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

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

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 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

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

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

where we used Maple to do the integration. It would be nice to check the independence of the result on the direction of $\mathbf{p}$, 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.

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

$$= 1 \tag{6}$$

Again, Maple was used for the integral.

To get the mean kinetic energy, we first calculate:

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

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

$$= \frac{\hbar^2}{a^2} \tag{9}$$

The kinetic energy is therefore

$$\langle T\rangle = \frac{\langle p^2\rangle}{2m} \tag{10}$$

$$= \frac{\hbar^2}{2ma^2} \tag{11}$$

$$= \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{m}{2\hbar^2} \tag{12}$$

$$= -E_1 \tag{13}$$

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.