Physics 451- Fall 2012

Homework #17

Due Tuesday, Nov. 6 by 7pm

Please place your assignment in the "Physics 451" slot across from N373 ESC.
We will have help sessions twice a week:
Tuesday session (with Jacob): from 2 pm to 5pm – room 363 MARB
Thursday session (with Peter): from 3pm to 6pm – room 393 CB

grading Total 40

<u>List of problems (from the textbook)</u>:

4.6

Spherical well:
4.7
4.8
4.9 (solve for bound state only)

$\boxed{4.6}$	10 pts
$\boxed{4.7}$	a) 4 pts (2 for [illegible], 2 for [illegible])
	b) 6 pts
$\boxed{4.8}$	a) 4 pts
	b) 6 pts
$\boxed{4.9}$	10 pts (6 for general solution + continuity, 4 for discussion on E, V_0)

Hints:

For problem 4.6, the trick is to integrate by-part l times in order to bring all the derivation on the same term. You should get l boundary terms plus on final integral. You can show that all the boundaries terms are zero because they all contain at least one factor (x^2-1) which becomes zero when you take the value at $x = -1$ and $x = 1$. You then need to take care of the final integral. Discuss the three cases $l > l'$, $l < l'$ (same result by symmetry) and $l = l'$. Remember that deriving an n^{th} order polynomial more than n times gives zero. For $l = l'$, we will need to calculate the integral. Use a change of variable $x = \cos\theta$

useful formulae: $\dfrac{d^n}{dx^n}\left(x^n\right) = n!$ and $\displaystyle\int_0^\pi \sin^{2l+1}\theta d\theta = 2\frac{2*4*6....(2l)}{1*3*5...(2l+1)} = 2\frac{\left(2^l l!\right)^2}{(2l+1)!}$

For problem 4.9: solve for a bound state only, write the solution inside and outside the spherical well. Use the continuity of u and du/dr at the boundary $r = a$. Show that these conditions are equivalent to solving an equation like $\sqrt{\left(\dfrac{z_0}{z}\right)^2 - 1} = -\tan^{-1}(z)$.

Discuss in which case there is a solution.

Homework # 17

Pb 4.6 $$P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

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

$$= \frac{1}{2^{\ell+\ell'}}\,\frac{1}{\ell!}\,\frac{1}{\ell'!}\underbrace{\int_{-1}^{+1} \frac{d^\ell}{dx^\ell}(x^2-1)^\ell\,\frac{d^{\ell'}}{dx^{\ell'}}(x^2-1)^{\ell'}\,dx}_{}$$

integration by parts : ℓ times until having all the derivation on same term

$$= \frac{1}{2^{\ell+\ell'}}\,\frac{1}{\ell!}\,\frac{1}{\ell'!}\left(\left[\frac{d^{\ell-1}}{dx^{\ell-1}}(x^2-1)^\ell\,\frac{d^{\ell'}}{dx^{\ell'}}(x^2-1)^{\ell'}\right]_{-1}^{+1} - \int_{-1}^{+1}\frac{d^{\ell-1}}{dx^{\ell-1}}(x^2-1)^\ell\,\frac{d^{\ell'+1}}{dx^{\ell'+1}}(x^2-1)^{\ell'}\,dx\right)$$

$$= \frac{1}{2^{\ell+\ell'}}\,\frac{1}{\ell'!}\,\frac{1}{\ell!}\left(\underbrace{\text{boundary terms}}_{0}\ \ldots + (-1)^\ell \int_{-1}^{+1}(x^2-1)^\ell\,\frac{d^{\ell'+\ell}}{dx^{\ell'+\ell}}(x^2-1)^{\ell'}\,dx\right)$$

- All the boundary terms are 0 because contain at least one factor (x^2-1) and taking the value at $x=\pm 1$ gives $(x^2-1)=0 \Rightarrow$ Boundary term $=0$

- Now for the last term the $(x^2-1)^{\ell'}$ is a polynomial in order $2\ell'$

If $\boxed{\ell > \ell'}$ then $\frac{d^{\ell+\ell'}}{dx^{\ell+\ell'}}(x^2-1)^{\ell'} = 0$ because $\ell+\ell' > 2\ell$

If $\boxed{\ell < \ell'}$ we just integrate by part the other way and find that same result.

Finally if $\boxed{l = l'}$, we have

$$\int_{-1}^{+1} P_l(x)\, P_l(x)\, dx = \frac{1}{2^{2l}(l!)^2}(-1)^l \int_{-1}^{+1} (x^2-1)^l \frac{d^{2l}}{dx^{2l}}(x^2-1)^l\, dx$$

But $\frac{d^{2l}}{dx^{2l}}(x^2-1)^l$ just leaves the first factor $= (2l)!$

$$\Rightarrow \int_{-1}^{+1} |P_l(x)|^2 dx = \frac{(-1)^l (2l)!}{2^{2l}\, l!\, l!} \int_{-1}^{+1} (x^2-1)^l\, dx$$

The integral can be done by change of variables:

let $X = \cos\theta \Rightarrow x^2 - 1 = -\sin^2\theta$ and $dx = -\sin\theta\, d\theta$

$$\Rightarrow \int_{-1}^{+1} (x^2-1)^l\, dx = \int_{\theta=\pi}^{\theta=0} (-\sin^2\theta)^l (-\sin\theta)\, d\theta = (-1)^l\, 2 \int_0^{\pi/2} \sin^{2l+1}\theta\, d\theta$$

$$\text{But} \int_0^{\pi/2} \sin^n\theta\, d\theta = \frac{n-1}{n}\int_0^{\pi/2} \sin^{n-2}\theta\, d\theta = \frac{(n-1)(n-3)\cdots}{n(n-2)\cdots}\,\frac{2}{1} \times$$

$$\text{So} \int_0^{\pi} \sin^{(2l+1)}\theta\, d\theta = \frac{(2l)(2l-2)\cdots 2}{(2l+1)(2l-1)\cdots 1} = \frac{2^l\, l!}{\left((2l+1)!/2^l l!\right)} = \frac{(2^l\, l!)^2}{(2l+1)!}$$

$$\Rightarrow \int_{-1}^{+1} |P_l(x)|^2 dx = \frac{(-1)^l (2l)!}{2^{2l}\, l!\, l!}(-1)^l\, 2\frac{(2^l\, l!)^2}{(2l+1)!} = 2\,\frac{2^{2l}}{2^{2l}}\,\frac{(2l)!}{(2l+1)!} = \frac{2}{2l+1}$$

$$\Rightarrow \boxed{\int_{-1}^{+1} P_l(x)\, P_{l'}(x)\, dx = \frac{2}{2l+1}\,\delta_{ll'}}$$

$\boxed{\text{Pb } \cancel{4}.7}$ $\mathcal{N}_\ell(x) = (-x)^{\ell+1}\left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x}$ Spherical Neumman function

a)

$$\mathcal{N}_0(x) = -\frac{\cos x}{x}$$

$$\mathcal{N}_1(x) = +x\frac{1}{x}\frac{d}{dx}\left(\frac{\cos x}{x}\right) = \frac{\cancel{x}}{x}\left(\frac{-\sin x}{x} - \frac{\cos x}{x^2}\right) = -\frac{\sin x}{x} - \frac{\cos x}{x^2}$$

$$\mathcal{N}_2(x) = -x^2\left(\frac{1}{x}\frac{d}{dx}\right)\left(\frac{1}{x}\frac{d}{dx}\left(\frac{\cos x}{x}\right)\right) = -x^2\left(\frac{1}{x}\frac{d}{dx}\right)\left(-\frac{\sin x}{x^2} - \frac{\cos x}{x^3}\right)$$

$$= +x\frac{d}{dx}\left(\frac{\sin x}{x^2} + \frac{\cos x}{x^3}\right)$$

$$= +x\left(\frac{\cos x}{x^2} - \frac{2\sin x}{x^3} - \frac{\sin x}{x^3} - \frac{3\cos x}{x^4}\right)$$

$$\mathcal{N}_2(x) = -\frac{3\sin x}{x^2} + \frac{\cos x}{x}\left(1 - \frac{3}{x^2}\right)$$

b) When $x \ll 1$ $\sin x \simeq x - \frac{x^3}{3!}$ and $\cos x \simeq 1 - \frac{x^2}{2}$

(or to a first order: $\sin x \simeq x$ and $\cos x \simeq 1$)

$\mathcal{N}_1(x) \simeq -\left(1 + \frac{1}{x^2}\right) \simeq -\frac{1}{x^2}$ $\longrightarrow$ Blows up when $x \to 0$

$\mathcal{N}_2(x) \simeq -\frac{3}{x} + \frac{1}{x}\left(1 - \frac{3}{x^2}\right) = -\frac{2}{x} - \frac{3}{x^3} \simeq -\frac{3}{x^3}$ when $x \to 0$

$\mathcal{N}_2(x)$ Blows up (diverge) when $x \to 0$

$\boxed{\text{Pb } 4.8}$

a) Radial equation with $l = 1$ (for $u = rR$)

$$\frac{d^2u}{dr^2} = \left[\frac{1\times 2}{r^2} - k^2\right] u \qquad \text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

Indeed:
$$u_1(r) = A_1\, r\, j_1(kr)$$
$$= A_1\, r \left(\frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr}\right)$$ (see p. 142)
$$= A_1 \left(\frac{\sin(kr)}{k^2 r} - \frac{\cos(kr)}{k}\right)$$

$$\frac{d^2u_1}{dr^2} = \frac{d}{dr}\left(A_1\right)\left(\frac{k\cos(kr)}{k^2 r} - \frac{\sin(kr)}{k^2 r^2} + \frac{k\sin(kr)}{k}\right)$$
$$= A_1\left(\frac{k}{k}\frac{(-\sin kr)}{r} - \frac{\cos kr}{k r^2} - \frac{k\cos(kr)}{k^2 r^2} + \frac{2\sin(kr)}{k^2 r^3} + k\cos(kr)\right)$$
$$= A_1\left(\frac{\sin kr}{k^2 r}\left(\frac{2}{r^2} - k^2\right) - \frac{\cos(kr)}{k}\left(\frac{2}{r^2} - k^2\right)\right)$$
$$= \underbrace{A_1\left(\frac{\sin kr}{k^2 r} - \frac{\cos(kr)}{k}\right)}_{u_1(r)}\left(\frac{2}{r^2} - k^2\right)$$

$$\Rightarrow \boxed{\frac{d^2u_1}{dr^2} = \left(\frac{2}{r^2} - k^2\right) u_1(r)}$$

4.8 (b) Allowed energies for the infinite spherical well, when $l = 1$

The radial solution is $R_{n1}(r) = \dfrac{u_1(r)}{r} = A_{n1}\, j_1(kr)$

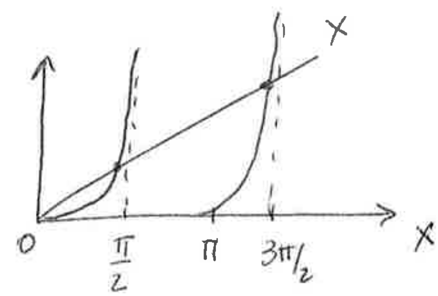
$$R_{n1}(r) = A_{n1}\left(\frac{\sin(kr)}{k^2 r^2} - \frac{\cos(kr)}{kr} \right)$$

The condition at boundary impose that $R_{n1}(a) = 0$

$$\Rightarrow \quad \frac{\sin(ka)}{k^2 a^2} - \frac{\cos ka}{ka} = 0$$

$$\Rightarrow \quad \frac{\sin(ka)}{ka} = \cos(ka) \quad \Rightarrow \quad \tan(ka) = ka$$

We need to solve for $\tan x = x$



For large X value: the solution is very close to $\frac{n\pi}{2}$

$$\Rightarrow \quad X \simeq \pi\left(n + \tfrac{1}{2}\right) \Rightarrow \quad ka \simeq \left(n + \tfrac{1}{2}\right)\pi \Rightarrow \quad k \simeq \left(n + \tfrac{1}{2}\right)\frac{\pi}{a}$$

$$\Rightarrow \quad \boxed{E_{n1} \simeq \frac{\pi^2 \hbar^2}{2ma^2}\left(n + \tfrac{1}{2}\right)^2}$$

$\boxed{\text{Pb 4.9}}$ Finite spherical Well

$$V = \begin{cases} -V_0 & \text{if } r \leq a \\ 0 & \text{if } r > a \end{cases}$$

Radial equation: $\quad l = 0$

$$\frac{d^2u}{dr^2} = -\frac{2m}{\hbar^2}(E+V_0)u$$ inside the sphere $r \lesssim a$

let $k' = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ $\Rightarrow$ solution $u(r) = A\sin(k'r) + B\cos(k'r)$

at $r=0$ the $\frac{\cos(k'r)}{r}$ blows up so not physically possible.

$$\Rightarrow \quad u(r) = A\sin(k'r)$$
$$R(r) = A\frac{\sin(k'r)}{r}$$

Outside the sphere: $r > a$

$$\frac{d^2u}{dr^2} = -\frac{2m}{\hbar^2}Eu \quad , \quad k = \frac{\sqrt{2mE}}{\hbar}$$

if $E>0$ solution $u(r) = Be^{-ikr} + Ce^{ikr}$

Boundary conditions at $r=a$: the particle can still go through the boundary and exist outside the sphere

We still have the continuity of u and u' at the boundary:

$$u_{r\leq a}(a) = u_{r>a}(a) \quad \text{and} \quad u'_{r\leq a}(a) = u'_{r>a}(a)$$

$$\begin{cases} A\sin(k'a) = B\cos(ka) + C\sin(ka) & (1) \\ k'A\cos(k'a) = k(-B\sin ka) + k(C\cos ka) & (2) \end{cases}$$

Combining (1) and (2)

$$A\left(k\sin(k'a)\sin(ka) + k'\cos(k'a)\sin(k'a)\right) = C\left(k\sin^2(ka) + k\cos^2(ka)\right)$$
$$= Ck$$

$\boxed{\text{Pb } 4.9}$ Finite spherical Well

$$V = \begin{cases} -V_0 & \text{if } r \leq a \\ 0 & \text{if } r > a \end{cases}$$

<u>Radial equation</u> : $\ell = 0$

Inside the sphere: $\dfrac{d^2u}{dr^2} = -\dfrac{2m}{\hbar^2}(E + V_0)u$

Outside the sphere $\dfrac{d^2u}{dr^2} = -\dfrac{2mE}{\hbar^2}u$

let's consider a <u>bound state</u> $-V_0 < E < 0$

- Solution inside the sphere $u(r) = A\sin(k'r) + B\cos(k'r)$ with $k' = \dfrac{\sqrt{2m(E+V_0)}}{\hbar}$

  physical condition $\Rightarrow$ $\dfrac{\cos(k'r)}{r}$ diverge at $r = 0$

  $\Rightarrow u(r) = A\sin(k'r)$ for $r \leq a$

- Solution outside the sphere: $u(r) = e^{-\kappa r}$ with $\kappa = \sqrt{\dfrac{-2mE}{\hbar^2}}$

<u>Condition at boundary</u> : $r = a$

Continuity of u : $A\sin(k'a) = e^{-\kappa a}$ (1)

Continuity of u' : $k'A\cos(k'a) = -\kappa e^{-\kappa a}$ (2)

Combining (1) and (2) $\Rightarrow$ $\boxed{\tan(k'a) = -\dfrac{k'}{\kappa}}$

change of variable: $z = k'a$

$k'^2 = \dfrac{2m(E+V_0)}{\hbar^2}$, $\kappa^2 = -\dfrac{2mE}{\hbar^2}$ $\Rightarrow$ $k'^2 = \dfrac{2mV_0}{\hbar^2} - \kappa^2$ $\Rightarrow \kappa^2 = \dfrac{2mV_0}{\hbar^2} - k'^2$

$\left(\dfrac{\kappa}{k'}\right)^2 = \dfrac{2mV_0}{\hbar^2 k'^2} - 1$, $\dfrac{\kappa}{k'} = \sqrt{\dfrac{2mV_0 a^2}{\hbar^2 z^2} - 1}$

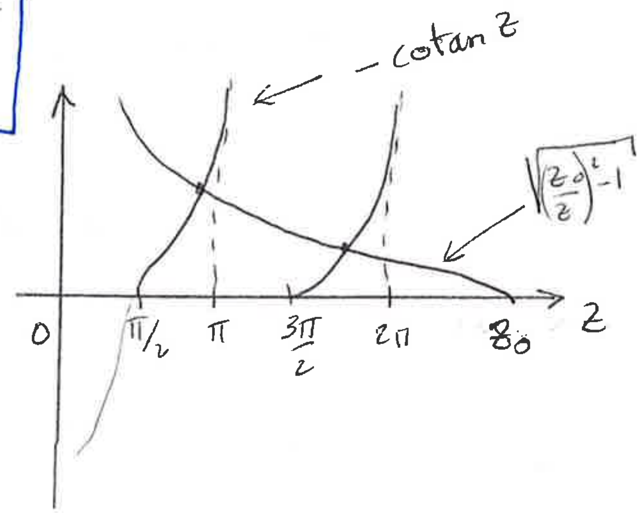
Calling $z_0 = \sqrt{\dfrac{2m V_0 a^2}{\hbar^2}}$

$$\Rightarrow \quad \frac{k}{k'} = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

$\Rightarrow$ We need to solve for $\tan z = -\dfrac{1}{\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}}$

OR $\boxed{\cot z = -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}}$

Grapical solution (see pb 2.29)



We have a solution only if $z_0 \geq \frac{\pi}{2}$

$$\Rightarrow \frac{2mV_0 a^2}{\hbar^2} \geq \frac{\pi^2}{4}$$

$$\Rightarrow \boxed{V_0 a^2 \geq \frac{\pi^2 \hbar^2}{8m}}$$

In that case the ground state energy is given by the intersectn between two graphs.

$$\frac{\pi}{2} \leq z \leq \pi$$

$$\frac{\pi}{2a} \leq k' \leq \frac{\pi}{a}$$

$$\frac{\pi^2}{4a^2} \leq \frac{2m(E+V_0)}{\hbar^2} \leq \frac{\pi^2}{a^2}$$

$$\boxed{-V_0 + \frac{\pi^2\hbar^2}{8ma^2} \leq E \leq -V_0 + \frac{\pi^2\hbar^2}{2ma^2}}$$