QUANTUM MECHANICS B (PHY5646)
HOMEWORK 19
(March 8, 2017)
Due on Thursday, March 21, 2017

PROBLEM 55

The Hamiltonian for a particle moving in the presence of a one dimensional 'quadratic- plus-quartic' potential is given by the following expression:

$$\hat{H} = \frac{\hat{P}^2}{2} + \frac{\hat{X}^2}{2} + \lambda \hat{X}^4,$$

where the Hamiltonian has been written in terms of properly scaled variables. We have shown in class that to first order in λ the energy of the system is given by

$$E_n = \left(n + \frac{1}{2}\right) + \frac{3}{4}\lambda(2n^2 + 2n + 1).$$

(a) Compute the *ground-state* energy of the system correct up to second order in λ. That is, evaluate the value of the dimensionless constant κ in the following expression:

$$E_0 = \frac{1}{2} + \frac{3}{4}\lambda + \kappa\lambda^2.$$

Before you start you should already know whether κ is positive or negative. After you compute the value κ comment on whether you think that the perturbative series will converge.

Solution:

$$E_n^{(2)} \quad = \quad \sum_{m \neq n} \frac{\left|\langle n_0|\hat{X}^4|m_0\rangle\right|^2}{E_n^0 - E_m^0}, \qquad m_0 > n_0$$

$$\hat{X}^4 = \frac{1}{4}\Big(\hat{a}^4 + \hat{a}^3\hat{a}^\dagger + \hat{a}^2\hat{a}^\dagger\hat{a} + \cancel{\hat{a}^2\hat{a}^{\dagger 2}} + \hat{a}\hat{a}^\dagger\hat{a}^2 + \cancel{\hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger} + \cancel{\hat{a}\hat{a}^{\dagger 2}\hat{a}} + \cancel{\hat{a}\hat{a}^{\dagger 3}} + \cancel{\hat{a}^\dagger\hat{a}^3}$$
$$+ \cancel{\hat{a}^\dagger\hat{a}^2\hat{a}^\dagger} + \cancel{\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}} + \cancel{\hat{a}^\dagger\hat{a}\hat{a}^{\dagger 2}} + \cancel{\hat{a}^{\dagger 2}\hat{a}^2} + \cancel{\hat{a}^{\dagger 2}\hat{a}\hat{a}^\dagger} + \cancel{\hat{a}^{\dagger 2}\hat{a}} + \cancel{\hat{a}^{\dagger 4}}\Big)$$

Terms with a and $a^\dagger$ of the same order vanish and also all terms leading with $a^\dagger$ vanish.

$$\hat{X}^4_{\text{eff}} = \frac{1}{4}\left(\hat{a}^4 + \hat{a}^3\hat{a}^\dagger + \hat{a}^2\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\hat{a}^2\right)$$

The eigenvalues $|m_0\rangle$ can be found for the only non-vanishing terms:

$\lvert m_0 = 2\rangle$	$\lvert m_0 = 4\rangle$
$\hat{a}^2\hat{a}^\dagger\hat{a}$	$\hat{a}^4$
$\hat{a}\hat{a}^\dagger\hat{a}^2$	
$\hat{a}^3\hat{a}^\dagger$	

$$\begin{aligned}
E_n^{(2)} &= \sum_{m\neq n} \frac{\left|\langle n_0|\hat{X}^4|m_0\rangle\right|^2}{E_n^0 - E_m^0} \\
&= \frac{\left|\langle 0|\hat{X}^4_{\text{eff}}|2\rangle\right|^2}{E_n^0 - E_m^0} + \frac{\left|\langle 0|\hat{X}^4_{\text{eff}}|4\rangle\right|^2}{E_n^0 - E_m^0} \\
&= \frac{\left|\frac{1}{4}\left(2\sqrt{2} + \sqrt{2} + 3\sqrt{2}\right)\right|^2}{\frac{1}{2} - \frac{5}{2}} + \frac{\left|\frac{1}{4}\left(2\sqrt{6}\right)\right|^2}{\frac{1}{2} - \frac{9}{2}} \\
&= -\frac{36}{16} - \frac{6}{16}
\end{aligned}$$

$$\boxed{\kappa = \frac{-21}{8}} \tag{1}$$

The perturbative series does seem to converge since the denominator appears to have a 2^n relationship which will eventually cause the energy to remain relatively unchanged with higher orders of λ

(b) Using a variational wave-function of the form

$$\phi(x) = \frac{1}{(\pi c^2)^{1/4}} \exp(-x^2/2c^2),$$

where c is the variational parameter, provide an estimate of the ground-state energy of the full Hamiltonian as a function of λ. For 'small' values of λ

compare your answer against the perturbative estimate obtained in part (a).

$$\begin{aligned}\hat{H}\left|\phi\right\rangle &= E_n\left|\phi\right\rangle \\ \langle\phi|\hat{H}|\phi\rangle &= \frac{1}{(\pi c^2)^{1/2}}\int_{-\infty}^{\infty} e^{-x^2/2c^2}\left[\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{x^2}{2}+\lambda x^4\right]e^{x^2/2c^2}\mathrm{d}x\end{aligned}$$

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{e^{-x^2/2c^2}}{2}\left(\frac{\partial^2}{\partial x^2}e^{x^2/2c^2}\right)\mathrm{d}x &= \frac{-1}{2c^2}\int_{-\infty}^{\infty}e^{-x^2/2c^2}\mathrm{d}x+\int_{-\infty}^{\infty}\left(\frac{x}{c^2}\right)^2\frac{e^{-x^2/2c^2}}{2}\mathrm{d}x \\ &= \frac{\sqrt{\pi}}{2c}-\frac{\sqrt{\pi}}{4c} \\ &= \frac{\sqrt{\pi}}{4c}\end{aligned}$$

$$\begin{aligned}\frac{1}{2}\int_{-\infty}^{\infty}x^2e^{-x^2/c^2}\mathrm{d}x &= \frac{\sqrt{\pi}}{4}c^2 \\ \lambda\int_{-\infty}^{\infty}x^4e^{-x^2/c^2}\mathrm{d}x &= \lambda\frac{3\sqrt{\pi}}{4}c^5\end{aligned}$$

$$\langle\phi|\hat{H}|\phi\rangle = \frac{1}{4}\left[\frac{1}{c^2}+c^2+3\lambda c^4\right]$$

$$\begin{aligned}\frac{\partial E_n}{\partial c} &= \frac{-2}{c^3}+2c=0, \qquad \lambda\to 0 \\ \frac{2}{c^3} &= 2c\end{aligned}$$

$$\boxed{c=1} \tag{2}$$

Plugging in 1 for c yields:

$$\boxed{E_0=\frac{1}{2}+\lambda\frac{3}{4}} \tag{3}$$

This matches closely with the given value for E_0

PROBLEM 56 - (Shankar 17.2.4)

An important result in atomic, condensed-matter, and nuclear physics is the *Thomas-Reiche-Kuhn* ("TRK") sum rule that states that:

$$M_1 \equiv \sum_{n'} (E_{n'} - E_n) \left| \langle n' | \hat{X} | n \rangle \right|^2 = \frac{\hbar^2}{2m}$$

where $|n\rangle$ and $|n'\rangle$ are exact eigenstates of a generic Hamiltonian given by

$$\hat{H} = \frac{\hat{P}^2}{2m} + \hat{V}(\hat{X}).$$

(a) Show that by eliminating the energy factor $(E_{n'} - E_n)$ in favor of $\hat{H}$, M_1 can be written as the expectation value in state $|n\rangle$ of a suitable "double commutator".

Solution:

$$\begin{aligned}
M_1 &= \sum_{n'} (E_{n'} - E_n) \langle n|X|n'\rangle \langle n'|X|n\rangle \\
&= \sum_{n'} \Big(\langle n|X\hat{H}|n'\rangle - \langle n|\hat{H}X|n'\rangle \Big) \langle n'|X|n\rangle \\
&= \sum_{n'} \langle X\hat{H} - \hat{H}X|n'\rangle \langle n'|X|n\rangle \\
&= \sum_{n'} \langle n| [X, H] |n'\rangle \langle n'|X|n\rangle \\
&= \langle n| [X, H] X|n\rangle
\end{aligned}$$

$$\begin{aligned}
M_1 &= \sum_{n'} \langle n|X|n'\rangle (E_{n'} - E_n) \langle n'|X|n\rangle \\
&= \sum_{n'} \langle n|X|n'\rangle \Big(\langle n'|\hat{H}X|n\rangle - \langle n'|X\hat{H}|n\rangle \Big) \\
&= \sum_{n'} \langle n|X|n'\rangle \Big(\langle n'| \Big[\hat{H}, X\Big] |n\rangle \Big) \\
&= \langle n|X \Big[\hat{H}, X\Big] n\rangle \\
&= -\langle n|X \Big[X, \hat{H}\Big] |n\rangle
\end{aligned}$$

$$
\begin{aligned}
2M_1 &= \langle n| \left[X, \hat{H}\right] X|n\rangle - \langle n|X \left[X, \hat{H}\right] |n\rangle \\
M_1 &= \frac{1}{2}\Big(\langle n| \left[X, \hat{H}\right] X - X \left[X, \hat{H}\right] |n\rangle\Big)
\end{aligned}
$$

$$
\boxed{M_1 = \frac{1}{2}\left\langle n\middle| \left[\left[X, \hat{H}\right], X\right] \middle|n\right\rangle} \tag{4}
$$

(b) Using this result, prove the TRK sum rule for the generic Hamiltonian given above. Note that this result holds *regardless* of the form of $\hat{V}$.

$$
\begin{aligned}
\left[X, \hat{P}\right]\psi &= X\hat{P}\psi - \hat{P}(X\psi) \\
&= X\frac{\hbar}{i}\frac{\partial}{\partial X}\psi - \frac{\hbar}{i}\frac{\partial}{\partial X}(X\psi) \\
&= -i\hbar\left[X\psi' - \psi - x\psi'\right] \\
&= i\hbar\psi \\
\left[X, \hat{H}\right] &= X\hat{H} - \hat{H}X \\
&= X\frac{\hat{P}^2}{2m} + XV(X) - \frac{\hat{P}^2}{2m} - V(X)X \\
&= \frac{1}{2m}\left[X, \hat{P}^2\right] + \cancel{[X, V(X)]} \\
\left[X, \hat{P}\hat{P}\right] &= X\hat{P}\hat{P} - \hat{P}\hat{P}X \\
&= X\hat{P}\hat{P} - \hat{P}X\hat{P} + \hat{P}X\hat{P} - \hat{P}\hat{P}X \\
&= \left[X, \hat{P}\right]\hat{P} + \hat{P}\left[X, \hat{P}\right] \\
&= 2i\hbar\psi \\
\left[X, \hat{H}\right] &= \frac{i\hbar p}{m} \\
M_1\psi &= \frac{1}{2}\left(\frac{i\hbar p}{m}(X\psi) - X\frac{i\hbar p}{m}\psi\right) \\
&= \frac{\hbar^2}{2m}\left(\psi + \cancel{X\psi'} - \cancel{X\psi'}\right) \\
&= \frac{\hbar^2}{2m}\psi
\end{aligned}
$$

$$
\boxed{\therefore M_1 = \frac{\hbar^2}{2m}} \tag{5}
$$

(c) Test the validity of the TRK sum rule in the particular case of the one-dimensional harmonic oscillator: $\hat{V}(\hat{X}) = \frac{1}{2}m\omega^2\hat{X}^2$.

Solution:

$$\begin{aligned}
\hat{X} &= \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger \\
\langle n'|\hat{X}|n\rangle &= \left\langle n' \middle| \left(\sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger\right) \middle| n \right\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\langle n'|n-1\rangle + \sqrt{n+1}\,\langle n'|n+1\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right) \\
\hat{X}^2 &= \frac{\hbar}{2m\omega}(\hat{a} + \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger) \\
&= \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \cancel{\hat{a}\hat{a}^\dagger} + \cancel{\hat{a}^\dagger\hat{a}} + \hat{a}^{\dagger 2}\right) \\
&= \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}^{\dagger 2}\right) \\
\left|\langle n'|\hat{X}|n\rangle\right|^2 &= \frac{\hbar}{2m\omega}\left[n\delta_{n',n-1} + (n+1)\delta_{n',n+1}\right]
\end{aligned}$$

For $E_{n'} = E_{n-1}$:

$$\begin{aligned}
&= \left[\left(n - 1 + \frac{1}{2}\right) - \left(n + \frac{1}{2}\right)\right]\hbar\omega \\
&= \left(n - \frac{1}{2} - n - \frac{1}{2}\right)\hbar\omega \\
&= -\hbar\omega
\end{aligned}$$

For $E_{n'} = E_{n+1}$:

$$\begin{aligned}
&= \left[\left(n + 1 + \frac{1}{2}\right) - \left(n + \frac{1}{2}\right)\right]\hbar\omega \\
&= \left(n + \frac{3}{2} - n - \frac{1}{2}\right)\hbar\omega \\
&= \hbar\omega
\end{aligned}$$

Plugging in the values $E_{n'}$, E_n, and $\left|\langle n'|\hat{X}|n\rangle\right|^2$ gives:

$$M_1 = \frac{\hbar}{2m\omega}\left[-n+(n+1)\right]\hbar\omega$$

$$\boxed{M_1 = \frac{\hbar^2}{2m}} \tag{6}$$

PROBLEM 57

The interaction of the electron spin with the magnetic field of the proton gives rise to the following interaction energy known as the *"spin-orbit"* interaction:

$$\hat{H}_{so} = \left(\frac{e^2}{2m^2c^2}\right)\frac{1}{r^3}\boldsymbol{S}\cdot\boldsymbol{L},$$

where m is the mass of the electron, and **S** and **L** are the spin and orbital angular momentum operators of the electron. In this problem you will calculate the first-order shift in the energy levels of the hydrogen atom due to the spin-orbit interaction. Given that the Coulomb potential is spherically symmetric, we can write the eigenstates of the hydrogen atom in terms of the spherical harmonics: $|nlm_l\rangle$, where l and m_l are the quantum numbers associated with $\hat{L}^2$ and $\hat{L}_z$. Now we have to incorporate the intrinsic spin-1/2 nature of the electron. We can do so in two ways: (a) the direct product basis: $|nlm_lm_s\rangle$ or (b) the total angular momentum basis: $|nljm\rangle$.

(a) Show that the spin-orbit operator is *diagonal* in the total angular momentum basis. That is, show that

$$\boldsymbol{S}\cdot\boldsymbol{L}\,|nljm\rangle = C_{lj}\,|nljm\rangle\,.$$

Provide an expression for C_{lj} and note that it is independent of both n and

m.

$$\begin{aligned}
\hat{J}^2 &= \left(\hat{S}+\hat{L}\right)\cdot\left(\hat{S}+\hat{L}\right) \\
&= \hat{S}^2 + 2\hat{S}\cdot\hat{L} + \hat{L}^2 \\
\hat{S}\cdot\hat{L} &= \frac{\hat{J}^2-\hat{S}^2-\hat{L}^2}{2} \\
\hat{S}\cdot\hat{L}\,|nljm\rangle &= \frac{1}{2}\left(j(j+1)-\frac{1}{2}\left(\frac{1}{2}+1\right)-l(l+1)\right)|nljm\rangle \\
&= \frac{1}{2}\left[j(j+1)-l(l+1)-\frac{3}{4}\right]|nljm\rangle \\
\langle n'l'j'm'|\,\hat{S}\cdot\hat{L}\,|nljm\rangle &= \frac{1}{2}\left[j(j+1)-l(l+1)-\frac{3}{4}\right]\langle n'l'j'm'|nljm\rangle
\end{aligned}$$

$$\boxed{\langle n'l'j'm'|\,\hat{S}\cdot\hat{L}\,|nljm\rangle = \frac{1}{2}\left[j(j+1)-l(l+1)-\frac{3}{4}\right]\hbar^2\delta_{n',n}\delta_{l',l}\delta_{j',j}\delta_{m',m}} \tag{7}$$

(b) Using *Kramer's rule*, one can evaluate the following matrix element in closed analytic form:

$$\left\langle nl\left|\frac{1}{r^3}\right|nl\right\rangle = \frac{2}{n^3 l(l+1)(2l+1)a_0^3},$$

where a_0 is the Bohr radius. Verify the validity of this expression for all the eigenstates with principal quantum numbers $n=1$ and $n=2$.

First, plugging in the possible values of n and l into the equation yields:

$$\begin{aligned}
\left\langle 10\left|\frac{1}{r^3}\right|10\right\rangle &= \frac{2}{(1)^3(0)(0+1)(2(0)+1)a_0^3} \\
&= \boxed{\frac{2}{0}} \quad \text{(indeterminate)} \\
\left\langle 20\left|\frac{1}{r^3}\right|20\right\rangle &= \frac{2}{(2)^3(0)(0+1)(2(0)+1)a_0^3} \\
&= \boxed{\frac{2}{0}} \quad \text{(indeterminate)} \\
\left\langle 21\left|\frac{1}{r^3}\right|21\right\rangle &= \frac{2}{(2)^3(1)(1+1)(2(1)+1)}a_0^3 \\
&= \boxed{\frac{1}{24a_0^3}}
\end{aligned}$$

Now solving for the expectation value of each state:

$\vert 10\rangle$	$\frac{2}{a_0^{3/2}}e^{-r/a_0}$
$\vert 20\rangle$	$\frac{1}{2\sqrt{2}a_0^{3/2}}\left[2-\frac{r}{a_0}\right]e^{-r/2a_0}$
$\vert 21\rangle$	$\frac{1}{2\sqrt{6}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$

$$\begin{aligned}
\left\langle 10\left|\frac{1}{r^3}\right|10\right\rangle &= \left(\frac{2}{a_0^{3/2}}\right)^2\int_0^\infty \frac{r^2}{r^3}e^{-2r/a_0}\mathrm{d}r \\
&= \boxed{\frac{4}{a_0^{3/2}}\int_0^\infty \frac{e^{-2r/a_0}}{r}\mathrm{d}r} \\
\left\langle 20\left|\frac{1}{r^3}\right|20\right\rangle &= \left(\frac{1}{2\sqrt{2}a_0^{3/2}}\right)^2\int_0^\infty \left[2-\frac{r}{a_0}\right]\frac{r^2}{r^3}e^{-r/a_0}\mathrm{dr} \\
&= \boxed{\frac{1}{8a_0^3}\left[\int_0^\infty \frac{2}{r}e^{-r/a_0}\mathrm{d}r - \int_0^\infty \frac{r}{a_0}e^{-r/a_0}\mathrm{d}r\right]}
\end{aligned}$$

	u	v'
+	r	e^{-r/a_0}
-	1	$-a_0e^{-r/a_0}$
+	0	$a_0^2e^{-r/a_0}$

$$
\begin{aligned}
&= \frac{1}{8a_0^3}\left[\left(\int_0^\infty \frac{2}{r}e^{-r/a_0}\mathrm{d}r\right) + a_0 e^{-r/a_0}\left(r+a_0\right)\right] \\
\left\langle 21\middle|\frac{1}{r^3}\middle|21\right\rangle &= \left(\frac{1}{2\sqrt{2}a_0^{3/2}}\right)^2 \frac{1}{a_0^2}\int_0^\infty \frac{r^4}{r^3}e^{-r/a_0}\mathrm{d}r \\
&= \frac{1}{24a_0^5}\int_0^\infty re^{-r/a_0}\mathrm{d}r \\
&= \frac{1}{24a_0^5}\left[-a_0 e^{-r/a_0}(r+a_0)\right]_0^\infty \\
&= \boxed{\frac{1}{24a_0^3}}
\end{aligned}
$$

(c) Using the results obtained in parts (a) and (b), conclude that the first-order shift in the energy levels of the hydrogen atom due to the spin-orbit interaction may be written as follows:

$$
E_{nlj}^{(1)} = \frac{\alpha^4 mc^2}{2n^3}\left[\frac{j(j+1)-l(l+1)-3/4}{l(l+1)(2l+1)}\right].
$$

Evaluate explicitly the first-order shift for all the eigenstates with principal quantum numbers $n = 1$, $n = 2$, and $n = 3$ - and compare it against the corresponding unperturbed value of the energy.

$$
a_0 \equiv \frac{\hbar}{mc\alpha}, \qquad e^2 \equiv c\alpha\hbar
$$

$$
\begin{aligned}
&\left\langle nljm\middle|\left(\frac{e^2}{2m^2c^2}\right)\frac{1}{r^3}\hat{S}\cdot\hat{L}\middle|nljm\right\rangle \\
&\qquad = \left(\frac{e^2}{2m^2c^2}\right)\frac{\hbar^2}{2}\left[j(j+1)-l(l+1)-\frac{3}{4}\right]\left\langle nljm\middle|\frac{1}{r^3}\middle|nljm\right\rangle \\
&\qquad = \left(\frac{e^2\hbar^2}{2m^2c^2n^3a_0^3}\right)\left[\frac{j(j+1)-l(l+1)-3/4}{l(l+1)(2l+1)}\right]
\end{aligned}
$$

$$
\boxed{\therefore E_{nlj}^{(1)} = \frac{\alpha^4 mc^2}{2n^3}\left[\frac{j(j+1)-l(l+1)-3/4}{l(l+1)(2l+1)}\right]} \tag{8}
$$

For $n = 1$, $l = 0$, $j = 1/2$:

$$\begin{aligned} E^1_{1,0,1/2} &= \frac{\alpha^4 mc^2}{2(1)^3}\left[\frac{\frac{1}{2}\left(\frac{1}{2}+1\right) - 0(0+1) - \frac{3}{4}}{0(0+1)(2(0)+1)}\right] \\ &= \boxed{\text{indeterminate}} \end{aligned}$$

Therefore $n = 2$, and $n = 3$ will also be indeterminate

For $n = 2$, $l = 1$, $j = 3/2$:

$$\begin{aligned} E^1_{2,1,3/2} &= \frac{\alpha^4 mc^2}{2(2)^3}\left[\frac{\frac{3}{2}\left(\frac{3}{2}+1\right) - 1(1+1) - \frac{3}{4}}{1(1+1)(2(1)+1)}\right] \\ &= \boxed{\frac{\alpha^4 mc^2}{3 \cdot 2^5}} \end{aligned}$$

It can be easily seen that for state $n = 3$, $l = 1$, $j = 3/2$:

$$\boxed{E^1_{3,1,3/2} = \frac{\alpha^4 mc^2}{4 \cdot 3^4}}$$

For $n = 3$, $l = 2$, $j = 5/2$:

$$\begin{aligned} E^1_{3,2,5/2} &= \frac{\alpha^4 mc^2}{2(3)^3}\left[\frac{\frac{5}{2}\left(\frac{5}{2}+1\right) - 2(2+1) - \frac{3}{4}}{2(2+1)(2(2)+1)}\right] \\ &= = \boxed{\frac{\alpha^4 mc^2}{10 \cdot 3^4}} \end{aligned}$$

The ground state energy values for an unperturbed Hamiltonian for a hydrogen atom are given by the equation $\frac{-13.6}{n^2}$. These values are much larger than the corresponding perturbed values.