Contour and Surface Maps of Atomic Orbitals

Let us look at a two dimensional way of graphing three dimensional atomic orbitals. The way to do this is to choose a two dimensional plane in which the function is represented. In other words, we take a "slice" through the function at a pre-determined plane.

Let us look at the 2px orbital in the XY plane. The complete expression for the 2px wave function is given in Table 11.5 (p. 522). We first pick the limits of the two-dimensional plane and define a grid on which the function is to be represented. Then we will plot the function as a contour and as a surface plot.

\[
\begin{align*}
  a &:= 15.0  \\
  b &:= 10.0  \\
  M &:= 40  \\
  N &:= 30  \\
  i &:= 0..M  \\
  j &:= 0..N
\end{align*}
\]

\[
x_i := -a + \left(\frac{i}{M}\right) (2a)  \\
y_j := -b + \left(\frac{j}{N}\right) (2b)  \\
r_{i,j} := \left[ (x_i)^2 + (y_j)^2 \right]^{\frac{1}{2}}
\]

\[
\psi_{2px_{i,j}} := \frac{1}{4\sqrt{2\pi}} r_{i,j} \exp \left( \frac{-r_{i,j}}{2} \right) \frac{x_i}{r_{i,j}}
\]

\[
\psi_{2px}
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\psi_{2px}
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