In[∘]:= $$\mathtt{f1}[\rho\_,\, n\_,\, l\_] := \sqrt{\left(\frac{2\,Z}{n\,a}\right)^{3} \frac{(n-l-1)\,!}{2\,n\,(n+l)\,!}}\ \mathtt{Exp}\left[\frac{-\mathtt{Abs}[\rho]}{n}\right] \left(\frac{2\,\mathtt{Abs}[\rho]}{n}\right)^{l} \mathtt{LaguerreL}\left[n-l-1,\, 2\,l+1,\, \frac{2\,\mathtt{Abs}[\rho]}{n}\right]$$

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 distance between adjacent atoms

In[∘]:=
```
Z = 11;
a = 1 / 137;
```

Let’s visualize maximally symmetric and antisymmetric wavefunctions φ+,φ- based e.g. on the 3d orbital. Sum over 200 adjacent lattice sites.

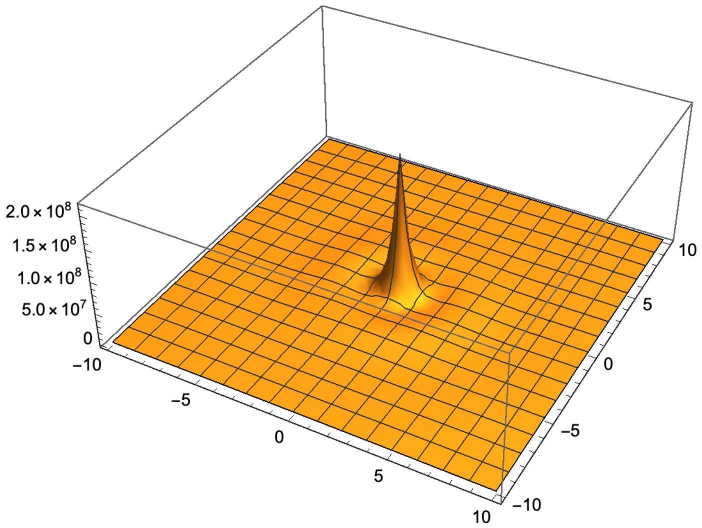
1-dimensional chain, and...

2 - dimensional lattice (simplified : only radial component of the wavefunction with radial symmetry):

In[∘]:= $$\mathtt{f3}[x\_,\, y\_,\, n\_,\, l\_] := \mathtt{f1}\left[\sqrt{x^2+y^2},\, n,\, l\right]^2;$$

In[∘]:=
```
Plot3D[f3[x, y, 4, 0], {x, -10, 10}, {y, -10, 10}, PlotRange → Full]
```

Out[∘]=



1s orbital

Let me define a lattice wavefunction as the sum of individual wavefunctions centered at each lattice site (d=7 times the Bohr radius).

|φ>= $\sum_i$ ci*|R(r-ri)>.

In the following the R(r) function is named by f1: the argument of the radial wavefunction is taken in its absolute value.

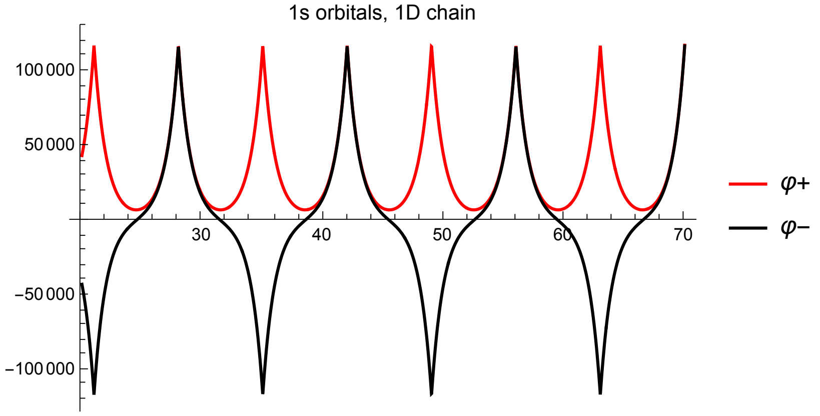
In[∘]:=
```
symm1s[r_] = Sum[f1[r - i * 7, 1, 0], {i, 0, 200}];

antisymm1s[r_] = Sum[(-1)^i f1[r - i * 7, 1, 0], {i, 0, 200}];
```

$$\text{symm1s}[r\_] = \sum_{i=0}^{200} \text{f1}[r - i * 7, 1, 0];$$

$$\text{antisymm1s}[r\_] = \sum_{i=0}^{200} (-1)^i\, \text{f1}[r - i * 7, 1, 0];$$

In[∘]:=
```
Plot[{symm1s[r], antisymm1s[r]}, {r, 20, 70},
 PlotRange → Full, PlotStyle → {Red, Black},
 PlotLabel → "1s orbitals, 1D chain", PlotLegends → {"φ+", "φ-"}]
```

Out[∘]=

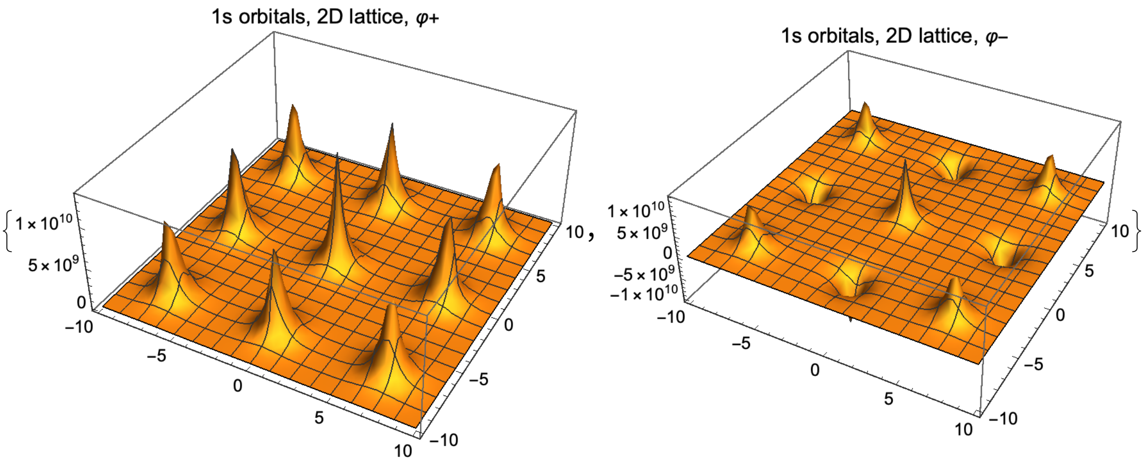


2D lattice: same as for the 1D chain, with an array of atoms spaced by d=7*b. The symmetric/antisymmetric functions are defined nased on f3[x,y].

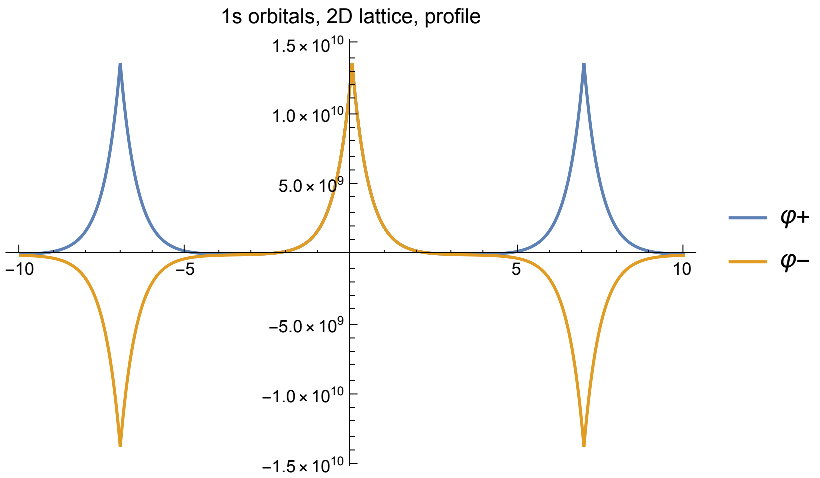
```
symm2d1s[x_, y_, n_, l_] := Sum[f3[x - 7 * i, y - 7 * j, n, l], {i, -5, 5}, {j, -5, 5}]
asymm2d1s[x_, y_, n_, l_] :=
 Sum[(-1)^(i+j) f3[x - 7 * i, y - 7 * j, n, l], {i, -5, 5}, {j, -5, 5}]
```

In[∘]:=
```
{Plot3D[symm2d1s[x, y, 1, 0], {x, -10, 10}, {y, -10, 10},
  PlotRange → Full, PlotLabel → "1s orbitals, 2D lattice, φ+"],
 Plot3D[asymm2d1s[x, y, 1, 0], {x, -10, 10}, {y, -10, 10},
  PlotRange → Full, PlotLabel → "1s orbitals, 2D lattice, φ-"]}
```

Out[∘]=



In[◦]:=
```
Plot[{symm2d1s[x, 0, 1, 0], asymm2d1s[x, 0, 1, 0]}, {x, -10, 10}, PlotRange → Full,
 PlotLabel → "1s orbitals, 2D lattice, profile", PlotLegends → {"φ+", "φ-"}]
```

Out[◦]=


2s orbital

2p orbital

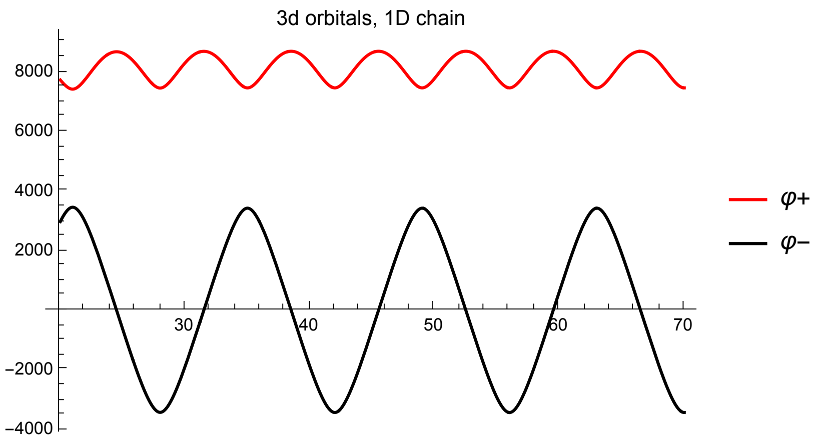
3s orbital

3d orbital

In[◦]:=
$$\text{symm3d}[r\_] = \sum_{i=0}^{200} \text{f1}[r - i * 7, 3, 2];$$

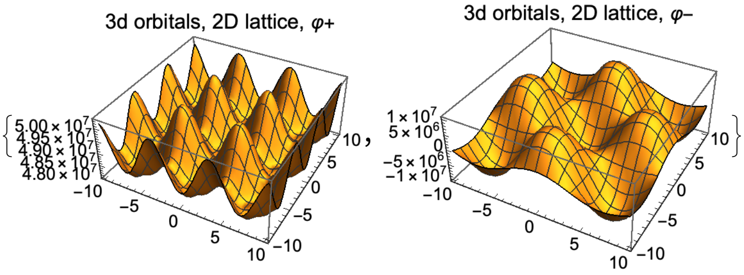
$$\text{antisymm3d}[r\_] = \sum_{i=0}^{200} (-1)^{i}\, \text{f1}[r - i * 7, 3, 2];$$

In[◦]:=
```
Plot[{symm3d[r], antisymm3d[r]}, {r, 20, 70},
 PlotRange → Full, PlotStyle → {Red, Black},
 PlotLabel → "3d orbitals, 1D chain", PlotLegends → {"φ+", "φ-"}]
```

Out[◦]=


In[∘]:=
```
{Plot3D[symm2d1s[x, y, 3, 2], {x, -10, 10}, {y, -10, 10},
   PlotRange → Full, PlotLabel → "3d orbitals, 2D lattice, φ+"],
  Plot3D[asymm2d1s[x, y, 3, 2], {x, -10, 10}, {y, -10, 10},
   PlotRange → Full, PlotLabel → "3d orbitals, 2D lattice, φ-"]}
```

Out[∘]=



In[∘]:=
```
Plot[{symm2d1s[x, 0, 3, 2], asymm2d1s[x, 0, 3, 2]}, {x, -10, 10}, PlotRange → Full,
  PlotLabel → "3d orbitals, 2D lattice, profile", PlotLegends → {"φ+", "φ-"}]
```

Out[∘]=