Quantum Mechanics FKA081/FIM400

Final Exam 28 October 2015

Next review time for the exam: December 2nd between 14:00-16:00 in my room.
(This info is also available on the course homepage.)

Examinator: Gabriele Ferretti tel. 031-7723168, 0721-582259, ferretti@chalmers.se

Allowed material during the exam:

- The course textbook J.J. Sakurai and Jim Napolitano, Modern Quantum Mechanics Second Edition.
  NB: The old version: J.J. Sakurai, Modern Quantum Mechanics is *also* allowed.
- A Chalmers approved calculator.

Write the final answers clearly marked by Ans: ...
and underline them.

You may use without proof any formula in the book.

The grades are assigned according to the table in the course homepage.

Problem 1

The nucleus of Li_7 (the most abundant isotope of Lithium) has spin 3/2. Consider the ion Li^{++} formed by a single electron orbiting such nucleus. Suppose the electron is in the orbital angular momentum state $l = 1$.

Q1 (*1 points*) Combine first the spin of the electron and the orbital angular momentum together and then combine the result with the spin of the nucleus to find all allowed total angular momenta of the ion.

Q2 (*1 points*) Repeat the same calculation combining first the two spins and then the orbital angular momentum and show that one gets the same final result.

Q3 (*1 points*) Check your calculation by showing that the dimensions of the various Hilbert spaces add up correctly.

Q4 (*1 points*) We see that the total angular momentum depends on the spin of the nucleus. Yet, in studying the atomic properties of Hydrogen-like atoms, we often ignore the nuclear spin. Why is that?

Problem 2

Consider an Hydrogen atom with the usual Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r}. \tag{1}$$

The finite size of the proton can be roughly approximated by a perturbation

$$V_1(r) = \begin{cases} +\frac{e^2}{r} + \frac{e^2 r^2}{2r_0^3} - \frac{3e^2}{2r_0} & \text{for } r \le r_0 \\ 0 & \text{for } r > r_0 \end{cases} \tag{2}$$

where r_0 is the radius of the proton.

Q1 (*2 points*) Compute the correction of the ground-state energy to first order in perturbation theory due to V_1.

Hints: Recall that the ground state wave-function is

$$\psi_{\text{g.s.}}(\mathbf{r}) = \frac{1}{\sqrt{\pi a_0^3}} \mathrm{e}^{-r/a_0} \tag{3}$$

(a_0 is the Bohr radius.) Don't do the integrals exactly! Since $r_0 \ll a_0$, you may approximate the exponential inside the integrand by 1!

Q2 (*1 point*) Given that $r_0 \approx 8.8 \times 10^{-16}$ m and $a_0 \approx 5.3 \times 10^{-11}$ m and that the unperturbed ground state energy is $-e^2/(2a_0) \approx -13.6$ eV compute the numerical value of the correction.

Q3 (*2 points*) Without any calculation, what can you say *qualitatively* on the higher order corrections? Should you use degenerate or non degenerate perturbation theory? Which levels (n, l, m_l, m_s) will be affected most?

Q4 (*1 point*) Why do you think V_1 has the form it has? Can you justify each term qualitatively?

Problem 3

Consider a spinless particle of mass m in a one dimensional infinite well:

$$H_0 = \frac{p^2}{2m} + U(x), \tag{4}$$

where

$$U(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases} \tag{5}$$

It is known that the energy eigenvalues of H_0 are (units $\hbar = 1$) $E_n^{(0)} = \frac{n^2\pi^2}{2mL^2}$.

At time $t = 0$ we turn on a potential given by

$$V(x) = \lambda\delta(x - L/2)e^{-t/\tau} \tag{6}$$

where $\lambda > 0$ is a small parameter, τ a constant and δ the Dirac delta-function.

Q1 (*1 point*) Show that, to first order in perturbation theory, no transition is allowed between the ground state ($n = 1$) and the excited states with n even.

Q2 (*2 point*) Compute the transition probability $P_{1\to n}$ between the ground state and states with n odd.

Q3 (*2 point*) How would you quantify the statement that λ must be "small" in terms of a relation between λ, L and τ? (Hint: What are the requirements on $P_{1\to n}$?)

Problem 4

Consider a sodium (Na) atom and let $\mathbf{L}$ and $\mathbf{S}$ be the orbital angular momentum and spin of the outer electron. Let as usual $\mathbf{J} = \mathbf{L} + \mathbf{S}$ and let j be its quantum number.

Let $\mathbf{S}_N$ be the spin operator of the nucleus, and let s_N be the spin of the nucleus. One can have the so-called hyperfine correction, given by the term $H_{\rm HF} = A\, \mathbf{S}_N \cdot (\mathbf{L} + \mathbf{S})$ for A a given positive constant much smaller than the constant appearing in the spin-orbit interaction.

Q1 (*2 points*) Compute the corrections to the spectrum of Na due to the hyperfine interaction for arbitrary spin of the nucleus.

Q2 (*2 points*) Show graphically how the diagram of Q1 is modified for the ground state level $(n, l) = (3, 0)$ in the case $s_N = 3/2$ (the realistic case for sodium).

Q3 (*1 points*) Could you use this interaction to measure the spin of a nucleus in general? How? (You do not need to be precise, just give the basic idea)

Problem 5

Consider a state described by the density matrix

$$\rho = \frac{1}{6} \begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix} \tag{7}$$

Q1 (*1 point*) Show that it corresponds to a pure state.

Q2 (*1 point*) Find the pure state it corresponds to.

Consider now the observable

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{8}$$

Q3 (*1 point*) Find its expectation value for the state described by ρ.

Q4 (*1 point*) Show that the probability of measuring the lowest eigenstate of A on the state described by ρ is zero.

Consider now another state described by the density matrix

$$\rho' = \frac{1}{12}\begin{pmatrix} 7 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix} \tag{9}$$

Q5 (*1 point*) is ρ' a pure state?

Q6 (*1 point*) Compute the probability of measuring the lowest eigenstate of A on the state described by ρ'.

Problem 6

A certain type of molecule in a constant electric field can assume two different orientation eigenstates $|\psi_1\rangle$ and $|\psi_2\rangle$ with energies $E_1 = -8.2 \times 10^{-5}$ eV and $E_2 = +8.2 \times 10^{-5}$ eV respectively. We have a sample of 10^6 such molecules all in their lower energy state.

At time $t = 0$ we turn on a varying field with period $T = 0.314$ ns and amplitude $\gamma = 4.1 \times 10^{-5}$ eV giving rise to the perturbation

$$V(t) = \gamma(e^{2\pi i t/T}|\psi_1\rangle\langle\psi_2| + e^{-2\pi i t/T}|\psi_2\rangle\langle\psi_1|) \tag{10}$$

Q1 (*2 points*) How long do we have to wait so that the maximum amount of molecules will be found in the excited state? (Use $\hbar = 4.1 \times 10^{-15}$ eV $\cdot$ s!)

Q2 (*2 points*) How many such molecules would we find at the time obtained in Q1?

PROBLEM 1

Q1: $\mathcal{H}_1 \otimes \mathcal{H}_{\frac{1}{2}} = \mathcal{H}_{\frac{1}{2}} \oplus \mathcal{H}_{\frac{3}{2}}$.

$$(\mathcal{H}_1 \otimes \mathcal{H}_{\frac{1}{2}}) \otimes \mathcal{H}_{\frac{3}{2}} = (\mathcal{H}_{\frac{1}{2}} \otimes \mathcal{H}_{\frac{3}{2}}) \oplus (\mathcal{H}_{\frac{3}{2}} \otimes \mathcal{H}_{\frac{3}{2}}) =$$

$$= (\mathcal{H}_1 \oplus \mathcal{H}_2) \oplus (\mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3) =$$

$$= \mathcal{H}_0 \oplus 2 \cdot \mathcal{H}_1 \oplus 2 \cdot \mathcal{H}_2 \oplus \mathcal{H}_3 .$$

Q2: $\mathcal{H}_{\frac{1}{2}} \otimes \mathcal{H}_{\frac{3}{2}} = \mathcal{H}_1 \oplus \mathcal{H}_2$

$$(\mathcal{H}_{\frac{1}{2}} \otimes \mathcal{H}_{\frac{3}{2}}) \otimes \mathcal{H}_1 = (\mathcal{H}_1 \otimes \mathcal{H}_1) \oplus (\mathcal{H}_2 \otimes \mathcal{H}_1)$$

$$= (\mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2) \oplus (\mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3) =$$

$$= \mathcal{H}_0 \oplus 2 \cdot \mathcal{H}_1 \oplus 2\mathcal{H}_2 \oplus \mathcal{H}_3 .$$

Q3: $\dim(\mathcal{H}_{\frac{1}{2}} \otimes \mathcal{H}_1 \otimes \mathcal{H}_{\frac{3}{2}}) = 2 \times 3 \times 4 = 24$

$\dim(\mathcal{H}_0 \oplus 2 \cdot \mathcal{H}_1 \oplus 2 \cdot \mathcal{H}_2 \oplus \mathcal{H}_3) = 1 + 2 \cdot 3 + 2 \cdot 5 + 7 = 24$

Q4: The atomic properties are controlled by $\mu = \mu_0 S$ etc. where $\mu_0 \propto \frac{1}{\text{mass}}$. Hence the nucleus contributes much less

PROBLEM 2

Q1: $E^{(1)} = \langle \psi_{gs} | V_1 | \psi_{gs} \rangle = \int d^3r \, |\psi_{gs}|^2 V_1 =$

$$= \int_0^{r_0} dr\, r^2 \cdot \underbrace{\int d^2\Omega}_{4\pi} \cdot \frac{1}{\pi a_0^3} e^{-2r/a_0} \left(\frac{e^2}{r} + \frac{e^2 r^2}{2r_0^3} - \frac{3e^2}{2r_0} \right) =$$

$$= \frac{4e^2}{a_0^3} \left(\int_0^{r_0} dr\, r\, e^{-2r/a_0} + \frac{1}{2r_0^2} \int_0^{r_0} dr\, r^4 e^{-2r/a_0} - \right.$$

$$\left. - \frac{3}{2r_0} \cdot \int_0^{r_0} dr\, r^2 e^{-2r/a_0} \right) = \frac{4e^2}{a_0^3} \left(\frac{r_0^2}{2} + \frac{1}{2r_0^2} \cdot \frac{r_0^5}{5} - \frac{3}{2r_0} \cdot \frac{r_0^3}{3} \right)$$

$$= \frac{2e^2 r_0^2}{5 a_0^3}$$

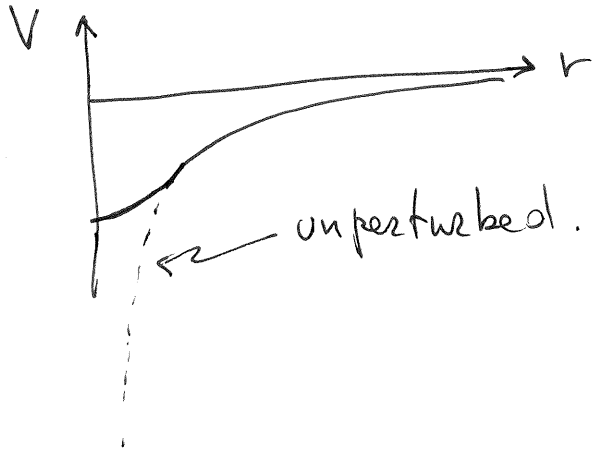
Q2: $E^{(1)} = \frac{2e^2 r_0^2}{5a_0^3} = \frac{4}{5} \cdot \frac{e^2}{2a_0} \cdot \left(\frac{r_0}{a_0} \right)^2 =$

$$= \frac{4}{5} \cdot 13.6\,eV \cdot \left(\frac{8.8 \times 10^{-16}\,m}{5.3 \times 10^{-11}\,m} \right)^2 \simeq 3 \times 10^{-9}\,eV.$$

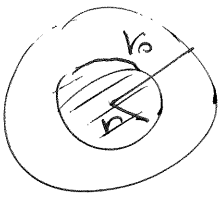
Q3: Since $R_{he}(r) \to 0$ as $r \to 0$ when $\ell \neq 0$ the only relevant corrections are for $\ell = 0$.

Also: $[L, V_1] = [S, V_1] = 0$ → non degenerate.

Q4 :



V must be continuous and dezivable at $r = r_0$.
Alternatively, use Gauss' law to get the potential inside a uniformly charged ball of radius r_0:



$$4\pi E r^2 = 4\pi \cdot \frac{e}{\frac{4\pi}{3} r_0^3} \cdot \frac{4\pi}{3} r^3$$

$$\Rightarrow E = \frac{e r}{r_0^3} = -\frac{\partial}{\partial r} U$$

$$U = -\frac{e r^2}{2 r_0^3} + \text{const} \quad \Rightarrow \underset{\text{ball.}}{V} = -eU = \frac{e^2 r^2}{2 r_0^3} + \text{const.}$$

I have to match this w/ the pot. outside.

$$V_{tot} = \begin{cases} -e^2/r & (r > r_0) \\ \frac{e^2 r^2}{2 r_0^3} - \frac{3}{2}\frac{e^2}{r_0} & (r < r_0) \end{cases}$$

$$\Rightarrow V_1 = \frac{e^2}{r} + \frac{e^2 r^2}{2 r_0^3} - \frac{3}{2}\frac{e^2}{r_0}.$$

PROBLEM 3

Q1: $\langle m|V|1\rangle = \int_0^L \left(\sqrt{\frac{2}{L}}\right)^2 \sin\frac{\pi n x}{L}\, \lambda\delta\left(x-\frac{L}{2}\right) \sin\frac{\pi x}{L}\, e^{-t/\tau}$

$= \lambda \cdot e^{-t/\tau} \cdot \frac{2}{L} \cdot \sin\left(\frac{\pi m}{L}\cdot\frac{L}{2}\right) \cdot \underbrace{\sin\left(\frac{\pi}{L}\cdot\frac{L}{2}\right)}_{1} =$

$= \frac{2\lambda}{L} e^{-t/\tau} \sin\frac{\pi}{2}\cdot m \quad = 0$ for n even.

(could also be proven by "parity" around $x=\frac{L}{2}$, not the origin).

Q2: $\omega_{n1} = \frac{(n^2-1)\pi^2}{2mL^2}$

$P_{1\to n} = (\quad) \cdot \left| \int_0^{+\infty} \frac{2\lambda}{L} e^{-\left(\frac{1}{\tau} - i\omega_{n1}\right)t} dt \right|^2 =$

$\left(\left|\sin\frac{\pi}{2}n\right| = 1\right)$

$= \left(\frac{2\lambda}{L}\right)^2 \cdot \frac{1}{\left|\frac{1}{\tau} - i\omega_{n1}\right|^2} = \left(\frac{2\lambda}{L}\right)^2 \cdot \frac{\tau^2}{1+\tau^2\omega_{n1}^2}.$

Q3. $P_{1\to n} < 1 \Rightarrow \lambda < L\omega_{n1}/2$ OR.

$\left(P_{1\to n} = \left(\frac{2\lambda}{L\omega_{n1}}\right)^2 \cdot \underbrace{\frac{\tau^2\omega_{n1}^2}{1+\tau^2\omega_{n1}^2}}_{<1}\right) < L/2\tau.$

depending on $\omega_{n1}\tau \gg 1$.

Case I:
ω_{21} is the smallest
$\Rightarrow \lambda < \frac{L}{2}\cdot\frac{3\pi^2}{2mL^2} = \frac{3\pi^2}{4}\frac{1}{mL} \simeq 7\frac{1}{mL}.$

Problem 4.

Q1: $H_{HF} = A\,\mathbb{S}_N \cdot \mathbb{J}$ set $\mathbb{J}_{TOT} = \mathbb{J} + \mathbb{S}_N$

$\mathbb{J}_{TOT}^2 = \mathbb{J}^2 + \mathbb{S}_N^2 + 2\,\mathbb{S}_N \cdot \mathbb{J}$ $\Rightarrow$ $H_{HF} = \frac{A}{2}\left(\mathbb{J}_{TOT}^2 - \mathbb{J}^2 - \mathbb{S}_N^2\right)$

$\Rightarrow E_{HF} = \frac{A}{2}\left(J_{TOT}(J_{TOT}+1) - j(j+1) - S_N(S_N+1)\right)$

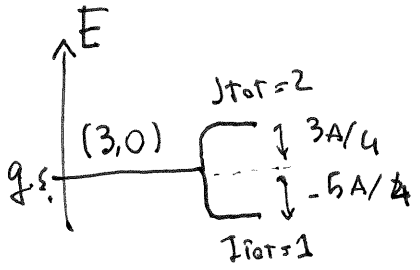
with $|j - S_N| \leq J_{TOT} \leq j + S_N$

Q2: $(n,\ell) = (3,0)$ $\Rightarrow$ $j = \frac{1}{2}$ only (and $E_{SO} = 0$.)

$\Rightarrow \left|\frac{1}{2} - \frac{3}{2}\right| \leq J_{TOT} \leq \frac{1}{2} + \frac{3}{2}$ $\Rightarrow$ $J_{TOT} = 1$ or 2.

For $J_{TOT} = 1$: $E_{HF} = \frac{A}{2}\left(1\cdot(1+1) - \frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{3}{2}\left(\frac{3}{2}+1\right)\right) = -\frac{5A}{4}$

For $J_{TOT} = 2$: $E_{HF} = \frac{A}{2}\left(2\cdot(2+1) - \frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{3}{2}\left(\frac{3}{2}+1\right)\right) = \frac{3A}{4}$.



Q3: The number and splitting of verious levels depend on S_N.

PROBLEM 5.

Q1 $\text{rank}(\rho) = 1$.

Alternatively $\rho^2 = \rho$.

Q2 the state must be the eigenvector of ρ w/ eigenvalue $= 1$: $\rho|\psi\rangle = 1 \cdot |\psi\rangle$

$$\frac{1}{6}\begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{cases} x+y+2z = 6x \\ x+y+2z = 6y \\ 2x+2y+4z = 6z \end{cases}.$$

set $x=1 \Rightarrow y=1,\ z=2$.

Properly normalized: $|\psi\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}$

as a check: $\rho = |\psi\rangle\langle\psi|$.

Q3:

$$\langle A \rangle = \langle\psi|A|\psi\rangle = \text{tr}(\rho A) = [A] = \frac{5}{3}$$

Q4:

The lowest eigenvalue/eigenvector of A: $a=-1$: $|a=-1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$

$$P = |\langle a=-1|\psi\rangle|^2 = \langle a=-1|\rho|a=-1\rangle = 0.$$

Q5. No it is a mixed state:
$\rho'^2 \neq \rho'$ or $\text{rank}\,\rho' > 1$.

Q6. $P = \langle a=-1|\,\rho'\,|a=-1\rangle =$

$$= \frac{1}{\sqrt{2}}(1,-1,0)\cdot\frac{1}{12}\begin{pmatrix}7 & 1 & 2\\ 1 & 1 & 2\\ 2 & 2 & 4\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\end{pmatrix} = \frac{1}{4}.$$

PROBLEM 6

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{8.2\cdot10^{-5}\,eV + 8.2\times10^{-5}\,eV}{4.1\times10^{-15}\,eV\cdot s} = 4\times10^{10}\,s^{-1}$$

$$\omega = \frac{2\pi}{T} = \frac{6.28}{3.14\times10^{-10}\,s} = 2\cdot10^{10}\,s^{-1}$$

$$\frac{\gamma}{\hbar} = \frac{4.1\times10^{-5}\,eV}{4.1\times10^{-15}\,eV\cdot s} = 10^{10}\,s^{-1}$$

$$\Omega = \sqrt{\left(\frac{\gamma}{\hbar}\right)^2 + \left(\frac{\omega-\omega_{21}}{2}\right)^2} = \sqrt{1 + \left(\frac{2-4}{2}\right)^2}\times10^{10}\,s^{-1}$$

$$= \sqrt{2}\cdot10^{10}\,s^{-1} = 1.41\times10^{10}\,s^{-1}.$$

Q1:
The probability is max for

$$\Omega\, t_{max} = \frac{\pi}{2} \quad \Rightarrow \quad t_{max} = 1.11\cdot10^{-10}\,s$$

$$= 0.111\,ns.$$

Q2: For each molecule the probability of flipping is:

$$P = \frac{(\gamma/\hbar)^2}{(\gamma/\hbar)^2 + \left(\frac{\omega-\omega_{21}}{2}\right)^2} = \frac{(\gamma/\hbar)^2}{\Omega^2} = \frac{1}{2}$$

There are thus $\simeq \frac{1}{2}\cdot10^6 = 500.000$ molecules in the excited state after 0.11 ns.