Going Backwards —

Some easier (?) problems in 3D

We did the H atom because it is so crucial to QM, but actually there are some easier (or seemingly easier) QM problems in 3D with central potentials:

(1) $V(r) = 0 \quad \forall r$

(2) $V(r) = 0 \quad r < r_0$ "infinite spherical well"
$\quad\;\; = \infty \quad r > r_0$

The sol'n to (1) is trivial in some sense (if we stick with cartesian coordinates)

$$\frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right)\psi(x,y,z) = E\psi(x,y,z)$$

separable $\quad \psi(x\,y\,z) = f(x)\,g(y)\,h(z)$

$$\qquad\qquad\qquad\quad \uparrow \qquad\;\; \uparrow \qquad\;\; \uparrow$$

$$\qquad\qquad\qquad\quad e^{ik_x x} \quad e^{ik_y y} \quad e^{ik_z z}$$

$$\psi(x,y,z) = e^{i\vec{k}\cdot\vec{r}}$$

$$E = \frac{\hbar^2}{2m}|k|^2 \longleftarrow k_x^2 + k_y^2 + k_z^2$$

But $V(r)=0$ is a central potential $[\hat{H},\hat{L}^2] = [\hat{H},\hat{L}_z]=0$ so we should be able to write solutions as $Y_{lm}(\theta,\phi)\,R(r)$!

The radial wave function obeys the eqn we wrote for Hydrogen atom but without the $-e^2/r$ term.

$$\left[-\frac{1}{r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{r^2}\right]R(r) = \frac{2mE}{\hbar^2}R(r)$$

If we define $E = \hbar^2k^2/2m$ and $x=kr$

$$\frac{d^2}{dx^2}R(x) + \frac{2}{x}\frac{dR}{dx} + \left(1 - \frac{l(l+1)}{x^2}\right)R(x) = 0$$

The soln of this eqn are "spherical Bessel functions"

$j_0(x) = \sin x/x$	$n_0(x) = -\dfrac{\cos x}{x}$
$j_1(x) = \sin x/x^2 - \cos x/x$	$n_1(x) =$
$j_2(x) = \left(3/x^3 - 1/x\right)\sin x - 3/x^2 \cos x$	$n_2(x) =$

Q: Do you notice anything about $n_l(x)$ compared to $j_l(x)$?

A: $n_l(x)$ behave badly at $x=0$!

Eg for $\ell = 0$ $\quad \frac{d^2}{dx^2}R + \frac{2}{x}\frac{dR}{dx} + R = 0$

$j_0 = \frac{\sin x}{x}$

$$\frac{d}{dx}\frac{\sin x}{x} = \frac{\cos x}{x} - \frac{\sin x}{x^2}$$

$$\frac{d^2}{dx^2}\frac{\sin x}{x} = -\frac{\sin x}{x} - \frac{\cos x}{x^2} - \frac{\cos x}{x^2} + \frac{2\sin x}{x^3}$$

$$\overset{\checkmark}{-\frac{\sin x}{x}} \overset{\checkmark\checkmark}{- \frac{2\cos x}{x^2}} \overset{\checkmark\checkmark\checkmark}{+ \frac{2\sin x}{x^3}} + \frac{2}{x}\left(\overset{\checkmark\checkmark}{\frac{\cos x}{x}} \overset{\checkmark\checkmark\checkmark}{- \frac{\sin x}{x^2}}\right) \overset{\checkmark}{+ \frac{\sin x}{x}} \overset{?}{=} 0$$

Math physics course : where these really come from...

I think about spherical Bessel as trig functions

which "decay". Anyway they are just special functions

like e^x, $\sin x$, $\ln x$ but less familiar. (If you think of e^x, $\sin x$, $\ln x$

as being <u>defined</u> by their power series

$$e^x = 1 + x + x^2/2 + x^3/3! + \ldots$$

Can similarly think of $j_\ell(x)$ as defined by their power series

$$j_0(x) = 1 - x^2/3! + x^4/5! \ldots$$

Bottom line Free particle Sch Eqn $V(r) = 0$ in 3D

$$e^{i\vec{k}\cdot\vec{r}} \qquad \text{(A)}$$

or

$$Y_{\ell m}(\theta,\phi)\, j_\ell(kr)$$
$$\text{(B)}$$
$$Y_{\ell m}(\theta,\phi)\, \eta_\ell(kr)$$

In case (A) we use $\hat{p}_x, \hat{p}_y, \hat{p}_z$ as operators which commute with $\hat{H}$. In case (B) we use $\hat{H}, \hat{L}^2$ and $\hat{L}_z$!

Should be able to expand one in terms of other! They are both complete sets. In fact, an amazing identity

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta)$$

Q what are those in terms of $Y_{\ell m}$?

A: $Y_{\ell 0}(\theta) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$

3D-5

$V = \infty \quad r \geq a$

We can do ∞ spherical well. Here it is better to use r, θ, ϕ!

Basis functions

$\phi_{k\ell m}(r,\theta,\phi) = j_\ell(kr) Y_{\ell m}(\theta,\phi) \qquad E = \hbar^2 k^2/2m$

What do we need to happen?

Well wave function must vanish at $r = a$,

so not any k is allowed. We must have $j_\ell(ka) = 0$

$j_0(x)$ vanishes at $x = \pi, 2\pi, \ldots$

$j_1(x)$ vanishes at $x = 4.49, 7.73, \ldots$

$j_2(x)$ vanishes at $x = 5.76, \ldots$

If we call $X_{\ell n}$ the nth root of $j_\ell(x)$

$$\phi_{n\ell m}(r,\theta,\phi) = j_\ell\left(\frac{X_{\ell n} r}{a}\right) Y_{\ell m}(\theta,\phi)$$

$$E_{n\ell} = \frac{\hbar^2}{2m} X_{\ell n}^2/a^2$$