HW6 solution[1] - Phys487 Spring 2015

Problem 6.12 (3 points)

For the potential $V = -e^2/(4\pi\epsilon_0 r)$, the Viral theorem states that $2\langle T\rangle = \langle \mathbf{r}\cdot\nabla V\rangle = -\langle V\rangle$. Therefore, $E = \langle T\rangle + \langle V\rangle = \langle V\rangle/2$. Using that $a = 4\pi\epsilon_0\hbar^2/(me^2)$ and $E = -\frac{m}{2\hbar^2}(\frac{e^2}{4\pi\epsilon_0})^2\frac{1}{n^2}$, we conclude that $\langle 1/r\rangle = 1/(n^2 a)$.

Problem 6.16 (6 points)

(a) $[\mathbf{L}\cdot\mathbf{S}, L_x] = [L_xS_x + L_yS_y + L_zS_z, L_x] = S_x[L_x, L_x] + S_y[L_y, L_x] + S_z[L_z, L_x] = 0 + S_y(-i\hbar L_z) + S_z(i\hbar L_y) = i\hbar(\mathbf{L}\times\mathbf{S})_z$. The same goes for L_y and L_y. Therefore, $[\mathbf{L}\cdot\mathbf{S}, \mathbf{L}] = i\hbar\,\mathbf{L}\times\mathbf{S}$
(b) We can simply relabel the variable $\mathbf{L}\leftrightarrow\mathbf{S}$. Therefore, $[\mathbf{L}\cdot\mathbf{S}, \mathbf{S}] = i\hbar\,\mathbf{S}\times\mathbf{L}$
(c) $[\mathbf{L}\cdot\mathbf{S}, \mathbf{J}] = [\mathbf{L}\cdot\mathbf{S}, \mathbf{L}] + [\mathbf{L}\cdot\mathbf{S}, \mathbf{S}] = i\hbar\,\mathbf{S}\times\mathbf{L} - i\hbar\,\mathbf{S}\times\mathbf{L} = 0$
(d) L^2 commutes with all components of $\mathbf{L}$ and $\mathbf{S}$. Therefore, $[\mathbf{L}\cdot\mathbf{S}, L^2] = 0$
(e) Likewise $[\mathbf{L}\cdot\mathbf{S}, S^2] = 0$
(f) $[\mathbf{L}\cdot\mathbf{S}, J^2] = [\mathbf{L}\cdot\mathbf{S}, L^2] + [\mathbf{L}\cdot\mathbf{S}, S^2] + 2[\mathbf{L}\cdot\mathbf{S}, \mathbf{L}\cdot\mathbf{S}] = 0$

Problem 6.19 (3 points)

The Mathematica code Simplify[mc^2 Series[$(1 + (\alpha/(n-(j+1/2)+\sqrt{(j+1/2)^2-\alpha^2}))^2)^{-1/2} - 1, \{\alpha, 0, 4\}], j \geq 0$] results in

$$\begin{aligned} E &= -\frac{mc^2\alpha^2}{2n^2} + \frac{mc^2(3+6j-8n)\alpha^4}{8(1+2j)n^2} \\ &= -\frac{mc^2\alpha^2}{2n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+1/2} - \frac{3}{4}\right)\right], \end{aligned}$$

which is the same as Eq. 6.67.

Problem 6.32 (6 points)

(a) Considering an unperturbed Hamiltonian $H(\lambda_0)$ for some fixed parameter λ_0. Under and infinitesimal change $d\lambda$, the perturbed Hamiltonian is $H' = H(\lambda_0 + d\lambda) - H(\lambda_0)$. The change in energy is given by Eq. 6.9

$$dE_n = E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle = \langle\psi_n^0|\frac{H(\lambda_0+d\lambda)-H(\lambda_0)}{d\lambda}|\psi_n^0\rangle d\lambda$$

After taking the limit $d\lambda \to 0$ the equation becomes

$$\frac{\partial E_n}{\partial\lambda} = \langle\psi_n|\frac{\partial H}{\partial\lambda}|\psi_n\rangle \tag{1}$$

(b) $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2$ and $E_n = (n+1/2)\hbar\omega$

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(i) $\lambda = \omega$, Eq. (1) leads to $(n+1/2)\hbar = \langle n|m\omega x^2|n\rangle$. Because $V = m\omega^2 x^2/2$, then $\langle V\rangle = (n+1/2)\hbar\omega/2$
(ii) $\lambda = \hbar$, Eq. (1) leads to $(n+1/2)\omega = 2\langle n|T|n\rangle/\hbar$ or $\langle T\rangle = (n+1/2)\hbar\omega/2$
(iii) $\lambda = m$, Eq. (1) leads to $\langle T\rangle = \langle V\rangle$

Therese results are consistent with problems 2.12 and 3.31.

Problem 6.34 (6 points)

demo 1 Eq. 4.53 implies that

$$u'' = \left[\frac{l(l+1)}{r^2} - \frac{2mE}{\hbar^2} - \frac{2m}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{r}\right]u$$

but $a = me^2/(4\pi\epsilon_0\hbar^2)$ and $E = -\hbar^2/(2ma^2n^2)$. Therefore,

$$u'' = \left[\frac{l(l+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right]u \tag{2}$$

demo 2

$$\int dr\, ur^s u'' = \int dr\, ur^2\left[\frac{l(l+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right]u = l(l+1)\langle r^{s-2}\rangle - \frac{2}{a}\langle r^{s-1}\rangle + \frac{\langle r^s\rangle}{n^2a^2} \tag{3}$$

But also

$$\int dr\, ur^s u'' = \underbrace{ur^s u'\Big|_0^\infty}_{0} - \int dr\,(ur^s)'u' = -\int dr\, u'r^s u' - s\int dr\, ur^{s-1}u' \tag{4}$$

The boundary term is zero because u and u' are finite at $r=0$ and decay exponentially as $r\to\infty$
demo 3: Integrating by parts

$$\int dr\,(ur^s)u' = \underbrace{(ur^s)u\Big|_0^\infty}_{0} - \int dr\,(ur^s)'u = -\int dr\, u'r^s u - s\int dr\, ur^{s-1}u$$

Therefore,

$$\int dr\, ur^s u' = -\frac{s}{2}\langle r^{s-1}\rangle \tag{5}$$

demo 4:

$$\int dr\, u'r^{s+1}u'' = \underbrace{u'r^{s+1}u'\Big|_0^\infty}_{0} - \int dr\,(u'r^{s+1})'u' = -\int dr\, u''r^{s+1}u' - (s+1)\int dr\, u'r^s u'$$

Therefore,

$$\int dr\, u'r^s u' = -\frac{2}{s+1}\int dr\, u'r^{s+1}u'' \tag{6}$$

Now, let us put everything together. Eqs. (3) and (4) imply that

$$l(l+1)\langle r^{s-2}\rangle - \frac{2}{a}\langle r^{s-1}\rangle + \frac{\langle r^s\rangle}{n^2a^2} = -\int dr\, u'r^s u' - s\int dr\, ur^{s-1}u'$$

Using Eqs. (5) and (6) for calculating the terms on the right side

$$l(l+1)\langle r^{s-2}\rangle - \frac{2}{a}\langle r^{s-1}\rangle + \frac{\langle r^s\rangle}{n^2a^2} = \frac{2}{s+1}\int dr\, u' r^{s+1} u'' + \frac{s(s-1)}{2}\langle r^{s-2}\rangle \tag{7}$$

Using Eqs. (2) and (5) on the first term of the right side

$$\begin{aligned}\frac{2}{s+1}\int dr\, u' r^{s+1} u'' &= \frac{2}{s+1}\left[l(l+1)\int dr\, u' r^{s-1} u - \frac{2}{a}\int dr\, u' r^s u + \frac{1}{n^2a^2}\int dr\, u' r^{s+1} u\right] \\ &= -l(l+1)\frac{s-1}{s+1}\langle r^{s-2}\rangle + \frac{2}{a}\frac{s}{s+1}\langle r^{s-1}\rangle - \frac{1}{n^2a^2}\langle r^s\rangle \end{aligned} \tag{8}$$

Finally, Eq. (8) into Eq. (7)

$$\frac{s+1}{n^2}\langle r^s\rangle - a(2s+1)\langle r^{s-1}\rangle + \frac{sa^2}{4}[(2l+1)^2 - s^2]\langle r^{s-2}\rangle = 0$$

Problem 6.35 (9 points)

(a)
For $s=0$

$$\frac{1}{n^2} - a\langle r^{-1}\rangle = 0 \implies \langle r^{-1}\rangle = \frac{1}{an^2}$$

For $s=1$

$$\frac{2}{n^2}\langle r\rangle - 3a + \frac{a^2}{4}[(2l+1)^2 - 1]\langle r^{-1}\rangle = 0 \implies \langle r\rangle = \frac{1}{a}[3n^2 - l(l+1)]$$

For $s=2$

$$\frac{3}{n^2}\langle r^2\rangle - 5a\langle r\rangle + \frac{a^2}{2}[(2l+1)^2 - 4] = 0 \implies \langle r^2\rangle = \frac{n^2a^2}{2}[5n^2 - 3l(l+1) + 1]$$

For $s=3$

$$\frac{4}{n^2}\langle r^3\rangle - 7a\langle r^3\rangle + \frac{3a^2}{4}[(2l+1)^2 - 9]\langle r\rangle = 0 \implies \langle r^3\rangle = \frac{n^2a^3}{8}[35n^4 + 25n^2 - 30l(l+1)n^2 + 3l^2(l+1)^2 - 6l(l+1)]$$

(b) For $s=-1$

$$a\langle r^{-2}\rangle - a^2 l(l+1)\langle r^{-3}\rangle = 0$$

(c) From Eq. 6.56 we know that

$$\langle r^{-2}\rangle = \frac{1}{(l+1/2)n^3a^2} \implies \langle r^{-3}\rangle = \frac{1}{l(l+1/2)(l+1)n^3a^3}$$

which agrees with Eq. 6.64.

Problem 6.37 (9 points)

(a) The unperturbed wave functions are

$$|nlm\rangle = |300\rangle, |31\text{-}1\rangle, |310\rangle, |311\rangle, |32\text{-}2\rangle, |32\text{-}1\rangle, |320\rangle, |321\rangle, |322\rangle$$

explicitly shown in Eq. 4.89, and the perturbation Hamiltonian is $H_s' = eE_{\text{ext}} r\cos\theta$.

First, we notice that $\langle nlm|H_s'|n'l'm'\rangle \propto \int_0^{2\pi} e^{i(m'-m)\phi} = 0$ for $m \neq m'$. Second, we notice that $\langle nlm|H_s'|n'l'm'\rangle \propto \int_0^{2\pi} |Y_l^m|^2 \cos\theta \sin\theta d\theta$, where $|Y_l^m|^2$ has only even powers of $\cos\theta$. Therefore, the θ integral has terms of the form $\int_0^{2\pi} (\cos\theta)^{2j+1} \sin\theta d\theta = 0$; i.e. all diagonal elements are zero.

We only need to calculate $\langle 300|H_s'|310\rangle$, $\langle 300|H_s'|320\rangle$, $\langle 310|H_s'|320\rangle$ and $\langle 31\pm1|H_s'|32\pm1\rangle$. We can implement ψ_{nlm} on Mathematica using the explicit solution in Eq. 4.89:

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ψ[n_, l_, m_, r_, θ_, ϕ_] := Sqrt[(2/(n a))^3 (n - l - 1)!/(2 n ((n + l)!))]
Exp[-r/(n a)] (2 r/(n a))^l LaguerreL[n - l - 1, 2 l + 1, 2 r/(n a)] SphericalHarmonicY[l, m, θ, ϕ]

Simplify[Integrate[Conjugate[ψ[3, 0, 0, r, θ, ϕ]] ψ[3, 1, 0, r, θ, ϕ] r^3 Cos[θ] Sin[θ],
  {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2 π}], {a ∈ Reals, a > 0}]

Out[7]= -3 √6 a
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The matrix elements, calculated using Mathematica, are

$$\langle nlm|H_s'|n'l'm'\rangle = -aeE_{\text{ext}} \begin{pmatrix} 0 & 3\sqrt{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3\sqrt{6} & 0 & 3\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 9/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 9/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The matrix elements are in the basis ordering $\{|300\rangle, |310\rangle, |320\rangle, |311\rangle, |321\rangle, |31\text{-}1\rangle, |32\text{-}1\rangle, |322\rangle, |32\text{-}2\rangle\}$.

(b) Using the function 'Eigenvalues[ ]' on Mathematica

3×3 submatrix $\rightarrow \{-9aeE_{\text{ext}}, 9aeE_{\text{ext}}, 0\}$

2×2 submatrix: $\rightarrow \{-9/2aeE_{\text{ext}}, 9/2aeE_{\text{ext}}\}$

Therefore,

0	degeneracy 3
$-9/2aeE_{\text{ext}}$	degeneracy 2
$9/2aeE_{\text{ext}}$	degeneracy 2
$-9aeE_{\text{ext}}$	degeneracy 1
$9aeE_{\text{ext}}$	degeneracy 1

Problem 7.1 (6 points)

Eq. 7.2 states $\psi(x) = (2b/\pi)^{1/4} e^{-bx^2}$, and 7.5 $\langle T \rangle = \hbar^2 b/(2m)$
(a) $V(x) = \alpha|x|$. Then

$$\langle V \rangle = 2\alpha\sqrt{\frac{2b}{\pi}} \int_0^\infty dx\, x e^{-2bx^2} = \frac{\alpha}{\sqrt{2\pi b}}$$

Minimization of $\langle H \rangle = \langle T \rangle + \langle V \rangle$ leads to $b = (m\alpha/(\sqrt{2\pi}\hbar^2))^{2/3}$. Therefore,

$$\langle H \rangle_{\min} = \frac{\hbar^2}{2m}\left(\frac{m\alpha}{\sqrt{2\pi}\hbar^2}\right)^{2/3} + \frac{\alpha}{\sqrt{2\pi}}\left(\frac{\sqrt{2\pi}\hbar^2}{m\alpha}\right)^{1/3} = \frac{3}{2}\left(\frac{\alpha^2\hbar^2}{2\pi m}\right)^{1/3}$$

(b) $V(x) = \alpha x^4$. Then

$$\langle V \rangle = 2\alpha\sqrt{\frac{2b}{\pi}} \int_0^\infty dx\, x^4 e^{-2bx^2} = 3\alpha/(16b^2)$$

Minimization of $\langle H \rangle$ leads to $b = (3\alpha m/(4\hbar^2))^{1/3}$. Therefore,

$$\langle H \rangle_{\min} = \frac{\hbar^2}{2m}\left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3} + \frac{3\alpha}{16}\left(\frac{4\hbar^2}{3\alpha m}\right)^{2/3} = \frac{3}{4}\left(\frac{3\alpha\hbar^4}{4m^2}\right)^{1/3}$$

Problem 7.2 (6 points)

Using 'Integrate[$A^2/(x^2+b^2)^2, \{x, -\infty, \infty\}$]' we conclude that $A = \sqrt{2b^3/\pi}$, and therefore,

$$\psi(x) = \sqrt{\frac{2b^3}{\pi}} \frac{1}{x^2+b^2}.$$

We need to calculate $\langle T \rangle$ and $\langle V \rangle$.

Using 'Integrate[$1/(x^2+b^2)$ D[$1/(x^2+b^2), \{x, 2\}], \{x, -\infty, \infty\}$]'

$$\langle T \rangle = -\frac{\hbar^2 b^3}{\pi m}\int_{-\infty}^\infty dx \frac{1}{x^2+b^2}\frac{d^2}{dx^2}\frac{1}{x^2+b^2} = \frac{\hbar^2}{4mb^2}$$

and 'Integrate[$x^2/(x^2+b^2)^2, \{x, -\infty, \infty\}$]'

$$\langle V \rangle = \frac{m\omega^2 b^3}{\pi}\int_0^\infty dx \frac{x^2}{(x^2+b^2)^2} = \frac{1}{2}m\omega^2 b^2$$

Therefore, maximization of $\langle H \rangle$ leads to $b = \hbar/(\sqrt{2}m\omega)$ and $\langle H \rangle_{\min} = \hbar\omega/\sqrt{2}$