

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

$$(0.1) \quad \phi(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \psi(\mathbf{r}) d^3\mathbf{r}$$

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

$$(0.2) \quad \psi_{100} = \frac{1}{\sqrt{\pi}a^{3/2}} e^{-r/a}$$

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

$$(0.3) \quad \phi(\mathbf{p}) = \frac{1}{\sqrt{\pi}a^3(2\pi\hbar)^{3/2}} \int_0^{2\pi} \int_0^\infty \int_0^\pi e^{-ipr\cos\theta/\hbar} e^{-r/a} r^2 \sin\theta d\theta dr d\phi$$
$$(0.4) \quad = \frac{1}{\pi} \left(\frac{2a}{\hbar}\right)^{3/2} \frac{1}{(1+a^2p^2/\hbar^2)^2}$$

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.

$$(0.5) \quad \int_0^{2\pi} \int_0^\infty \int_0^\pi \phi^2(\mathbf{p}) p^2 \sin \theta d\theta dp d\phi = \frac{1}{\pi^2} \left(\frac{2a}{\hbar} \right)^3 \int_0^{2\pi} \int_0^\infty \int_0^\pi \frac{p^2 \sin \theta d\theta dp d\phi}{(1 + a^2 p^2 / \hbar^2)^4}$$

$$(0.6) \quad = 1$$

Again, Maple was used for the integral.

To get the mean kinetic energy, we first calculate:

$$(0.7) \quad \langle p^2 \rangle = \int_0^{2\pi} \int_0^\infty \int_0^\pi \phi^2(\mathbf{p}) p^4 \sin \theta d\theta dp d\phi$$

$$(0.8) \quad = \frac{1}{\pi^2} \left(\frac{2a}{\hbar} \right)^3 \int_0^{2\pi} \int_0^\infty \int_0^\pi \frac{p^4 \sin \theta d\theta dp d\phi}{(1 + a^2 p^2 / \hbar^2)^4}$$

$$(0.9) \quad = \frac{\hbar^2}{a^2}$$

The kinetic energy is therefore

$$(0.10) \quad \langle T \rangle = \frac{\langle p^2 \rangle}{2m}$$

$$(0.11) \quad = \frac{\hbar^2}{2ma^2}$$

$$(0.12) \quad = \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{m}{2\hbar^2}$$

$$(0.13) \quad = -E_1$$

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.