Physics 828: Homework Set No. 5

Due date: Friday, February 17, 2011, 1:00pm in PRB M2043 (Biao Huang's office)

Total point value of set: 60 points

Problem 1 (10 pts.): Exercise 12.5.12 (Shankar, p. 338)

Problem 2 (10 pts.): Exercise 12.5.13 (Shankar, p. 338)

Problem 3 (10 pts.): Exercise 12.6.1 (Shankar, p. 340)

Problem 4 (10 pts.): Exercise 12.6.8 (Shankar, p. 349)

Problem 5 (20 pts.): Exercise 12.6.9 (Shankar, p. 349)

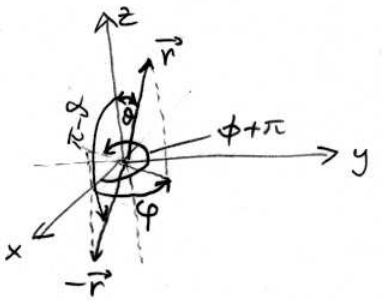
Exercise 12.5.12 (p. 338)

$[\hat{L}^2, \hat{\pi}] = [\hat{L}_z, \hat{\pi}] = 0 \Rightarrow$ common set of eigenstates for $\hat{L}^2, \hat{L}_z$ and $\hat{\pi}$.

Since $|\ell m\rangle \leftrightarrow \langle \vartheta, \varphi | \ell m \rangle = Y_{\ell m}(\vartheta, \varphi)$ completely classifies the common eigenstates of $\hat{L}^2, \hat{L}_z$, with no remaining degeneracy, the states $|\ell m\rangle$ should automatically be eigenstates of $\hat{\pi}$.

Under parity $\hat{\pi}$: $\vec{r} \overset{\hat{\pi}}{\longmapsto} -\vec{r}$

$(x, y, z) \longmapsto (-x, -y, -z)$



$r\sin\vartheta\cos\varphi \longmapsto -r\sin\vartheta\cos\varphi = r\sin(\pi-\vartheta)\cos(\varphi+\pi)$

$r\sin\vartheta\sin\varphi \longmapsto -r\sin\vartheta\sin\varphi = r\sin(\pi-\vartheta)\sin(\varphi+\pi)$

$r\cos\vartheta \longmapsto -r\cos\vartheta = r\cos(\pi-\vartheta)$

hence $\vartheta \overset{\hat{\pi}}{\longmapsto} \pi - \vartheta$

$\varphi \longmapsto \varphi + \pi$ ✓

$$Y_{\ell\ell}(\vartheta,\varphi) = (-1)^\ell \sqrt{\frac{(2\ell+1)!}{4\pi}} \frac{1}{2^\ell \ell!} \sin^\ell(\vartheta)\, e^{i\ell\varphi}$$

$$\overset{\hat{\pi}}{\longmapsto} (-)^\ell \sqrt{\frac{(2\ell+1)!}{4\pi}} \frac{1}{2^\ell \ell!} \underbrace{\sin^\ell(\pi-\vartheta)}_{=\sin^\ell\vartheta} \underbrace{e^{i\ell(\varphi+\pi)}}_{=(e^{i\pi})^\ell e^{i\ell\varphi} = (-)^\ell e^{i\ell\varphi}}$$

$$= (-)^\ell Y_{\ell\ell}(\vartheta,\varphi)$$

Next $Y_{\ell,m-1}(\vartheta,\varphi) \sim L_- Y_{\ell m}(\vartheta,\varphi) = -\hbar e^{-i\varphi}\left(\frac{\partial}{\partial\vartheta} - i\frac{\cos\vartheta}{\sin\vartheta}\frac{\partial}{\partial\varphi}\right) Y_{\ell m}$

Under the transformation $\vartheta \to \pi - \vartheta$, $\varphi \to \varphi + \pi$

$$L_- \longmapsto -\hbar e^{-i\varphi} \underbrace{e^{-i\pi}}_{(-1)} \left(\underbrace{\frac{\partial}{\partial(\pi-\vartheta)}}_{-\frac{\partial}{\partial\vartheta}} - i \underbrace{\frac{\cos(\pi-\vartheta)}{\sin(\pi-\vartheta)}}_{\frac{-\cos\vartheta}{+\sin\vartheta}} \underbrace{\frac{\partial}{\partial(\varphi+\pi)}}_{\frac{\partial}{\partial\varphi}} \right)$$

$$= -\hbar e^{-i\varphi}\left(\frac{\partial}{\partial\vartheta} - i\cot\vartheta\frac{\partial}{\partial\varphi}\right) = L_- \Rightarrow$$

$\Rightarrow [\hat{L}_-, \hat{\pi}] = 0$

So we can write the following chain of arguments:

$\underline{\ell = m}$: $\hat{\pi}|\ell\ell\rangle = (-1)^\ell |\ell\ell\rangle$

$\underline{m \to m-1}$: $\hat{\pi}|\ell, m-1\rangle = \hat{\pi} \frac{1}{\hbar\sqrt{(\ell+m)(\ell-m+1)}} \hat{L}_- |\ell m\rangle$

$= \frac{\hat{L}_-}{\hbar\sqrt{(\ell+m)(\ell-m+1)}} \underbrace{\hat{\pi}|\ell m\rangle}_{=(-1)^\ell |\ell m\rangle}$

$= (-1)^\ell \frac{\hat{L}_-}{\hbar\sqrt{(\ell+m)(\ell-m+1)}} |\ell m\rangle = (-1)^\ell |\ell, m-1\rangle$

Hence $\boxed{\hat{\pi}|\ell m\rangle = (-1)^\ell |\ell m\rangle \quad \forall\, \ell, m}$

Exercise 12.5.13 (p. 338)

$$\psi(x,y,z) = N(x+y+2z)\,e^{-\alpha r} \qquad r = \sqrt{x^2+y^2+z^2}$$

$$= N(r\sin\vartheta\sin\varphi + r\cos\varphi + 2r\cos\vartheta)\,e^{-\alpha r}$$

$$= N r e^{-\alpha r}(\sin\vartheta(\sin\varphi+\cos\varphi) + 2\cos\vartheta)$$

(1)

$$Y_{1,\pm1}(\vartheta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\vartheta\, e^{\pm i\varphi} \qquad (12.5.39)$$

$$= \mp\sqrt{\frac{3}{8\pi}}\,\frac{r\sin\vartheta(\cos\varphi \pm i\sin\varphi)}{r}$$

$$= \mp\sqrt{\frac{3}{4\pi}}\,\frac{x \pm iy}{\sqrt{2}\,r}$$

$$Y_{10}(\vartheta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\vartheta = \sqrt{\frac{3}{4\pi}}\,\frac{z}{r}$$

$$\Rightarrow Y_{11} + Y_{1,-1} = \sqrt{\frac{3}{8\pi}}\left(\frac{-x-iy}{r} + \frac{x-iy}{r}\right) = -2i\,\frac{y}{r}\sqrt{\frac{3}{8\pi}}$$

$$\Rightarrow \boxed{y = i\sqrt{\frac{8\pi}{3}}\,r\,\frac{Y_{11}+Y_{1,-1}}{2} = i\sqrt{\frac{4\pi}{3}}\,r\left(\frac{Y_{1,-1}+Y_{11}}{\sqrt{2}}\right)}$$

$$Y_{11} - Y_{1,-1} = \sqrt{\frac{3}{8\pi}}\left(\frac{-x-iy}{r} - \frac{x-iy}{r}\right) = -2\sqrt{\frac{3}{8\pi}}\,\frac{x}{r}$$

$$\Rightarrow \boxed{x = -\sqrt{\frac{8\pi}{3}}\,r\,\frac{Y_{1,-1}-Y_{11}}{2} = \sqrt{\frac{4\pi}{3}}\,r\left(\frac{Y_{1,-1}-Y_{11}}{\sqrt{2}}\right)}$$

$$\boxed{z = \sqrt{\frac{4\pi}{3}}\,r\,Y_{10}}$$

(2) $$\Rightarrow x+y+2z = \sqrt{\frac{8\pi}{3}}\,r\left(\frac{Y_{1,-1}-Y_{11}}{2} + i\,\frac{Y_{1,-1}+Y_{11}}{2} + \frac{2}{\sqrt{2}}Y_{10}\right)$$

$$= \sqrt{\frac{4\pi}{3}}\,r\left(Y_{1,-1}\,\frac{1+i}{\sqrt{2}} + Y_{11}\,\frac{i-1}{\sqrt{2}} + 2Y_{10}\right)$$

$$= \left(c(\ell_z=-1)\,Y_{1,-1} + c(\ell_z=1)\,Y_{11} + c(\ell_z=0)\,Y_{10}\right)\sqrt{\frac{4\pi}{3}}\,r$$

The probabilities for finding a given value of l_z are $\sim |c(l_z)|^2$

$$|c(l_z=0)|^2 = 4$$

$$|c(l_z=1)|^2 = \frac{i-1}{\sqrt{2}} \cdot \frac{-i-1}{\sqrt{2}} = \frac{1+i-i+1}{2} = 1$$

$$|c(l_z=-1)|^2 = \frac{(1+i)(1-i)}{2} = 1$$

These add up to 6; hence

$$P(l_z=0) = \frac{4}{6} = \frac{2}{3}$$

$$P(l_z=-1) = \frac{1}{6} = P(l_z=+1)$$

Exercise 12.6.1 (p.340)

$$\psi_E(r,\vartheta,\varphi) = A\, e^{-r/a_0} \quad \Rightarrow u_E(r) = r e^{-r/a_0}$$

(1) ψ_E is independent of ϑ, φ $\Rightarrow \psi_E(r,\vartheta,\varphi) \sim e^{-r/a_0} Y_{00}(\vartheta,\varphi)$

$\Rightarrow$ The state $|\psi_E\rangle$ is an angular momentum eigenstate with $\ell = 0$ and $m = 0$.

(2) Assume $V(r) \xrightarrow[r\to\infty]{} 0$

Schrödinger equation:

$$\left(\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2}(E - V(r))\right) r e^{-r/a_0} = 0$$

$$\frac{d^2}{dr^2}\left(r e^{-r/a_0}\right) = \frac{d}{dr}\left(-\frac{r}{a_0} e^{-r/a_0} + e^{-r/a_0}\right)$$

$$= -\frac{1}{a_0} e^{-r/a_0} + \frac{r}{a_0^2} e^{-r/a_0} - \frac{1}{a_0} e^{-r/a_0}$$

$$= \frac{1}{a_0}\left(\frac{r}{a_0} - 2\right) e^{-r/a_0}$$

$$\Rightarrow \frac{1}{a_0}\left(\frac{r}{a_0} - 2\right) e^{-r/a_0} = -\frac{2\mu E}{\hbar^2} r e^{-r/a_0} + \frac{2\mu}{\hbar^2} V(r) r e^{-r/a_0}$$

$$\Rightarrow \frac{1}{a_0}\left(\frac{1}{a_0} - \frac{2}{r}\right) = -\frac{2\mu E}{\hbar^2} + \frac{2\mu}{\hbar^2} V(r)$$

Take $r \to \infty$, use $V(r) \to 0$:

$$\frac{1}{a_0^2} = -\frac{2\mu E}{\hbar^2} \quad \Rightarrow \quad \boxed{E = -\frac{\hbar^2}{2\mu a_0^2}}$$

(3) Back to the full Schrödinger equation:

(remember, $\ell = 0$, hence no centrifugal potential)

$$\frac{1}{a_0^2} - \frac{2}{r a_0} = + \frac{1}{a_0^2} + \frac{2\mu}{\hbar^2} V(r)$$

$$\Rightarrow \boxed{V(r) = \frac{\hbar^2}{2\mu}\left(-\frac{2}{a_0 r}\right) = -\frac{\hbar^2}{\mu a_0 r}}$$

Exercise 12.6.8 (p. 349)

Spherical box of radius r_0: $V(r) = \lim_{V_0 \to \infty} V_0 \, \Theta(r - r_0)$

Schrödinger equation:

$$\psi_{Eem}(r, \vartheta, \varphi) = \frac{u_{Ee}(r)}{r} Y_{em}(\vartheta, \varphi)$$

$$\left[\frac{d^2}{dr^2} + \underbrace{\frac{2\mu}{\hbar^2}(E - V(r))}_{k^2} - \frac{\ell(\ell+1)}{r^2} \right] u_{Ee}(r) = 0$$

For $r < r_0$: $\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} \right] u_{Ee}(r) = 0$

For $r \geq r_0$: $u_{Ee}(r) \equiv 0$

Change variables $\rho = kr$

$$\left(-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} \right) u_{Ee}(\rho) = 0$$

$\Rightarrow$ solution is that for a free particle, but with a boundary condition: $R_{Ee}(r_0) = 0$

The solution must be regular at $r = 0$

$$\Rightarrow \boxed{\begin{array}{l} \psi_{n\ell m}(r, \vartheta, \varphi) = N j_\ell(k_{n\ell} r) \, Y_{\ell m}(\vartheta, \varphi) \\ \text{with } k_{n\ell} r_0 = n^{\text{th}} \text{ zero of } j_\ell(x) \end{array}}$$

For $\ell = 0$: $j_0(\rho) = \frac{\sin \rho}{\rho}$

$\Rightarrow \psi_{n0m}(r) = N_n \frac{\sin(k_n r)}{r}$ with $k_n r_0 = n\pi$ $(n = 1, 2, 3 \ldots)$

$$\Rightarrow k_n^2 r_0^2 = n^2\pi^2 \Rightarrow \frac{2\mu r_0^2}{\hbar^2} E_n = n^2\pi^2$$

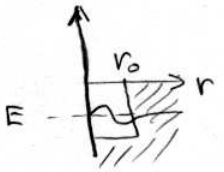
$$\Rightarrow \boxed{E_n = \frac{\hbar^2 n^2 \pi^2}{2\mu r_0^2}}$$

μ = mass of particle

Exercise 12.6.9 (p. 349)

$V(r) = -V_0\,\theta(r-r_0)$ spherical well

$\psi_E(r,\vartheta,\varphi) = \frac{u_E(r)}{r}$ for $\ell=0$ states



$-V_0 < E < 0$ for bound states:

Schrödinger equation for $\ell=0$:

$$\left(\frac{d^2}{dr^2} + \frac{2\mu(V_0-|E|)}{\hbar^2}\right) u_E(r) = 0 \qquad r < r_0$$

$$\left(\frac{d^2}{dr^2} - \frac{2\mu|E|}{\hbar^2}\right) u_E(r) = 0 \qquad r \geq r_0$$

define $\kappa^2 = \frac{2\mu|E|}{\hbar^2} > 0$, $k^2 = \frac{2\mu(V_0-|E|)}{\hbar^2} > 0$

$$\Rightarrow u_E(r) = \begin{cases} A\sin(kr) + B\cos(kr) & r < r_0 \\ Ce^{-\kappa r} + De^{\kappa r} & r \geq r_0 \end{cases}$$

Normalizability $\rightarrow$ $B=0$, $D=0$

At $r=r_0$: Continuity of ψ:

$$A\sin(kr_0) = Ce^{-\kappa r_0}$$

Continuity of ψ':

$$Ak\cos(kr_0) = -\kappa Ce^{-\kappa r_0}$$

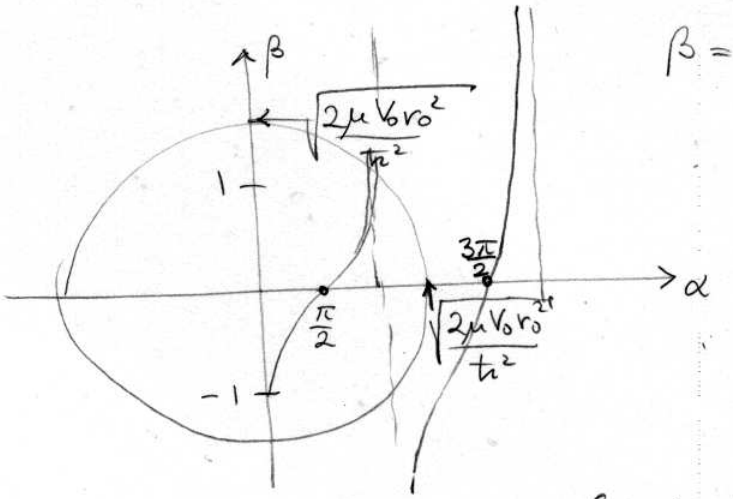
Divide by each other:

$$\frac{1}{k}\tan(kr_0) = -\frac{1}{\kappa} \Rightarrow \boxed{\frac{k}{\kappa} = -\tan(kr_0)}$$ ✓

or $\frac{\kappa r_0}{k r_0} = -\cot(kr_0)$

Define $\beta = kr_0$, $\alpha = kr_0$

$\alpha^2 + \beta^2 = \frac{2\mu r_0^2 V_0}{\hbar^2}$ and $\beta = -\alpha \cot\alpha$



$\beta = 0$ at $\cos\alpha = 0 \Leftrightarrow \alpha = (2n+1)\frac{\pi}{2}$

Only $\alpha > 0$, $\beta > 0$ are physical

If $\sqrt{\frac{2\mu r_0^2 V_0}{\hbar^2}} < \frac{\pi}{2}$, then the two curves do not intersect in the first quadrant → no bound state.

⇒ No bound state if

$$\boxed{V_0 < \frac{\pi^2 \hbar^2}{8\mu r_0^2}} \; V$$

If V_0 is large, the circle above is big and intersects with several branches of the $\alpha\cot\alpha$ function → several bound state.