# UNIVERSITY OF OSLO
## FACULTY OF MATHEMATICS AND NATURAL SCIENCES

**Solution to exam in:** FYS3110, Quantum mechanics

**Day of exam:** Dec. 1. 2014

**Permitted material:** Approved calculator, D.J. Griffiths: "Introduction to Quantum Mechanics", the printed notes: "Time evolution of states in quantum mechanics", "Symmetry and degeneracy" and "WKB connection formulae", one handwritten A4-sheet(2 pages) with your own notes, and K. Rottmann: "Matematisk formelsamling"

## Problem 1

**1.1** The variational method is a method for calculating an upper bound on the ground state energy. The method is based on the inequality $\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$ which holds for any $|\psi\rangle$, or equivalently $\langle\psi|H|\psi\rangle \geq E_0$ which holds for any *normalized* state $|\psi\rangle$. In the variational method one calculates the left hand side of the inequality for a guessed trial state $|\psi\rangle$. The obtained number is then an upper bound on the ground state energy. One can also calculate the left hand side for several trial states. The best (least) upper bound on the ground state energy is then the minimum of all these.

**1.2** For arbitrary states $|\psi_1\rangle$ and $|\psi_2\rangle$ we have

$$\langle\psi_1|(\hat{A}\hat{B})^\dagger|\psi_2\rangle = \langle\psi_2|\hat{A}\hat{B}|\psi_1\rangle^* = \left(\sum_k \langle\psi_2|\hat{A}|k\rangle\langle k|\hat{B}|\psi_1\rangle\right)^* = \sum_k \langle\psi_2|\hat{A}|k\rangle^*\langle k|\hat{B}|\psi_1\rangle^*$$
$$= \sum_k \langle\psi_1|\hat{B}^\dagger|k\rangle\langle k|\hat{A}^\dagger|\psi_2\rangle = \langle\psi_1|\hat{B}^\dagger\hat{A}^\dagger|\psi_2\rangle.$$

Since this holds for all states $|\psi_1\rangle$ and $|\psi_2\rangle$ we have the operator identity: $\underline{\left(\hat{A}\hat{B}\right)^\dagger = \hat{B}^\dagger\hat{A}^\dagger}$. q.e.d.

For Hermitean operators: $\hat{A}^\dagger = \hat{A}$ and $\hat{B}^\dagger = \hat{B}$. Then using $\hat{O}^\dagger = (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A}$. $\hat{O}^\dagger = \hat{O} \implies \hat{B}\hat{A} = \hat{A}\hat{B} \implies \underline{\left[\hat{A},\hat{B}\right] = 0}$. q.e.d.

## Problem 2

**2.1** For $g = 0$ the system is like the Hydrogen atom, but with the energy scale $\underline{E_1 = -\frac{m}{2\hbar^2}|qQ|^2}$ and effective Bohr radius $a = \frac{\hbar^2}{m|Qq|}$. We can denote the states as in the

Hydrogen problem by $|nlm\rangle$ and the energy depends only on $n$, $E_n = E_1/n^2$. The lowest energy state is $|100\rangle$ with energy $\underline{E_{gs} = E_1 = -\frac{m}{2\hbar^2}|qQ|^2}$ and is unique, so the degree of degeneracy is $\underline{1}$. The second lowest energy level has energy $\underline{E_{ex} = E_1/4 = -\frac{m}{8\hbar^2}|qQ|^2}$. There are $\underline{4}$ states with this energy: $|200\rangle, |21-1\rangle, |210\rangle$ and $|21+1\rangle$.

**2.2** The ground state wave function is $\langle r, \theta, \phi|100\rangle = \sqrt{\frac{1}{\pi a^3}}e^{-r/a}$ where the effective Bohr radius is $a = \frac{\hbar^2}{m|qQ|}$. Non-degenerate perturbation theory gives

$$\begin{aligned}\Delta E = \langle 100|gr^2|100\rangle &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dr r^2 \frac{1}{\pi a^3} g r^2 e^{-2r/a} = g\frac{4\pi}{\pi a^3}\int_0^{\infty} dr r^4 e^{-2r/a} \\ &= g\frac{4}{a^3}\left(\frac{a}{2}\right)^5 \underbrace{\int_0^{\infty} du u^4 e^{-u}}_{4!} = 3ga^2 = 3g\frac{\hbar^4}{m^2q^2Q^2}\end{aligned}$$

Therefore the ground state energy is $\underline{E_g = -\frac{m}{2\hbar^2}q^2Q^2 + 3g\frac{\hbar^4}{q^2Q^2m^2} + \mathcal{O}(g^2)}$.

**2.3** The perturbed system is still rotational symmetric. This means that the eigenstates can be characterized by the quantum numbers $l$ and $m$. States with different $m$-values are degenerate because $m$ is the quantum number of $L_z$ and rotational invariance implies that the energy cannot depend on the choice of z-axis. The $l$ degeneracy that exists in the unperturbed case is a special consequence of the Coulomb potential and is not expected to hold for a potential that falls off differently than $1/r$. Thus the first excited level which have four states ($n = 2$) will split into $\underline{\text{two}}$ levels, one with three states $l = 1, m = 0, \pm 1$ and the other with a single state $l = 0, m = 0$.

One can also calculate this explicitly to first order in $g$. Degenerate perturbation theory requires one to calculate all the matrix elements $\langle 2l'm'|r^2|2lm\rangle$. The rotational symmetry of $V_K$ manifests itself in the fact that $V_K$ only depends on $r$ and not on the angles. This means that only matrix elements with $m' = m$ and $l' = l$ will be non-zero. Therefore the matrix is diagonal so that the $|2lm\rangle$'s are good states, and we can read off the energy corrections as the diagonal matrix elements. The wave functions $\langle r\theta\phi|21m\rangle$ differ from each other only by a factor $e^{im\phi}$ which implies that the matrix elements $\langle 211|r^2|211\rangle = \langle 210|r^2|210\rangle = \langle 21-1|r^2|21-1\rangle$ are all equal. The only one that can be different is $\langle 210|r^2|210\rangle$. Thus the four-fold energy level can be split into maximally $\underline{\text{two}}$ sublevels by the perturbation $V_K$.

The actual numbers are

$$\begin{aligned}
\langle 210|gr^2|210\rangle &= g\underbrace{\int_0^{2\pi} d\phi}_{2\pi}\int_0^{\pi} d\theta \sin\theta \int_0^{\infty} drr^2 r^2 \frac{3}{4\pi}\cos^2\theta \frac{1}{24}a^{-3}\left(\frac{r}{a}\right)^2 e^{-r/a} \\
&= g\frac{3}{48}\underbrace{\int_0^{\pi} d\theta \sin\theta\cos^2\theta}_{2/3} a^{-3}\int_0^{\infty} drr^4\left(\frac{r}{a}\right)^2 e^{-r/a} = g\frac{1}{24}a^2\underbrace{\int_0^{\infty} duu^6 e^{-u}}_{6!} \\
&= 30ga^2 = 30\left(\frac{\hbar^2}{mqQ}\right)^2 \\
\langle 200|gr^2|200\rangle &= g\underbrace{\int_0^{2\pi} d\phi\int_0^{\pi} d\theta\sin\theta}_{4\pi}\int_0^{\infty} drr^2 r^2\frac{1}{4\pi}\frac{1}{2}a^{-3}\left(1-\frac{r}{2a}\right)^2 e^{-r/a} \\
&= g\frac{1}{2}a^2\int_0^{\infty} duu^4\left(1-\frac{u}{2}\right)^2 e^{-u} \\
&= g\frac{1}{2}a^2\left(\underbrace{\int_0^{\infty} duu^4 e^{-u}}_{4!} - \underbrace{\int_0^{\infty} duu^5 e^{-u}}_{5!} + \frac{1}{4}\underbrace{\int_0^{\infty} duu^6 e^{-u}}_{6!}\right) \\
&= 42ga^2 = 42g\left(\frac{\hbar^2}{mqQ}\right)^2
\end{aligned}$$

**2.4** For $Q = 0$ the Hamiltonian is that of a 3D harmonic oscillator with $\frac{1}{2}m\omega^2 = g$ or equivalently $\omega = \sqrt{2g/m}$. The energy levels for $Q = 0$ is given by $E_{n_x,n_y,n_z} = \hbar\omega\left(n_x + n_y + n_z + 3/2\right)$ where the states are direct product of 1D harmonic oscillator states $|n_x, n_y, n_z\rangle = |n_x\rangle \otimes |n_y\rangle \otimes |n_z\rangle$. The unperturbed ground state is unique and has the energy $E^0_{000} = \frac{3}{2}\hbar\omega$ and the wave function

$$\psi_{000}\left(\vec{r}\right) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar}\left(x^2+y^2+z^2\right)} = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar}r^2} = \left(\frac{1}{\pi}\sqrt{\frac{2gm}{\hbar^2}}\right)^{3/4} e^{-\sqrt{\frac{2gm}{\hbar^2}}r^2/2}$$

where we have used the wave function for the ground state of three independent 1D harmonic oscillators. The inverse quadratic length scale $\frac{m\omega}{\hbar} = \sqrt{\frac{2gm}{\hbar^2}}$. The ground state is unique, so

the energy correction to first order is

$$\begin{aligned}\Delta E_{000} &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dr r^2 \psi^*_{000}(\vec{r}) \frac{-|qQ|}{r} \psi_{000}(\vec{r}) \\ &= -|qQ| 4\pi \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} \int_0^{\infty} \underbrace{dr r}_{\frac{1}{2}dr^2} e^{-\frac{m\omega}{\hbar}r^2} \\ &= -|qQ| 2\pi \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} \left(\frac{m\omega}{\hbar}\right)^{-1} \underbrace{\int_0^{\infty} d\left(\frac{m\omega}{\hbar}r^2\right) e^{-\frac{m\omega}{\hbar}r^2}}_{1} \\ &= -|qQ| \frac{2}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar}\right)^{1/2} = \underline{-|qQ| \frac{2}{\sqrt{\pi}} \left(\frac{2gm}{\hbar^2}\right)^{1/4}}\end{aligned}$$

Thus the energy correct to order $\mathcal{O}(Q)$ is

$$\underline{E = \frac{3}{2}\hbar \left(\frac{2g}{m}\right)^{1/2} - \frac{2}{\sqrt{\pi}}|qQ| \left(\frac{2gm}{\hbar^2}\right)^{1/4}}$$

**2.5** According to first order time-dependent perturbation theory the probability amplitude to find the system in the energy eigenstate $f$ starting from the energy eigenstate $i$ at $t = 0$ after the field has vanished is

$$a_f = \frac{1}{i\hbar} \int_0^{t_1} dt \langle f| - q\vec{E}_0 \cdot \vec{r}|i\rangle e^{i\left(E_f - E_i\right)t/\hbar}$$

where the integral is cut off at $t_1$ as the electric field is only non-zero in this time period. The electric field is polarized in the $z$-direction, thus $\vec{E}_0 \cdot \vec{r} = E_0 z$. In first order perturbation theory there will only be transitions to states $f$ for which $\langle f|z|i\rangle \neq 0$. The initial state is the ground state of the 3D harmonic oscillator $|n_x = 0, n_y = 0, n_z = 0\rangle$. The operator $z$ can be written as a combination of creation and annihilation operators $z = \sqrt{\frac{\hbar}{2m\omega}}\left(a_z + a_z^\dagger\right)$ which means that $z|000\rangle = \sqrt{\frac{\hbar}{2m\omega}}|001\rangle$ and implies that the only non-zero matrix element is

$$\langle 001|z|000\rangle = \sqrt{\frac{\hbar}{2m\omega}}$$

thus the only possible excited final state is $|f\rangle = |001\rangle$ which has energy $\frac{5}{2}\hbar\omega$, and therefore $E_f - E_i = \hbar\omega$. We therefore have

$$a_f = -qE_0\sqrt{\frac{\hbar}{2m\omega}} \frac{1}{i\hbar} \int_0^{t_1} dt e^{i\omega t} = \frac{qE_0}{\left(2m\hbar\omega\right)^{1/2}} \frac{e^{i\omega t_1} - 1}{\omega} = \frac{2iqE_0}{\left(2m\hbar\omega^3\right)^{1/2}} e^{i\omega t_1/2} \underbrace{\frac{e^{i\omega t_1/2} - e^{-i\omega t_1/2}}{2i}}_{\sin\omega t_1/2}$$

The probability is

$$P_{i\to f} = |a_f|^2 = \frac{4q^2E_0^2}{2m\hbar\omega^3}\sin^2\left(\frac{\omega t_1}{2}\right) = \underline{\frac{q^2E_0^2}{\hbar}\left(\frac{m}{2g^3}\right)^{1/2}\sin^2\left(\sqrt{\frac{g}{2m}}t_1\right)}$$

## Problem 3

**3.1** $H^{so} = \frac{b}{\hbar^2}\vec{S}\cdot\vec{L} = \frac{b}{2\hbar^2}\left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2\right)$. Eigenstates are $|JLS\rangle$ with energy $E_{JLS} = \frac{b}{2}\left(J(J+1) - L(L+1) - S(S+1)\right)$. For fixed $L$ and $S$ the total angular momentum takes values $J \in \{|L-S|, |L-S|+1, \ldots, L+S\}$.

Two successive energy levels have J values that differ by unity. Let $J_1$ and $J_2$ be the two such successive values with $J_2$ the largest, so that $J_1 = J_2 - 1$. The energy splitting between these two levels is then $\Delta E = E_{J_2LS} - E_{J_1LS} = \frac{b}{2}\left(J_2(J_2+1) - (J_2-1)(J_2-1+1)\right) = \underline{bJ_2}$, thus $\Delta E$ is proportional to $J_2$ which is the largest of the two. q.e.d.

**3.2** The number of levels corresponds to the number of different $J$ values. If $L > S$ the total number of $J$ values is $2S+1$, while if $L < S$ the total number of different $J$ values is $2L+1$. $2L+1$ is however always an odd number, thus the fact that there are four levels implies $L > S$ and $2S+1 = 4 \implies \underline{S = 3/2}$.

In order to determine $J$ we can form energy differences between successive energy levels (in eV): $\Delta E_{10} = E_1 - E_0 = 1.70\times10^{-2}$, $\Delta E_{21} = E_2 - E_1 = 2.38\times10^{-2}$, $\Delta E_{32} = E_3 - E_2 = 3.06\times10^{-2}$. and use the fact shown in **3.1** that these energy differences are proportional to the largest of the $J$ values involved. Lets label the different $J$ values in increasing order $\{J_0, J_1, J_2, J_3\} = \{J_0, J_0+1, J_0+2, J_0+3\}$. We do not a priori know the sign of $b$ so we do not know if the lowest energy correspond to $J_0$ or $J_3$. If $b > 0$: $\Delta E_{10} \propto J_1$ and $\Delta E_{32} \propto J_3$, while if $b < 0$: $\Delta E_{10} \propto J_3$ and $\Delta E_{32} \propto J_1$. Thus to find the sign of $b$ we can investigate the ratio

$$\frac{\Delta E_{32}}{\Delta E_{10}} = \begin{cases} \frac{J_3}{J_1} = \frac{J_0+3}{J_0+1} > 1, & b > 0 \\ \frac{J_1}{J_3} = \frac{J_0+1}{J_0+3} < 1, & b < 0 \end{cases}$$

Using the numbers given we find $\Delta E_{32}/\Delta E_{10} = 1.8 > 1 \implies \underline{b > 0}$, thus the sign of $b$ is positive, and the lowest energy level corresponds to $J_0$. (With this knowledge we can also

find the precise value of $b$ because $\Delta E_{32} - \Delta E_{21} = b\,(J_3 - J_2) = b \implies b = 6.8 \times 10^{-3} eV$). To find the numerical value of $J_0$ we can solve the energy ratio $\Delta E_{32}/\Delta E_{10}$ for $J_0$. One ratio is enough, but we give all the possibilities here

$$\begin{aligned}
\frac{\Delta E_{21}}{\Delta E_{10}} &= \tfrac{2.38}{1.70} = 1.40 = \tfrac{J_0+2}{J_0+1} = 1 + \tfrac{1}{J_0+1} \implies J_0 = 1.5 \\
\frac{\Delta E_{32}}{\Delta E_{10}} &= \tfrac{3.06}{1.70} = 1.80 = \tfrac{J_0+3}{J_0+1} = 1 + \tfrac{2}{J_0+1} \implies J_0 = 1.5 \\
\frac{\Delta E_{32}}{\Delta E_{21}} &= \tfrac{3.06}{2.38} = 1.286 = \tfrac{J_0+3}{J_0+2} = 1 + \tfrac{1}{J_0+2} \implies J_0 = 1.5
\end{aligned}$$

All of these give $J_0 = 1.5$. Thus we conclude that $J_0 = 3/2$. Now $J_0 = |L - S|$, and since $L > S$: $\underline{L = 3}$.

——THE END