRange → All]
```

Out[∘]=


Gaussian orbitals (GTOs)

In[∘]:=
```
SimplifiedGTO[r_, R_] := 1 / (E ^ ((Abs@(r - R)) ^ 2) * Sqrt[Pi])
```

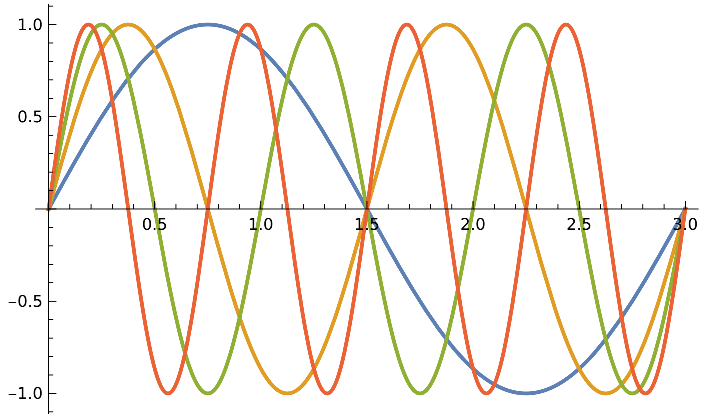
In[∘]:=
```
Plot[{SimplifiedGTO[r, 0], SimplifiedGTO[r, 2], SimplifiedGTO[r, 0] + SimplifiedGTO[r, 2]},
  {r, 0, 10}, PlotRange → All]
```

Out[∘]=


Plane Waves

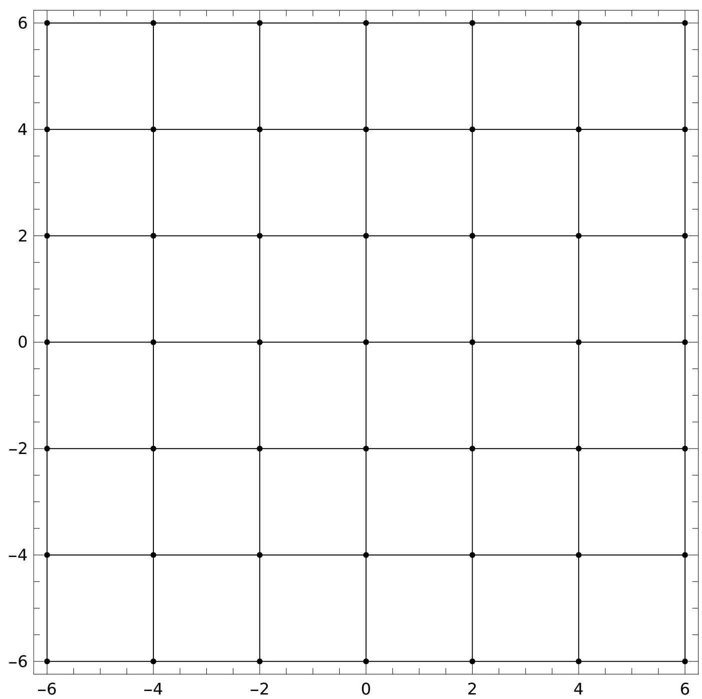
In[∘]:=
```
Plot[Evaluate@Table[Sin[x nx 2 Pi / 3], {nx, 1, 4}], {x, 0, 3}]
```

Out[∘]=

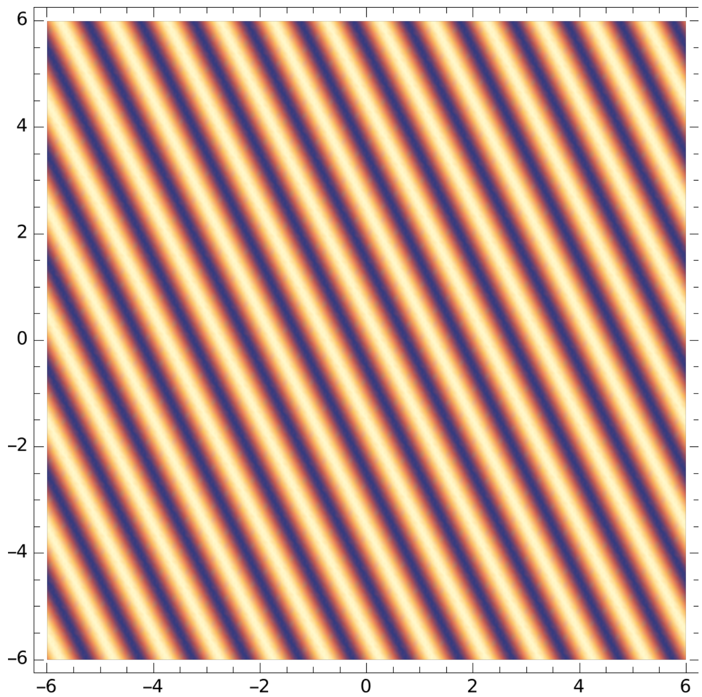


In[∘]:=
```
L = 2;
n = 3;
basis = L * LatticeData["SquareLattice", "Basis"] // Normal;
points = Tuples[Range[-n, n], 2].basis;
lines = Select[Subsets[points, {2}], Norm[#[[1]] - #[[2]]] == L &];
g1 = Graphics[{Point[points], Line@lines}, Frame → True]
```

Out[∘]=



In[∘]:=
```
d1 = DensityPlot[Sin[x 2 × 2 Pi / L + y 2 Pi / L], {x, - n L, n L}, {y, - n L, n L}, PlotPoints → 50]
```

Out[∘]=


In[∘]:=
```
Show[d1, g1]
```

Out[∘]=