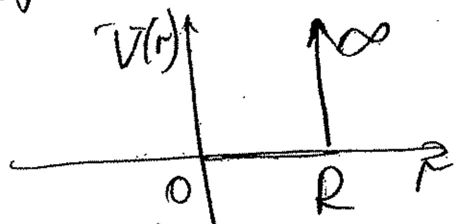
Lecture #6

Examples of dealing with particles in spherically-symmetric potentials

Example 1

Consider a particle enclosed in a sphere of zero potential with infinitely high potential walls defining its surface of radius R. Find the energy levels.



Solution:

Since we deal with a central potential $\Rightarrow$

$$\Psi(r,\theta,\varphi) = \underbrace{R(r)}_{\frac{u_\ell(r)}{r}} Y_\ell^m(\theta,\varphi) \quad ; \quad u_\ell(0) = 0 \text{ — keeps } R(r) \text{ finite}$$

$$u_\ell(R) = 0 \text{ — Bound. cond.}$$

The equation for $u_\ell(r)$ is:

$$-\frac{\hbar^2}{2\mu}\frac{d^2u_\ell(r)}{dr^2} + V_{eff}(r)\,u_\ell(r) = E u_\ell(r) \quad \leftarrow \text{Lecture \#4}$$

$$V_{eff}(r) = \underbrace{V(r)}_{=0} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}$$

$\Downarrow$

$$\frac{d^2u_\ell(r)}{dr^2} + \left[\frac{2\mu E}{\hbar^2} - \frac{\ell(\ell+1)}{r^2}\right]u_\ell(r) = 0 \qquad (7.1)$$

If we consider s-states $\Rightarrow l=0 \Rightarrow$ (2)

Eq. (7.1) is reduced to $\frac{d^2 u_0(r)}{dr^2} + \underbrace{\frac{2\mu E}{\hbar^2}}_{k^2} u_0(r) = 0$

$\Downarrow$

$u_0(r) = C_1 \sin kr + C_2 \cos kr$

$u_0(0) = 0 \Rightarrow C_2 = 0$

$u_0(R) = 0 \Rightarrow \sin kR = 0 \Rightarrow kR = \pi n,$

$n = 1, 2, \ldots$

$$k_n = \frac{\pi n}{R}$$

$$E_n = \frac{\hbar^2 k_n^2}{2\mu} = \frac{\hbar^2}{2\mu}\left(\frac{\pi n}{R}\right)^2$$

$\leftarrow$ similar to a 1D particle-in-the-box problem!

$\psi_{ns} = \tilde{C}\,\frac{\sin kr}{r}$

Let's now go back to Eq. (7.1) and try to solve it for arbitrary l.

Change of variables: $z = kr = \sqrt{\frac{2\mu E}{\hbar^2}}\, r$

Substitute this $\Rightarrow$ $u_l(r) = z^{1/2}\, \eta_l(z)$

into (7.1)

$\uparrow$ new variable $\quad \uparrow$ new function

$\Downarrow$

$$\frac{d^2 \eta_l(z)}{dz^2} + \frac{1}{z}\frac{d\eta_l(z)}{dz} + \left(1 - \frac{(l+\frac{1}{2})^2}{z^2}\right)\eta_l(z) = 0 \qquad (7.2)$$

Eq. (7,2) is one of the forms of <u>Bessel</u> ③ equation $\Rightarrow$ solutions are Bessel functions of $\left(l+\frac{1}{2}\right)$-order $\Rightarrow$

$$\eta_l(z) = C_1 J_{l+\frac{1}{2}}(z) + C_2 J_{-(l+\frac{1}{2})}(z)$$

$$\Downarrow$$

$$u_l(r) = \sqrt{kr}\left(C_1 J_{l+\frac{1}{2}}(kr) + C_2 J_{-(l+\frac{1}{2})}(kr)\right)$$

$$\Downarrow$$

$$R_l(r) = \sqrt{\frac{k}{r}}\left(C_1 J_{l+\frac{1}{2}}(kr) + C_2 J_{-(l+\frac{1}{2})}(kr)\right)$$

Introduce <u>spherical Bessel functions</u> $\Rightarrow$

$$j_l(z) = \sqrt{\frac{\pi}{2}}\,\frac{J_{l+\frac{1}{2}}(z)}{\sqrt{z}}$$

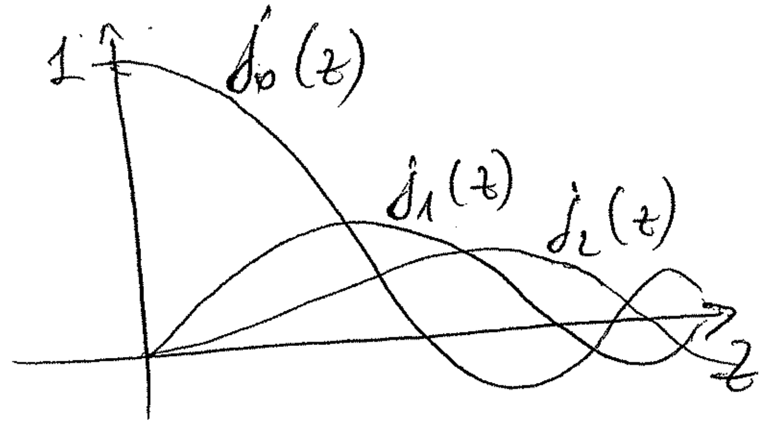
$$n_l(z) = \sqrt{\frac{\pi}{2}}\,(-1)^{l+1}\,\frac{J_{-(l+\frac{1}{2})}(z)}{\sqrt{z}}$$

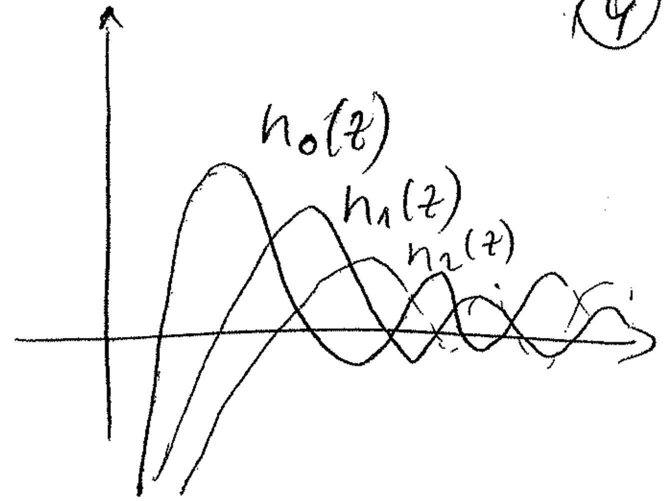
<u>Properties:</u> $\quad z \to 0 \Rightarrow j_l(z) \to \frac{z^l}{(2l+1)!!}$

$$n_l(z) \to -\frac{(2l-1)!!}{z^{l+1}}$$

$$z \to \infty \Rightarrow j_l(z) \to \frac{1}{z}\cos\left[z - \frac{\pi(l+1)}{2}\right]$$

$$n_l(z) \to \frac{1}{z}\sin\left[z - \frac{\pi(l+1)}{2}\right]$$





$$j_0(z) = \frac{\sin z}{z}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}$$

$$j_2(z) = \left(\frac{3}{z^3} - \frac{1}{z}\right)\sin z - \frac{3}{z^2}\cos z$$

$$n_0(z) = -\frac{\cos z}{z}$$

$$n_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}$$

$\vdots$

See A.5 (pp. 450 – 454) of Sakurai

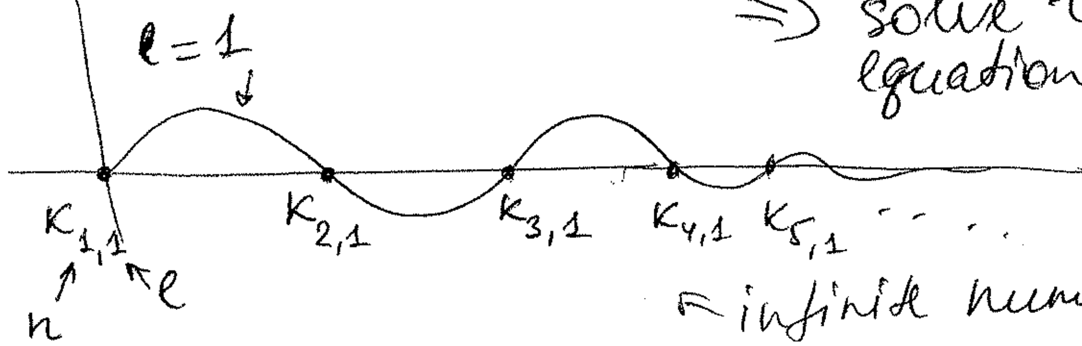
Back to our problem $\Rightarrow$

$$u_\ell(r) = kr\left(\tilde{C}_1 j_\ell(kr) + \tilde{C}_2 n_\ell(kr)\right)$$

$u_\ell(0) = 0 \Rightarrow \tilde{C}_2 = 0$ (since $n_\ell(z) \underset{z\to 0}{\rightarrow} \frac{1}{z^{\ell+1}}$, $u_\ell(z) \underset{z\to 0}{\rightarrow} \frac{1}{z^\ell}$)

$u_\ell(R) = 0 \Rightarrow \underline{j_\ell(kR) = 0}$

$\Rightarrow$ solve transcendental equation to find $k_{n,\ell}$'s



← infinite number of $k_{n,\ell}$

For example, for $l=1 \Rightarrow$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z} \Rightarrow j_1(K_{n,1}R) = 0 \Rightarrow$$

$$\tan(K_{n,1}R) = K_{n,1}R$$ $\Rightarrow$ solve for K_n's graphically or numerically

Then, $E_{n,l} = \frac{\hbar^2}{2\mu} K_{n,l}^2$

note that energy levels depend on l (since K_n's are different for each l)
no "accidental" degeneracy as in the case of Coulomb potential

Example 2

The hydrogen atom is in a stationary $|n,l,m\rangle$ state. Calculate the expectation value of $\underline{P}^4$!

momentum

Solution:

Since $\hat{H} = \frac{\vec{P}^2}{2\mu} - \frac{e^2}{r} \Rightarrow \vec{P}^2 = 2\mu\left(\hat{H} + \frac{e^2}{r}\right) \Rightarrow$

$$\langle n,l,m|\vec{P}^4|n,l,m\rangle = 4\mu^2 \langle n,l,m|\left(\hat{H}+\frac{e^2}{r}\right)^2|n,l,m\rangle$$

$$= 4\mu^2\left(\underbrace{\langle \hat{H}^2\rangle}_{=E_n^2} + e^2\langle \hat{H}\frac{1}{r}\rangle + e^2\langle \frac{1}{r}\hat{H}\rangle + e^4\langle\frac{1}{r^2}\rangle\right)$$

$(\hat{H}|n,l,m\rangle = E_n|n,l,m\rangle)$ $=$

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$$= 4\mu^2 \left(E_n^2 + 2e^2 E_n \left\langle \frac{1}{r} \right\rangle + e^4 \left\langle \frac{1}{r^2} \right\rangle \right) =$$

$$\langle n,l,m \,|\, \hat{H} \frac{1}{r} \,|\, n,l,m \rangle \qquad E_n = -\frac{E_I}{n^2}$$

$$\langle n,l,m \,|\, E_n$$

$$= \frac{\mu^4 e^8}{\hbar^4 n^4} \left[\frac{8n}{2l+1} - 3 \right]$$

HW!