Quantum Mechanics FKA081/FIM400

Final Exam 19 August 2014

Next review time for the exam: September 26 any time (9-18) in my room.
NB: If you want to come to the review you must collect your exam before at the "Kansli" in Origo 5th floor. (This info is also available on the course homepage.)

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

Allowed material during the exam:

- The course textbook J.J. Sakurai and Jim Napolitano, Modern Quantum Mechanics Second Edition (2010).
  NB: The old red cover version: J.J. Sakurai, Modern Quantum Mechanics Revised Edition (1994) 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

Consider a spinless particle in one dimension in an arbitrary state $|\psi\rangle$ and denote by x and p the position and momentum operator respectively.
Q1 (*1 points*) Show that $\langle\psi|xp|\psi\rangle$ can never be equal to $\langle\psi|px|\psi\rangle$.
Q2 (*2 points*) Show that neither $\langle\psi|xp|\psi\rangle$ nor $\langle\psi|px|\psi\rangle$ can ever be real. (In particular, they can never be zero.)
Q3 (*2 points*) Find the linear combination of $\langle\psi|xp|\psi\rangle$ and $\langle\psi|px|\psi\rangle$ that is always real and give an example where this combination vanishes.

Problem 2

Consider the following hamiltonian for a two state system (units of eV understood, no need to write them.)

$$H_1 = \begin{pmatrix} 1 & a \\ a & 2 \end{pmatrix} \tag{1}$$

Q1 (*2 points*) For generic small a make a graph comparing the exact eigenvalues with second order in perturbation theory

Consider now instead

$$H_2 = \begin{pmatrix} 1 & a \\ a & 1 \end{pmatrix} \tag{2}$$

Q2 (*3 points*) Discuss the most important differences that arise in this case and the reason for them.

Problem 3

Consider two states $|\psi_0\rangle$ and $|\psi_E\rangle$ of energy 0 and $E > 0$ respectively. At times $t < 0$ the system is in the ground state $|\psi_0\rangle$. Between time $t = 0$ and time $t = T$, we turn on a perturbation H' mixing the two states, i.e.

$$\langle\psi_0|H'|\psi_E\rangle = \langle\psi_E|H'|\psi_0\rangle = \epsilon \ll E, \quad \langle\psi_0|H'|\psi_0\rangle = \langle\psi_E|H'|\psi_E\rangle = 0. \tag{3}$$

Q1 (*2 points*) Use first order perturbation theory to find the probability that the system is in the excited state after $t > T$.

Now consider the same system with the following experimental values:

$$\Omega = \frac{E}{\hbar} = 1.00 \times 10^{12} \text{ Hz}, \quad \omega = \frac{\epsilon}{\hbar} = 2.00 \times 10^{11} \text{ Hz}, \quad T = 3.00 \times 10^{-12} \text{ s}$$

Q2 (*1 points*) Give the numerical answer to probability found in **Q1**.
Q3 (*4 points*) Solve the problem numerically with the above values *without* using perturbation theory and check how well the result agrees with perturbation theory.

(*Hints:* You never need to use the value of $\hbar$ if you always work with frequencies. Consider the exact total hamiltonian $(1/\hbar)H$ in the interval between 0 and T. It's OK if you get negative eigenfrequencies, they just arise because we chose the energy of the unperturbed ground state to be zero.)

Problem 4

Consider a nucleus of spin $s = 5/2$ subjected to the following Hamiltonian: (γ and β are constants)

$$H = \left(\beta S_x^2 + \gamma(S_y^2 + S_z^2)\right) \tag{4}$$

Q1 (*2 points*) Find the spectrum of H.
Q2 (*2 points*) Find the degeneracy of the eigenvalues in the spectrum of H.

Problem 5

Consider the two observables:

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}, \qquad B = \begin{pmatrix} 2 & x \\ x & 3 \end{pmatrix} \tag{5}$$

Q1 (*1 point*) For what value of x can they be simultaneously diagonalized?
Q2 (*1 point*) Find the eigenvalues of A and B for x found in **Q1**.
Q3 (*2 points*) How are the eigenvalues found in **Q2** paired? In other words, which pairs correspond to the same eigenvector?

Problem 6

In the ground state of a hydrogen atom, the electron is subjected at $t > 0$ to the perturbation

$$H' = gr\cos\theta \mathrm{e}^{-\gamma t} \tag{6}$$

where r and θ are the usual polar coordinates of the electron, g is a small parameter and $\gamma > 0$. You may ignore the spin degree of freedom in this problem and use lowest order perturbation theory.
Q1 (*2 points*) Which of the states $|n, l, m\rangle$ can be excited by this perturbation?
Q2 (*3 points*) What is the probability for the electron to be found in the first excited state ($n = 2$) state at $t = +\infty$?

You may use the fact that

$$\int_0^\infty r^3 \mathcal{R}_{21}(r)\mathcal{R}_{10}(r)\,\mathrm{d}r = \frac{2^7\sqrt{2}}{3^4\sqrt{3}}a_0,$$
$$\langle Y_{10}|\cos\theta|Y_{00}\rangle = \frac{1}{\sqrt{3}}$$

where a_0 is the Bohr radius and $\mathcal{R}_{nl}(r)$ are the radial wave functions.

PROBLEM 1

Q1: $\langle\psi|xp|\psi\rangle - \langle\psi|px|\psi\rangle =$

$= \langle\psi|[x,p]|\psi\rangle = i\hbar\langle\psi|\psi\rangle = i\hbar \neq 0$

Q2: $\langle\psi|xp|\psi\rangle^* = \langle\psi|(xp)^\dagger|\psi\rangle =$

$= \langle\psi|p^\dagger x^\dagger|\psi\rangle = \langle\psi|px|\psi\rangle$

$\Rightarrow \mathrm{Re}(\langle\psi|xp|\psi\rangle) = \mathrm{Re}(\langle\psi|px|\psi\rangle)$

$\mathrm{Im}(\langle\psi|xp|\psi\rangle) = -\mathrm{Im}(\langle\psi|px|\psi\rangle)$

By Q1: $2\,\mathrm{Im}(\langle\psi|xp|\psi\rangle) = i\hbar \neq 0.$

Q3: By Q2: $\langle\psi|xp|\psi\rangle + \langle\psi|px|\psi\rangle \in \mathbb{R}$

on a <u>real</u> wave function;

$$\langle\psi|xp|\psi\rangle = -i\int_{-\infty}^{+\infty} dx\, \psi(x)\, x\, \psi'(x)$$

purely imaginary. Same for $\langle\psi|px|\psi\rangle$

Thus the sum (which is real) must be zero.

PROBLEM 2

Q1. Exact sol: $\begin{vmatrix} 1-E & a \\ a & 2-E \end{vmatrix} = 0$

$$\Rightarrow E^2 - 3E + 2 - a^2 = 0 \Rightarrow E_{1,2} = \frac{3 \pm \sqrt{1+4a^2}}{2}$$

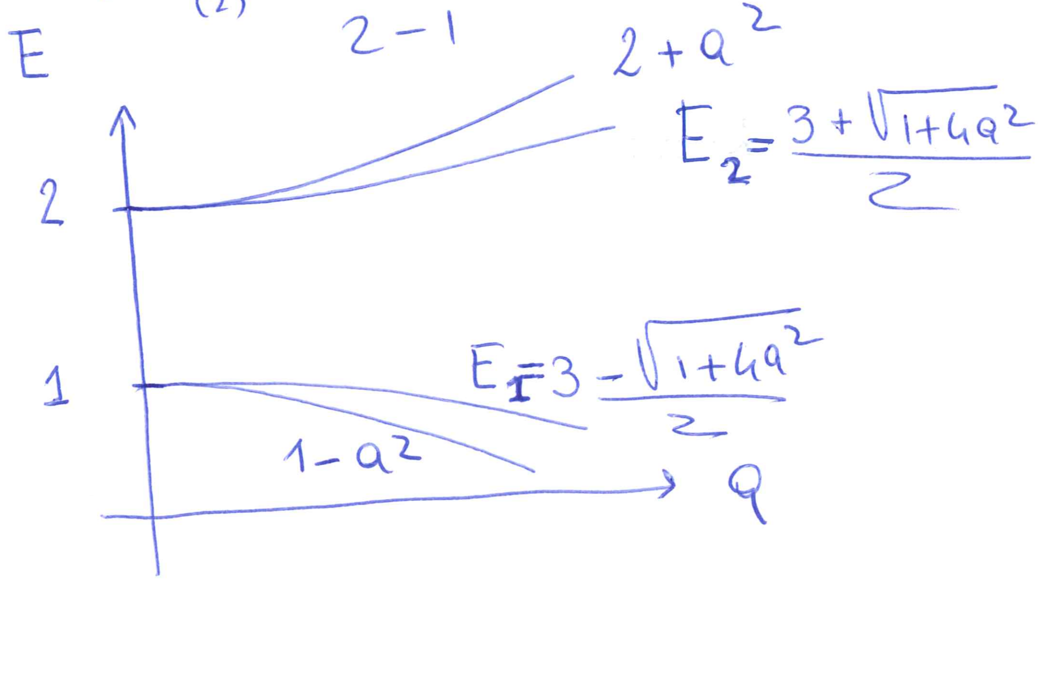
Pert. theory: $H_0 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$ $H' = \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}$

$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $|2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ eigenstates of H_0.

I order: $\langle 1 | H' | 1 \rangle = \langle 2 | H' | 2 \rangle \equiv 0$.

II order: $\Delta E^{II}_{(1)} = \dfrac{a^2}{1-2} = -a^2$

$$\Delta E^{II}_{(2)} = \frac{a^2}{2-1} = +a^2$$



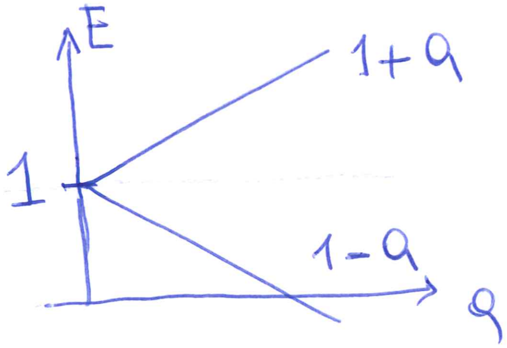
Q2: Exact sol: $\begin{vmatrix} 1-E & a \\ a & 1-E \end{vmatrix} = 0$

$$\Rightarrow E^2 - 2E + 1 - a^2 = 0 \Rightarrow E_{1,2} = 1 \pm a$$

The exact sol. is the same as the one that is found in <u>degenerate first order</u> pert. theory:

$$H_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad H' = \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}$$

(eigenvalues of H': $\pm a$).



Differences between Q1 and Q2:

.) Non-degenerate vs. degenerate.

..) II order vs. I order.
($\Delta E \propto a^2$ $\quad$ $\Delta E \propto a$)

...) Approx v.s exact
$[H_0, H'] \neq 0$ $\quad$ $[H_0, H'] = 0$.

PROBLEM 3.

Q1

$$C^{(1)}_{\text{excited}}(t) = \frac{-i}{\hbar} \int_0^t \langle \psi_E | V(t') | \psi_0 \rangle e^{i\frac{Et'}{\hbar}} dt'$$

where $V(t') = \begin{cases} \epsilon & \text{for } t' \in [0, T] \\ 0 & \text{otherwise} \end{cases}$.

for $t > T$

$$C^{(1)}_{\text{excited}}(t) = -\frac{i}{\hbar} \int_0^T \epsilon \, e^{\frac{iEt'}{\hbar}} = \frac{\epsilon}{E}\left(1 - e^{\frac{iET}{\hbar}}\right).$$

$$P_{\text{excite}} = |c^{(1)}_{\text{excite}}(t)| = \frac{4\epsilon^2}{E^2} \sin^2\left(\frac{ET}{2\hbar}\right).$$

Q2

Numerically

$$P_{\text{excite}} = \frac{4 \times (0.2)^2}{1^2} \sin^2\left(\frac{1.3}{2}\right) \simeq 0.159$$

Q3 For $t \in [0, T]$ the hamiltonian is:

$$\frac{1}{\hbar} H = \begin{pmatrix} 0 & \epsilon \\ \epsilon & E \end{pmatrix} = \begin{pmatrix} 0 & 0{,}2 \\ 0{,}2 & 1. \end{pmatrix} \times 10^{+12} \, Hz.$$

eigenvectors: $\phi_1 = \begin{pmatrix} 0{,}189 \\ 0{,}982 \end{pmatrix}$ with $\omega_1 = 1{,}04 \cdot 10^{12} \, Hz$

and $\phi_2 = \begin{pmatrix} -0{,}982 \\ 0{,}189 \end{pmatrix}$ with $\omega_2 = -3{,}85 \times 10^{10} \, Hz$

The normalized solution that matches $\psi_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ when $t=0$ is:

$$\psi(t) = 0{,}189 \, \phi_1 e^{-i\omega_1 t} - 0{,}982 \, \phi_2 e^{-i\omega_2 t}$$

$$\langle \psi_E | \psi(T) \rangle = 0{,}189 \times 0.982 \times e^{-i\omega_1 T} - 0{,}982 \times 0{,}189 \times e^{-i\omega_2 T}$$

$$P_{exact} = |\langle \psi_E | \psi(T) \rangle|^2 = 0{,}138$$

The perturbative result is $\approx 15\%$ off.

PROBLEM 4.

Q1/2: write $H = \gamma \vec{S}^2 + (\beta - \gamma) S_x^2$

where $\vec{S}^2 = S_x^2 + S_y^2 + S_z^2$

$[\vec{S}^2, S_x^2] = 0$ hence they can be simultaneously diagonalized.

The possible eigenvalues of S_x^2 are the same as those of S_z^2 (just relable the axes).

Hence the spectrum is:

$$E = \gamma s(s+1) + (\beta - \gamma) m^2$$

where $s = 5/2$ and $m = -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$

$$E = \begin{cases} \frac{5}{2}\gamma + \frac{25}{4}\beta & m = \pm\frac{5}{2} \quad \text{doubly deg.} \\ \frac{13\gamma}{2} + \frac{9\beta}{4} & m = \pm\frac{3}{2} \quad \text{" "} \\ \frac{17\gamma}{2} + \frac{\beta}{4} & m = \pm\frac{1}{2} \quad \text{" "} \end{cases}$$

PROBLEM 5

Q1: $[A,B] = \begin{pmatrix} 0 & 1-x \\ -1+x & 0 \end{pmatrix} = 0 \Leftrightarrow x = 1.$

Q2: $\det(A - a\mathbb{1}) = a^2 - 3a + 1 = 0$

$\Rightarrow a_{1,2} = \dfrac{3 \pm \sqrt{5}}{2}$

$\det(B - b\mathbb{1}) = b^2 - 5b + 5 = 0$

$\Rightarrow b_{1,2} = \dfrac{5 \pm \sqrt{5}}{2}$

Q3: The easiest way is to find an eigenvector of A:

$Av = a_1 v \Rightarrow \begin{pmatrix} 1 - \frac{3+\sqrt{5}}{2} & 1 \\ 1 & 2 - \frac{3+\sqrt{5}}{2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$

$\Rightarrow \alpha = 1, \beta = \frac{1+\sqrt{5}}{2}$ up to unimportant normaliz.

$Bv = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1+\sqrt{5}}{2} \end{pmatrix} = \begin{pmatrix} \frac{5+\sqrt{5}}{2} \\ \frac{5+3\sqrt{5}}{2} \end{pmatrix} = \frac{5+\sqrt{5}}{2} \cdot v$

$\Rightarrow$ Pairs: $\left(\frac{3+\sqrt{5}}{2}, \frac{5+\sqrt{5}}{2}\right)$ and $\left(\frac{3-\sqrt{5}}{2}, \frac{5-\sqrt{5}}{2}\right)$

PROBLEM 6

Q1: $\langle \psi_{n\ell m} | H' | \psi_{1,0,0} \rangle \propto \langle Y_{\ell m} | \cos\theta | Y_{00} \rangle$

$\Rightarrow$ only $m=0$, $\ell=1$ contribute.

(You can see this by noticing that $Y_{00} = \text{const.}$ and $\cos\theta \propto Y_{1,0}$ and using $\perp$ of $Y_{\ell m}$)

Q2:

$$P_{1\to 2} = \frac{1}{\hbar^2} \left| \int_0^{+\infty} dt\, e^{i\omega_{21} t} \langle \psi_{210} | H' | \psi_{100} \rangle \right|^2 =$$

$$= \frac{1}{\hbar^2} \left| \int_0^{+\infty} dt\, e^{i\omega_{21} t} g e^{-\gamma t} \cdot \int_0^{\infty} dr\, r^2 R_{21}(r) \cdot r \cdot R_{10}(r) \times \right.$$

$$\left. \times \langle Y_{10} | \cos\theta | Y_{00} \rangle \right|^2 =$$

$$= \frac{g^2}{\hbar^2} \cdot \left| \frac{1}{\gamma - i\omega_{21}} \right|^2 \cdot \left(\frac{2^7 \sqrt{2}}{3^4 \sqrt{3}} a_0 \right)^2 \cdot \left(\frac{1}{\sqrt{3}} \right)^2 =$$

$$= \frac{2^{15}}{3^{10}} \cdot \frac{g^2}{\hbar^2} \cdot \frac{1}{\gamma^2 + \omega_{21}^2} a_0^2 \quad // \left(\omega_{21} = \frac{3e^2}{8a_0} \right)$$