PHYS 606 – Spring 2015 – Homework IX – Solution

Problem [1]

(a) $\frac{d}{d\xi}\left((1-\xi^2)\frac{dP}{d\xi}\right) + \lambda P = 0 \qquad (\text{case } m=0)$

Ansatz $P(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$

$$\Rightarrow \sum_{j=2}^{\infty} j(j-1)a_j(1-\xi^2)\xi^{j-2} + \sum_{j=1}^{\infty} j a_j(-2\xi)\xi^{j-1} + \sum_{j=0}^{\infty}\lambda a_j \xi^j = 0$$

$$\Rightarrow \sum_{j=0}^{\infty}\left((j+2)(j+1)a_{j+2} - j(j-1)a_j - 2j a_j + \lambda a_j\right)\xi^j = 0$$

$$\Rightarrow a_{j+2} = \frac{-\lambda + j(j+1)}{(j+1)(j+2)}\, a_j \qquad \forall j \in \mathbb{N}$$

For $\lambda = \ell(\ell+1)$ with some $\ell \in \mathbb{N}$ the power series terminates and $P(\xi)$ is a polynomial.

Otherwise, for large j $\frac{a_{j+2}}{a_j} \simeq \frac{j}{j+2} \Rightarrow a_j \sim \frac{1}{j}$; at $\xi = \pm 1$ $P(\xi) \sim \sum_{j=0}^{\infty} \frac{1}{j}(-1)^j$ which diverges.

(b) $P_\ell(\xi) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{d\xi^\ell}(\xi^2-1)^\ell$ is a polynomial of degree ℓ $\left\{\begin{matrix}\text{even for even } \ell \\ \text{odd for odd } \ell\end{matrix}\right\}(*)$

Term of degree j ($j \le \ell$) is (neglect overall normalization): $\frac{d^\ell}{d\xi^\ell}\binom{\ell}{\frac{\ell+j}{2}}\xi^{2\frac{\ell+j}{2}}(-1)^{\frac{\ell-j}{2}}$

(note: $\ell+j$ always even because of $(*)$)

Term of degree $j+2$ is: $\frac{d^\ell}{d\xi^\ell}\binom{\ell}{\frac{\ell+j+2}{2}}\xi^{2\frac{\ell+j+2}{2}}(-1)^{\frac{\ell-j-2}{2}}$

$$\Rightarrow \frac{a_{j+2}}{a_j} = (-1)\frac{(\ell+j+2)(\ell+j+1)}{(j+1)(j+2)}\underbrace{\frac{\frac{\ell+j}{2}!\;\frac{\ell-j}{2}!}{\frac{\ell+j+2}{2}!\;\frac{\ell-j-2}{2}!}}_{\frac{(\ell-j)}{(\ell+j+2)}} = -\frac{\ell(\ell+1)-j(j+1)}{(j+1)(j+2)}$$

Same recursion relation as in (a) for $\lambda = \ell(\ell+1)$! $\Rightarrow$ The $P_\ell(\xi)$ are the solutions to Legendre's equation for $m=0$.

(c) $P_0(\xi) = 1 \qquad P_1(\xi) = \xi$

$$P_2(\xi) = \frac{1}{8}\frac{d^2}{d\xi^2}\left(\xi^4 - 2\xi^2 + 1\right) = \frac{1}{2}\left(3\xi^2 - 1\right)$$

$$P_3(\xi) = \frac{1}{8\cdot 6}\frac{d^3}{d\xi^3}\left(\xi^6 - 3\xi^4 + 3\xi^2 - 1\right) = \frac{1}{2}\left(5\xi^3 - 3\xi\right)$$

(d) Assume $\ell \geq \ell'$

(otherwise start partial integration in the next line with other term)

$$\int_{-1}^{+1} P_\ell(\xi) P_{\ell'}(\xi)\, d\xi = \frac{1}{2^\ell 2^{\ell'} \ell! \ell'!}\int_{-1}^{+1} \frac{d^\ell}{d\xi^\ell}(\xi^2-1)^\ell \frac{d^{\ell'}}{d\xi^{\ell'}}(\xi^2-1)^{\ell'}\, d\xi$$

$$\underset{\ell\times\text{ part. int.}}{=} \frac{1}{2^\ell 2^{\ell'} \ell! \ell'!}\int_{-1}^{+1} (-1)^\ell (\xi^2-1)^\ell \frac{d^{\ell+\ell'}}{d\xi^{\ell+\ell'}}(\xi^2-1)^{\ell'}\, d\xi$$

boundary terms have terms $\frac{d^n}{d\xi^n}(\xi^2-1)^m$ with $n<m$ which have left-over factors (ξ^2-1) after differentiation which vanish at $\xi = \pm 1$.

$\ell + \ell' \geq 2\ell' \Rightarrow$ integrand vanishes except for $\ell = \ell'$

$$\Rightarrow \int_{-1}^{+1} P_\ell(\xi) P_{\ell'}(\xi)\, d\xi = \frac{1}{(2^\ell \ell!)^2}\int_{-1}^{+1} (1-\xi^2)^\ell (2\ell)!\, d\xi \quad \delta_{\ell\ell'}$$

$$\int_{-1}^{+1} (1-\xi^2)^\ell d\xi \underset{\substack{\xi = \sin u \\ d\xi = \cos u\, du}}{=} 2\int_0^{\pi} \cos^{2\ell+1} u\, du = 2\,\frac{2\ell(2\ell-1)\cdots 2}{(2\ell+1)(2\ell-1)\cdots 3}\underbrace{\int_0^{\pi}\cos u\, du}_{=1}$$

Here: use recursive formula for powers of trig fcts. $\int \cos^n u\, dx = \frac{1}{n}\cos^{n-1} u \sin u + \frac{n-1}{n}\int \cos^{n-2} u\, du$

Boundary terms have at least one cos sin factor and disappear for $u = 0, u = \pi$

$$\Rightarrow \int_{-1}^{+1} P_\ell(\xi) P_{\ell'}(\xi)\, d\xi = \delta_{\ell\ell'}\,\frac{2(2\ell)!}{2^\ell \cancel{2^\ell}\, \ell! \cancel{\ell!}}\,\frac{\cancel{2^\ell}\, \cancel{\ell!}}{(2\ell+1)\cdots 3} =$$

$$= \frac{2}{2\ell+1}\,\delta_{\ell\ell'}\,\underbrace{\frac{2\ell(2\ell-2)\cdots 2\cdot(2\ell-1)(2\ell-3)\cdots 3}{2^\ell \ell! \quad (2\ell-1)\cdots 3}}_{=1}$$

(e) Introduce $\tilde{P}_\ell^m(\xi) = \frac{d^m}{d\xi^m} P_\ell(\xi)$; then $P_\ell^m(\xi) = (1-\xi^2)^{m/2} \tilde{P}_\ell^m(\xi)$

We have shown that for the $P_\ell(\xi)$: $\frac{d}{d\xi}\left((1-\xi^2)\frac{d}{d\xi}\right)P_\ell(\xi) + \lambda P_\ell(\xi) = 0$

for $\lambda = \ell(\ell+1)$

Differentiate m-times w.r.t. ξ:

$$\frac{d}{d\xi}\left((1-\xi^2)\frac{d}{d\xi}\right)\frac{d^m}{d\xi^m} P_\ell + \lambda \frac{d^m}{d\xi^m} P_\ell + \frac{d}{d\xi}\left(m(-2\xi)\frac{d^m}{d\xi^m}\right) P_\ell + \binom{m}{2}(-2)\frac{d^m}{d\xi^m} P_\ell = 0$$

$\Rightarrow$ The $\tilde{P}_\ell^m$ satisfy

$$(1-\xi^2)\frac{d^2}{d\xi^2}\tilde{P}_\ell^m - 2\xi(m+1)\frac{d}{d\xi}\tilde{P}_\ell^m + \left(\lambda - 2m - m(m-1)\right)\tilde{P}_\ell^m = 0 \qquad (*)$$

On the other hand from Legendre's DE:

$$(1-\xi^2)\,\frac{m}{2}\left(\frac{m}{2}-1\right)(-2\xi)^2(1-\xi^2)^{\frac{m}{2}-2}\tilde{P}_\ell^m + (1-\xi^2)\,\frac{m}{2}(-2)(1-\xi^2)^{\frac{m}{2}-1}\tilde{P}_\ell^m$$

$$+2(1-\xi^2)\frac{m}{2}(-2\xi)(1-\xi^2)^{\frac{m}{2}-1}\frac{d}{d\xi}\tilde{P}_\ell^m + (1-\xi^2)(1-\xi^2)^{\frac{m}{2}}\frac{d^2}{d\xi^2}\tilde{P}_\ell^m$$

$$+4\xi^2\frac{m}{2}(1-\xi^2)^{\frac{m}{2}-1}\tilde{P}_\ell^m - 2\xi(1-\xi^2)^{\frac{m}{2}}\frac{d}{d\xi}\tilde{P}_\ell^m - m^2(1-\xi^2)^{\frac{m}{2}-1}\tilde{P}_\ell^m + \lambda(1-\xi^2)^{\frac{m}{2}}\tilde{P}_\ell^m = 0$$

This is the same as $(*) * (1-\xi^2)^{\frac{m}{2}}$ $\Rightarrow$ The P_ℓ^m satisfy Legendre's equation.

Problem [2]

(a) (i) $[L_j, L_k] = \varepsilon_{j\ell m}\varepsilon_{kno}[r_\ell p_m, r_n p_o] = \varepsilon_{j\ell m}\varepsilon_{kno}\left(r_\ell r_n \underbrace{[p_m, p_o]}_{=0} + r_\ell[p_m, r_n]p_o + \underbrace{[r_\ell, r_n]}_{=0} p_o p_m + r_n[r_\ell, p_o]p_m\right)$

$$= i\hbar\,\varepsilon_{j\ell m}\varepsilon_{kno}\left(-\delta_{mn} r_\ell p_o + \delta_{\ell o} r_n p_m\right)$$

$$= i\hbar\left[(\delta_{jk}\delta_{\ell o} - \delta_{jo}\delta_{k\ell})r_\ell p_o - (\delta_{jk}\delta_{mn} - \delta_{jn}\delta_{km})r_n p_m\right]$$

$$= i\hbar\left(-r_k p_j + r_j p_k\right) = i\hbar\,\varepsilon_{jk\ell} L_\ell$$

(ii) $[L_j, L^2] = \underbrace{[L_j, L_j^2]}_{=0} + \sum_{i\neq j}[L_j, L_i^2] = \sum_{i\neq j}\left(L_i[L_j, L_i] + [L_j, L_i]L_i\right)$

$$= \sum_{i\neq j}(i\hbar)\,\varepsilon_{jik}\left(L_i L_k + L_k L_i\right) = 0$$

antisymmetric in i,k symmetric in i,k

(b) Spherical coordinates:
$$\begin{pmatrix} r = \sqrt{x^2+y^2+z^2} \\ \phi = \arctan \frac{y}{x} \\ \theta = \arccos \frac{z}{\sqrt{x^2+y^2+z^2}} \end{pmatrix}$$

Unit vectors:

$$\hat{r} = \sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z}$$
$$\hat{\theta} = \cos\theta\cos\phi\,\hat{x} + \cos\theta\sin\phi\,\hat{y} - \sin\theta\,\hat{z}$$
$$\hat{\phi} = -\sin\phi\,\hat{x} + \cos\phi\,\hat{y}$$

Jacobi matrix:
$$J = \frac{\partial(r,\theta,\phi)}{\partial(x,y,z)} = \begin{pmatrix} \frac{x}{r} & \frac{y}{r} & \frac{z}{r} \\ \frac{1}{r^2}\frac{xz}{\sqrt{x^2+y^2}} & \frac{1}{r^2}\frac{yz}{\sqrt{x^2+y^2}} & -\frac{1}{r^2}\sqrt{x^2+y^2} \\ \frac{-y/x^2}{1+y^2/x^2} & \frac{1/x}{1+y^2/x^2} & 0 \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \frac{1}{r}\cos\theta\cos\phi & \frac{1}{r}\cos\theta\sin\phi & -\frac{1}{r}\sin\theta \\ -\frac{1}{r}\frac{\sin\phi}{\sin\theta} & \frac{1}{r}\frac{\cos\phi}{\sin\theta} & 0 \end{pmatrix}$$

$$\frac{\partial}{\partial x} = J_{11}\frac{\partial}{\partial r} + J_{21}\frac{\partial}{\partial\theta} + J_{31}\frac{\partial}{\partial\phi} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial}{\partial\theta} - \frac{1}{r}\sin\phi\frac{\partial}{\partial\phi}$$

$\frac{\partial}{\partial y}$, $\frac{\partial}{\partial z}$ similarly

$$\Rightarrow \nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}$$

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r}\frac{\partial}{\partial r}$$
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \qquad \text{(standard form)}$$

(c)
$$L_x = (-i\hbar)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = -i\hbar\Big[r\sin\theta\sin\phi\left(\cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}\right)$$
$$- r\cos\theta\left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\phi\frac{\partial}{\partial\theta} + \frac{1}{r}\frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\phi}\right)\Big]$$
$$= -i\hbar\left[-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]$$

Similarly $L_y = -i\hbar\left[\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$L^2 = -\hbar^2\left[\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\theta^2} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + \cot\theta\frac{\partial}{\partial\theta}\right] = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]$$

(d) $L_z Y = m\hbar Y \quad ; \quad L^2 Y = \lambda \hbar^2 Y$

Separation ansatz $Y(\theta,\phi) = \Phi(\phi)\,\Theta(\theta)$

$\Rightarrow -i\hbar \frac{\partial}{\partial\phi} \Phi = m\hbar \Phi \quad \Rightarrow \Phi(\phi) = e^{im\phi}$

Φ is 2π-periodic in ϕ, i.e. $\Phi(\phi+2\pi) = \Phi(\phi) \Rightarrow e^{im2\pi} = 1 \Rightarrow m$ integer!

$L^2 Y = -\hbar^2 \left[\frac{1}{\sin^2\theta}(-m^2) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right)\right] \Theta = \lambda\hbar^2 \Theta$

Substitute $\xi = \cos\theta \Rightarrow \sin\theta = \sqrt{1-\xi^2} \; ; \; \frac{\partial}{\partial\theta} = -\sin\theta \frac{\partial}{\partial\xi}$

$\Rightarrow \frac{\partial}{\partial\xi}\left((1-\xi^2)\frac{\partial}{\partial\xi}\right)\Theta(\xi) - \frac{m^2}{1-\xi^2}\Theta(\xi) + \lambda\,\Theta(\xi) = 0$ Legendre's equation from [1]

$\Rightarrow Y(\theta,\phi) = e^{im\phi}\, P_l^m(\cos\theta)$ (up to proper normalization)

Problem [3]

(a) $\langle H \rangle [\psi_\pm^0] = (N_\pm^0)^2 \left(2\int_{\mathbb{R}} \psi_0(x-a) H \psi_0(x-a)\,dx \pm 2\int_{\mathbb{R}} \psi_0(x-a) H \psi_0(x+a)\,dx \right)$

with $(N_\pm^0)^2 = \left[\underbrace{2\int_{\mathbb{R}} \psi_0^2(x-a)\,dx}_{=1} \pm 2\int_{\mathbb{R}} \psi_0(x-a)\psi_0(x+a)\,dx \right]^{-1} =$

$= \left[2\left(1 \pm e^{-\frac{m\omega}{\hbar}a^2}\right)\right]^{-1}$

$\int_{\mathbb{R}} \psi_0(x-a) H \psi_0(x-a)\,dx = \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \left(-\frac{\hbar^2}{2m} \int_{\mathbb{R}} e^{-\frac{m\omega}{\hbar}(x-a)^2}\left(-\frac{m\omega}{\hbar} + \frac{m^2\omega^2}{\hbar^2}(x-a)^2\right)dx \right.$

$\left. + \frac{1}{2}m\omega^2 \int_{\mathbb{R}} e^{-\frac{m\omega}{\hbar}(x-a)^2} (|x|-a)^2\,dx \right)$

$= \frac{1}{4}\hbar\omega + \frac{1}{2}m\omega^2 \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \int_{\mathbb{R}} e^{-\frac{m\omega}{\hbar}(x-a)^2} (|x|-a)^2\,dx$

$$\int_{\mathbb{R}} \psi_0(x-a) H \psi_0(x+a)\, dx = \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \left(-\frac{\hbar^2}{2m} \int_{\mathbb{R}} e^{-\frac{m\omega}{\hbar}x^2} \left(-\frac{m\omega}{\hbar} + \frac{m^2\omega^2}{\hbar^2}(x+a)^2\right) dx \; e^{-\frac{m\omega}{\hbar}a^2} \right.$$

$$\left. + \frac{1}{2} m\omega \int_{\mathbb{R}} e^{-\frac{m\omega}{\hbar}x^2} (|x|-a)^2 dx \; e^{-\frac{m\omega}{\hbar}a^2} \right)$$

$$= e^{-\frac{m\omega}{\hbar}a^2} \left[\frac{1}{4}\hbar\omega - \frac{1}{4} m\omega^2 a^2 + \frac{1}{2} m\omega^2 \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \int_{\mathbb{R}} e^{-\frac{m\omega}{\hbar}x^2} (|x|-a)^2 dx \right]$$

(b) Two remaining integrals for $a \to \infty$ (with $\alpha = \sqrt{\frac{m\omega}{\hbar}}\, a$, $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$)

$$I_1 = \int_{\mathbb{R}} \psi_0(x-a) H \psi_0(x-a)\, dx = \frac{1}{2}\hbar\omega \left[\frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-(\xi-\alpha)^2} \underbrace{(|\xi|-\alpha)^2}_{(\xi-\alpha)^2 + \underbrace{2\alpha(\xi-|\xi|)}_{\substack{4\alpha\xi \text{ for } \xi\le 0 \\ 0 \text{ for } \xi \ge 0}}} d\xi \right]$$

$$= \frac{1}{2}\hbar\omega \left[1 + \frac{4\alpha}{\sqrt{\pi}} \int_{-\infty}^{0} \xi\, e^{-(\xi-\alpha)^2} d\xi \right]$$

Integrand peaked at $\xi = \alpha \to \infty$ $\Rightarrow$ integral dominated by $\xi \approx 0$

$$\Rightarrow e^{-(\xi-\alpha)^2} \approx e^{-\alpha^2} e^{2\xi\alpha}$$

$$\Rightarrow I_1 = \frac{1}{2}\hbar\omega \left[1 + \frac{4\alpha}{\sqrt{\pi}} e^{-\alpha^2} \int_{-\infty}^{0} \xi e^{2\xi\alpha} d\xi \right] \underset{\text{part. int.}}{=} \frac{1}{2}\hbar\omega \left[1 - \frac{1}{\sqrt{\pi}\,\alpha} e^{-\alpha^2} \right]$$

$$I_2 = \int_{\mathbb{R}} \psi_0(x-a) H \psi_0(x+a)\, dx = \frac{1}{2}\hbar\omega\, e^{-\alpha^2} \left[1 + \frac{4\alpha}{\sqrt{\pi}} \int_{0}^{\infty} \xi\, e^{-\xi^2} d\xi \right]$$

$$= \frac{1}{2}\hbar\omega\, e^{-\alpha^2} \left[1 - \frac{2\alpha}{\sqrt{\pi}} \right]$$

$$\langle H \rangle = (N_\pm^0)^2 (2I_1 \pm 2I_2) \approx \frac{1}{2}\hbar\omega \, \frac{1 - \frac{1}{\sqrt{\pi}\alpha} e^{-\alpha^2} \pm e^{-\alpha^2}\left(1 - \frac{2\alpha}{\sqrt{\pi}}\right)}{1 \pm e^{-\alpha^2}}$$

$$\underset{\alpha\to\infty}{\approx} \frac{1}{2}\hbar\omega \left[1 \mp \frac{2\alpha}{\sqrt{\pi}} e^{-\alpha^2} \right]$$