PHYS 606 – Spring 2017 – Homework IX – Solution

Problem [1]

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

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

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

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

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

For $\lambda = \ell(\ell+1)$ with some $\ell \in N$ 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 $l \geq l'$

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

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

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

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 $\xi = \pm 1$.

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

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

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

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 $u = 0$, $u = \pi$

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

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

(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]

$L_z Y = m\hbar Y$; $L^2 Y = \lambda\hbar^2 Y$

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

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

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]

$\Rightarrow Y(\theta,\phi) = e^{im\phi}\,P_\ell^m(\cos\theta)$ (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 $\alpha = \sqrt{\frac{m\omega}{\hbar}}\, a$, $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$)

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

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

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

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

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

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

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

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

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

Problem [4]

$|\phi_i\rangle = \sum_j S_{ji} |\psi_j\rangle$, or, without indices $\phi = S^T \psi$

(a) Obviously $S_{ji} = \langle \psi_j | \phi_i \rangle$. Proof: $\sum_j |\psi_j\rangle\langle\psi_j|\phi_i\rangle \underset{\uparrow \text{ completeness}}{=} |\phi_i\rangle$

(b) Show that $SS^\dagger = \mathbb{1}$:

$$\sum_j S_{ij}(S^\dagger)_{jk} = \sum_j \langle\psi_i|\phi_j\rangle\langle\psi_k|\phi_j\rangle^* = \sum_j \langle\psi_i|\phi_j\rangle\langle\phi_j|\psi_k\rangle \overset{\text{completeness}}{\overset{!}{=}} \langle\psi_i|\psi_k\rangle = \delta_{ik}$$

indices switched because transpose taken (recall: $\dagger = T^*$ for matrices)

(c) $$\tilde{A}_{ij} \equiv \langle\phi_i|A|\phi_j\rangle = \sum_{k,l} \underbrace{\langle\phi_i|\psi_k\rangle}_{(S^\dagger)_{ik}} \underbrace{\langle\psi_k|A|\psi_l\rangle}_{A_{kl}} \underbrace{\langle\psi_l|\phi_j\rangle}_{S_{lj}} = \sum_{k,l} S^\dagger_{ik} A_{kl} S_{jl}$$

[similar to argument in (b)]

without indices: $\tilde{A} = S^\dagger A S$

These kind of changes between (orthonormal) bases are called similarity transformations.