

MOMENTUM SPACE IN 3-D

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.42.

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

$$\phi(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \psi(\mathbf{r}) d^3\mathbf{r} \quad (1)$$

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

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \quad (2)$$

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

$$\phi(\mathbf{p}) = \frac{1}{\sqrt{\pi a^3} (2\pi\hbar)^{3/2}} \int_0^{2\pi} \int_0^\infty \int_0^\pi e^{-ipr \cos \theta / \hbar} e^{-r/a} r^2 \sin \theta d\theta dr d\phi \quad (3)$$

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

where we used Maple to do the integration. It would be nice to check the independence of the result on the direction of \mathbf{p} , but unfortunately, choosing any other direction gives an intractable integral. For example, if we took \mathbf{p} to be along the x axis, so that $\mathbf{p} = [p, 0, 0]$, then since $\mathbf{r} = [x, y, z]$ we have $\mathbf{r} \cdot \mathbf{p} = xp = rp \sin \theta \cos \phi$. 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 θ and ϕ via the spherical harmonic, the direction of \mathbf{p} *does* matter, so the calculation above doesn't apply in those cases. The integrals, even in the case where we take \mathbf{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 $\phi^2(\mathbf{p})$ over p -space in three dimensions.

$$\int_0^{2\pi} \int_0^\infty \int_0^\pi \phi^2(\mathbf{p}) p^2 \sin \theta d\theta dp d\phi = \frac{1}{\pi^2} \left(\frac{2a}{\hbar} \right)^3 \int_0^{2\pi} \int_0^\infty \int_0^\pi \frac{p^2 \sin \theta d\theta dp d\phi}{(1 + a^2 p^2 / \hbar^2)^4} \quad (5)$$

$$= 1 \quad (6)$$

Again, Maple was used for the integral.

To get the mean kinetic energy, we first calculate:

$$\langle p^2 \rangle = \int_0^{2\pi} \int_0^\infty \int_0^\pi \phi^2(\mathbf{p}) p^4 \sin \theta d\theta dp d\phi \quad (7)$$

$$= \frac{1}{\pi^2} \left(\frac{2a}{\hbar} \right)^3 \int_0^{2\pi} \int_0^\infty \int_0^\pi \frac{p^4 \sin \theta d\theta dp d\phi}{(1 + a^2 p^2 / \hbar^2)^4} \quad (8)$$

$$= \frac{\hbar^2}{a^2} \quad (9)$$

The kinetic energy is therefore

$$\langle T \rangle = \frac{\langle p^2 \rangle}{2m} \quad (10)$$

$$= \frac{\hbar^2}{2ma^2} \quad (11)$$

$$= \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{m}{2\hbar^2} \quad (12)$$

$$= -E_1 \quad (13)$$

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.