MOMENTUM SPACE IN 3-D

We can generalize the 1-d definition of momentum space to 3-d, so the momentum space wave function is

\[ \phi(p) = \frac{1}{(2\pi \hbar)^{3/2}} \int e^{-ipr/\hbar} \psi(r) \, d^3r \tag{1} \]

As an example, we can calculate this function for the ground state of hydrogen:

\[ \psi_{100} = \frac{1}{\sqrt{\pi a^{3/2}}} e^{-r/a} \tag{2} \]

Since \( \psi_{100} \) is spherically symmetric, the integral above should be the same for a given magnitude \( p \) regardless of the direction of \( p \). Taking \( p \) along the polar axis means that \( p \cdot r = pr \cos \theta \), so

\[ \phi(p) = \frac{1}{\sqrt{\pi a^{3/2}}(2\pi \hbar)^{3/2}} \int_{-\infty}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} e^{-ipr \cos \theta/\hbar} e^{-r/a} \, r^2 \sin \theta \, d\theta \, dr \, d\phi \tag{3} \]

\[ = \frac{1}{\pi} \left( \frac{2a}{\hbar} \right)^{3/2} \frac{1}{(1 + a^2 p^2 / \hbar^2)^2} \tag{4} \]

where we used Maple to do the integration. It would be nice to check the independence of the result on the direction of \( p \), but unfortunately, choosing any other direction gives an intractable integral. For example, if we took \( p \) to be along the \( x \) axis, so that \( p = [p, 0, 0] \), then since \( r = [x, y, z] \) we have \( r \cdot p = xp = rp \sin \theta \cos \phi \). Since this factor appears in the exponent, there’s no analytic integral that I know of as a solution.

Also, since any hydrogen wave function with a non-zero \( l \) number has a dependence on the angles \( \theta \) and \( \phi \) via the spherical harmonic, the direction of \( p \) does matter, so the calculation above doesn’t apply in those cases. The integrals, even in the case where we take \( p \) along the polar axis, are all horrible anyway, so it’s doubtful we could get a closed solution even in that special case.
To check normalization, we integrate $\phi^2(p)$ over $p$-space in three dimensions.

\[
\int_0^{2\pi} \int_0^\infty \int_0^{\pi} \phi^2(p)p^2 \sin \theta d\theta dp d\phi = \frac{1}{\pi^2} \left( \frac{2a}{\hbar} \right)^3 \int_0^{2\pi} \int_0^\infty \int_0^{\pi} p^2 \sin \theta d\theta dp d\phi \frac{(1 + a^2p^2/\hbar^2)^4}{(1 + a^2p^2/\hbar^2)^4}
\]

\[= 1\quad \text{(5)}\]

Again, Maple was used for the integral.

To get the mean kinetic energy, we first calculate:

\[
\langle p^2 \rangle = \int_0^{2\pi} \int_0^\infty \int_0^{\pi} \phi^2(p)p^4 \sin \theta d\theta dp d\phi
\]

\[= \frac{1}{\pi^2} \left( \frac{2a}{\hbar} \right)^3 \int_0^{2\pi} \int_0^\infty \int_0^{\pi} p^4 \sin \theta d\theta dp d\phi \frac{(1 + a^2p^2/\hbar^2)^4}{(1 + a^2p^2/\hbar^2)^4}
\]

\[= \frac{\hbar^2}{a^2}\quad \text{(8)}\]

The kinetic energy is therefore

\[
\langle T \rangle = \frac{\langle p^2 \rangle}{2m}
\]

\[= \frac{\hbar^2}{2m a^2}\quad \text{(10)}\]

\[= \left( \frac{e^2}{4\pi\varepsilon_0} \right)^2 \frac{m}{2\hbar^2}\quad \text{(12)}\]

\[= -E_1\quad \text{(13)}\]

where we’ve used the formula for the energy levels in the last line. This agrees with the result of the 3-d virial theorem.