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Det matematisk-naturvitenskapelige fakultet

Solution to Exam in: FYS3110 - Quantum mechanics.

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Max score: 54 points

Problem 1

1a)(6 points) A quantum state

- is the description of the system/object at a specific instant in time.
- contains information about all the *probabilities* for different measurement outcomes for *all* possible types of measurements that can be performed on the system/object.
- is represented mathematically as a normalized complex vector, a ket.

The first point is also true for a classical state, –it is also the description of a system/object at a specific time. In contrast, the other two points are different for a classical state. A classical state is *defined* in terms of a set of definite measurement values. Thus there are no probabilities encoded in a classical state. (There can be uncertainties/probabilitites as to which classical state the system/object is in, but not in the classical state itself.) Mathematically a classical state is represented as a point in a set, not as a complex vector. (Thus there is no meaning attached to adding classical states together.)

Grading: To get full score the answer must contain at least the 2nd and 3rd bullet points, and the contrast to classical states must be stated. The first bullet point is of course also true, but one can argue that it is obvious so we will not penalize answers that fails to mention it. If the answer contains one or more statements that are directly wrong among otherwise correct statements this will qualify for a deduction of 1-2 points. Minor typos and formulations that are only partially transparent will not be penalized significantly.

1b)(6 points) $[\hat{C}, \hat{A}] = 0$ means that a common complete set of simultaneous eigenstates of $\hat{A}$ and $\hat{C}$ can be constructed. The eigenstates of $\hat{A}$ are already given and is unique since the eigenvectors belonging to different eigenvalues of a hermitian operator are orthogonal, this means that they are also eigenstates of $\hat{C}$;

$$\begin{aligned}\hat{C}|1\rangle &= c_1|1\rangle \\ \hat{C}|2\rangle &= c_2|2\rangle\end{aligned}\tag{1}$$

But by the same logic, the states $|\pm\rangle$ are also eigenstates of $\hat{C}$, that is

$$\begin{aligned}\hat{C}|+\rangle &= c_+|+\rangle \\ \hat{C}|-\rangle &= c_-|-\rangle\end{aligned}\tag{2}$$

Now

$$\hat{C}|\pm\rangle = \frac{1}{\sqrt{2}} \left(\hat{C}|1\rangle \pm \hat{C}|2\rangle \right) = \frac{1}{\sqrt{2}} (c_1|1\rangle \pm c_2|2\rangle) = c_{\pm}|\pm\rangle\tag{3}$$

Taking the inner product with the bras $\langle 1|$ and $\langle 2|$ in the last equality we get

$$\frac{c_1}{\sqrt{2}} = c_{\pm} \frac{1}{\sqrt{2}}\tag{4}$$

$$\pm \frac{c_2}{\sqrt{2}} = \pm c_{\pm} \frac{1}{\sqrt{2}}\tag{5}$$

which implies

$$c_1 = c_2 = c_+ = c_-\tag{6}$$

thus the eigenvalues of $\hat{C}$ must all be degenerate. (The problem text does not mention that $\hat{C}$ is hermitian, thus this degenerate eigenvalue does not need to be real.) Nothing particular can be said about the eigenstates of $\hat{C}$ other than the fact that they are general superpositions of $|1\rangle$ and $|2\rangle$.

Grading: To get full score, sound arguments must be provided for why the eigenvalues are degenerate. The correct answer alone (eigenvalues of $\hat{C}$ are degenerate) gives a maximum of 2 points. A partial credit of 2 points is given if the answer states that commuting operators share a common set of eigenstates. Also a partial (bonus) credit of 1 point is given for commenting that the eigenvalues are in general complex since $\hat{C}$ is not explicitly specified to be a hermitian operator. No deductions are made for not commenting on this.

Problem 2

2a)(2 points) An linear operator in a two-dimensional Hilbert space is defined by its action on two orthonormal states as follows:

$$\hat{T}|1\rangle = |2\rangle, \quad \hat{T}|2\rangle = i|1\rangle$$

Calculate $\langle 2|\hat{T}^\dagger|1\rangle$

Select one alternative:

- 1
- i
- -1
- -i

Correct answer: -i

Explanation: $\langle 2|\hat{T}^\dagger|1\rangle = \langle 1|\hat{T}|2\rangle^* = \langle 1|i|1\rangle^* = -i$.

2b)(2 points) A Hilbert space is spanned by three orthonormal kets $|1\rangle, |2\rangle, |3\rangle$. The eigenstates of the operator

$$\hat{H} = \frac{1}{2} (|1\rangle + |2\rangle) (\langle 1| + \langle 2|) + |3\rangle\langle 3|$$

in this Hilbert space are

Select one or more alternatives:

- $|3\rangle$
- $\frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)$
- $\frac{1}{\sqrt{2}} (|1\rangle - |2\rangle)$
- $|1\rangle$

Correct answers: $\frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)$, $\frac{1}{\sqrt{2}} (|1\rangle - |2\rangle)$, $|3\rangle$

Explanation: Apply the Hamiltonian to all the alternatives. Those states that gives a number times the state itself are eigenstates. Note that the eigenvalue can be zero.

2c)(2 points) The angular momentum states with angular momentum 1 and Lz-component -1, 0 and +1 are denoted $|-\rangle, |0\rangle, |+\rangle$ respectively.

When combining two angular momentum 1 states, the state with total angular momentum 1 and total Lz-component 0 is

Select one alternative

- $\frac{1}{\sqrt{2}} (|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle)$

- $\frac{1}{\sqrt{3}} (|+\rangle \otimes |-\rangle - |0\rangle \otimes |0\rangle + |-\rangle \otimes |+\rangle)$
- $\frac{1}{\sqrt{2}} (|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle)$
- $\frac{1}{\sqrt{3}} (|+\rangle \otimes |-\rangle + |0\rangle \otimes |0\rangle + |-\rangle \otimes |+\rangle)$

Correct answer: $\frac{1}{\sqrt{2}} (|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle)$.

Explanation: Use the Clebsch-Gordan table 1×1 and look for the entry $L = 1$ and $L_z = 0$.

2d)(2 points)

A system of three spin-1/2s

Select one or more alternatives:

- can never form a total spin-1 state.
- cannot exist because of the Pauli principle.
- have in total 8 orthonormal spin states.
- cannot have negative energy eigenvalues.

Correct answers: “can never form a total spin-1 state” and “have in total 8 orthonormal spin states”.

2e)(2 points) Two indistinguishable spin-1 bosons are located in a three dimensional harmonic oscillator potential. There are no interactions between the bosons. What is the ground state degeneracy?

Select one alternative:

- 1
- 3
- 6
- 9

Correct answer: 6

Explanation: A state with indistinguishable bosons must always be symmetric under the interchange of particle and spin coordinates. In the lowest energy state both particles are

in the ground state of the 3D harmonic oscillator so that their spatial part is $|000\rangle \otimes |000\rangle$. In addition the particles have spin, so we must construct *symmetric* combinations of these. This can be achieved by constructing the total spin states which have a well-defined symmetry under the interchange of the spins. From the Clebsch-Gordan table for combining two spin-1s it follows that the five total spin-2 states and the total spin-0 state are all symmetric. Thus the answer is $5 + 1 = 6$.

2f)(2 points) An electron (with spin-1/2) in a Coulomb potential is in the state

$$\frac{1}{\sqrt{2}} (|n=3, l=2, m=2\rangle \otimes |\uparrow\rangle + |n=3, l=2, m=0\rangle \otimes |\downarrow\rangle)$$

at time $t = 0$.

The probability density for finding the electron

Select one or more alternatives:

- is 0 at the origin.
- is smaller in the x-direction than in the z-direction.
- varies with the azimuthal angle ϕ .
- varies with time.

Correct answers: “is 0 at the origin” and “is smaller in the x-direction than in the z-direction”.

Explanation: The probability density is found by taking the expectation value of the operator $|r, \theta, \phi\rangle\langle r, \theta, \phi| \otimes \hat{I}$ in the given state at time t . Now this state is an energy eigenstate because it is a linear combination of $n = 3$ states which both have the same energy $E_1/3^2$. Therefore this is a stationary state, thus expectation values will not depend on time which immediately excludes the alternative “varies with time”, and so we can evaluate the expectation value at $t = 0$. This gives

$$\begin{aligned} P(r, \theta, \phi) &= \frac{1}{2} (|R_{32}(r)Y_2^2(\theta, \phi)|^2 + |R_{32}(r)Y_2^0(\theta, \phi)|^2) \\ &= \frac{1}{2} |R_{32}(r)|^2 (|Y_2^2(\theta, \phi)|^2 + |Y_2^0(\theta, \phi)|^2) \\ &= \frac{1}{2} \left| \frac{4}{81\sqrt{30}} \right|^2 a^{-3} \left(\frac{r}{a} \right)^4 e^{-2r/3a} \left(\frac{15}{32\pi} \sin^4 \theta + \frac{5}{16\pi} (3 \cos^2 \theta - 1)^2 \right) \end{aligned}$$

where we used expression for R_{nl} and Y_l^m from Griffiths. This expression is 0 at the origin $r = 0$. Also it does not depend on ϕ . The last thing we need to check is the magnitude in the

x and z directions. The x-direction is defined by $\theta = \pi/2$ and $\phi = 0$, while the z-direction is defined by $\theta = 0$ ($\phi = 0$). In these cases we get

$$P(r, \theta = \pi/2, \phi = 0) = \frac{1}{2} \left| \frac{4}{81\sqrt{30}} \right|^2 a^{-3} \left(\frac{r}{a} \right)^4 e^{-2r/3a} \left(\frac{15}{32\pi} + \frac{5}{16\pi} \right)$$

$$P(r, \theta = 0, \phi = 0) = \frac{1}{2} \left| \frac{4}{81\sqrt{30}} \right|^2 a^{-3} \left(\frac{r}{a} \right)^4 e^{-2r/3a} \left(\frac{5}{4\pi} \right)$$

from which it follows that $P(r, \theta = \pi/2, \phi = 0) < P(r, \theta = 0, \phi = 0)$ which is the same as stating “is smaller in the x-direction than in the z-direction”.

2g)(2 points) Use Hund’s rules to determine which of the following total angular momentum states has the lowest energy: ${}^3D_1, {}^3F_4, {}^1P_{1/2}, {}^3S_1$. It is also known that the outermost subshell is less than half-filled.

Select one alternative:

- ${}^3D_1$
- ${}^3F_4$
- ${}^1P_{1/2}$
- ${}^3S_1$

Correct answer: ${}^3F_4$

Explanation: Hund’s first rule selects as lowest energy candidate the states with highest total spin. These are ${}^3D_1, {}^3F_4$ and ${}^3S_1$. Then Hund’s second rule selects the lowest energy candidate to be the one with largest total L . This is ${}^3F_4$ as it has $L = 4$.

2h)(2 points) The variational principle

Select one or more alternatives:

- can be used to find a lower bound on the ground state energy.
- declares that the expectation value of the Hamiltonian in any normalized state is greater than or equal to the ground state energy.
- can be used to determine if a single electron can bind two protons.
- can be used to find exact energy eigenstates of a Hamiltonian.

Correct answers: “Declares that the expectation value of the Hamiltonian in any normalized state is g
and “Can be used to determine if a single electron can bind two protons.”

2i)(2 points) A Hydrogen atom is located in a spatially uniform electric field with polarization in the z-direction and a magnitude that oscillates in time. This time-varying electric field can within first order time-dependent perturbation theory cause transitions between the Hydrogen $|n = 4, l = 0, m = 0\rangle$ state and

Select one or more alternatives:

- $|300\rangle$
- $|310\rangle$
- $|311\rangle$
- $|211\rangle$

Correct answer: $|310\rangle$.

Explanation: When the electric field is spatially uniform and polarized in the z-direction one will only get transitions to states where the transition matrix element $\langle nlm|z|400\rangle \neq 0$. This implies that $m = 0$. In addition the l dipole selection rule $\Delta l = \pm 1$ implies that $l = 1$.

Problem 3

3a)(6 points) Before the pulse, the spin-1/2 is in its the ground state, which is $|\uparrow\rangle$ with energy $E_i = -\gamma B_z \hbar/2$. The excited state has energy $E_f = \gamma B_z \hbar/2$. Therefore $E_f - E_i = \gamma B_z \hbar$.

The first-order perturbative expression for the transition amplitude for exciting the system is

$$a_{\uparrow \rightarrow \downarrow} = \frac{1}{i\hbar} \int_0^T dt e^{i\gamma B_z t} \langle \downarrow | (-\alpha) \Gamma \hat{S}_x | \uparrow \rangle$$

writing $\hat{S}_x = \frac{1}{2} (\hat{S}^+ + \hat{S}^-)$ and using the fact that $\hat{S}^+ |\uparrow\rangle = \hbar |\downarrow\rangle$ we get

$$\langle \downarrow | (-\alpha) \Gamma \hat{S}_x | \uparrow \rangle = -\frac{\alpha \Gamma \hbar}{2}$$

then

$$\begin{aligned} a_{\uparrow \rightarrow \downarrow} &= \frac{\alpha \Gamma}{2i} \int_0^T dt e^{i\gamma B_z t} = -\frac{\alpha \Gamma}{2i} \frac{1}{i\gamma B_z} (e^{i\gamma B_z T} - 1) = -\frac{\alpha \Gamma}{2i} \frac{1}{i\gamma B_z} e^{i\gamma B_z T/2} (e^{i\gamma B_z T/2} - e^{-i\gamma B_z T/2}) \\ &= -\frac{\alpha \Gamma}{i\gamma B_z} e^{i\gamma B_z T/2} \sin\left(\frac{\gamma B_z T}{2}\right). \end{aligned}$$

which means that the excitation probability

$$P_{\uparrow \rightarrow \downarrow} = |a_{\uparrow \rightarrow \downarrow}|^2 = \left| \frac{\alpha \Gamma}{\gamma B_z} \right|^2 \sin^2 \left(\frac{\gamma B_z T}{2} \right).$$

This reaches its (first) maximum for $\frac{\gamma B_z T}{2} = \frac{\pi}{2}$ which implies $T = \frac{\pi}{\gamma B_z}$.

Grading: 1 point is given for writing down the general formula for the transition probability. Then additional credit is given for connecting the information given in the problem to the general formula. 1 point is given for the correct answer to the last question. Minor algebraic errors are penalized by 1-2 points.

Problem 4

4a)(6 points) The Hamiltonian in the harmonic approximation is

$$H^0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{D}{a^2} x^2 - D \quad (7)$$

We recognize this as the harmonic oscillator Hamiltonian with a constant term $-D$ and

$$\frac{1}{2} m \omega^2 = \frac{D}{a^2} \implies \omega = \sqrt{\frac{2D}{ma^2}} = \sqrt{\frac{4}{\hbar^2} \frac{D \hbar^2}{2ma^2}} = \frac{2}{\hbar} \sqrt{DE_R} \quad (8)$$

where we have rewritten the expression for ω in terms of D and the recoil energy $E_R = \frac{\hbar^2}{2ma^2}$.

The energy eigenvalues are

$$E_n = -D + \hbar \omega \left(n + \frac{1}{2} \right) = \underline{-D + 2\sqrt{DE_R} \left(n + \frac{1}{2} \right)} \quad (9)$$

where $n \in \{0, 1, 2, \dots\}$.

Grading: To obtain full score the answer must be written as above. Failure to identify ω in terms of D and E_R is penalized by 2 points. Failure to take into account the constant is penalized by 1 point (No penalty is made if one leaves the constant out, but mention that the constant shifts the zero of energy). Minor algebraic errors are penalized by 1-2 points.

4b)(6 points) The perturbation is

$$H^1 = D \left(-\left(\frac{x}{a}\right)^3 + \frac{7}{12} \left(\frac{x}{a}\right)^4 + \dots \right) \quad (10)$$

Following the hint we write the position operator x as harmonic oscillator ladder operators, and insert the value of ω

$$\frac{x}{a} = \sqrt{\frac{\hbar}{2ma^2\omega}} (a^\dagger + a) = \sqrt{\frac{\hbar^2}{4ma^2\sqrt{DE_R}}} (a^\dagger + a) = \sqrt{\frac{E_R}{2\sqrt{DE_R}}} (a^\dagger + a) = \frac{1}{\sqrt{2}} \left(\frac{E_R}{D}\right)^{1/4} (a^\dagger + a) \quad (11)$$

The first order perturbative correction to the ground state energy is

$$E_0^1 = \langle 0 | H^1 | 0 \rangle \quad (12)$$

Then inserting the expression for H^1 , we see that all terms x^p with p odd will give zero as an odd number of creation/annihilation operators acting on the unperturbed ground state $|0\rangle$ will always give a state different from $|0\rangle$. Thus the lowest order term that contributes is

$$\langle 0 | \frac{7D}{12} \left(\frac{x}{a}\right)^4 | 0 \rangle = \frac{7D}{12} \left(\frac{1}{\sqrt{2}}\right)^4 \frac{E_R}{D} \langle 0 | (a^\dagger + a)^4 | 0 \rangle = \frac{7 \cdot 3}{12 \cdot 4} E_R = \frac{7}{16} E_R \quad (13)$$

where we have used the fact that the matrix element is

$$\langle 0 | (a^\dagger + a)^4 | 0 \rangle = \langle 1 | (a^\dagger + a)^2 | 1 \rangle = \langle 1 | (a^\dagger a + a a^\dagger) | 1 \rangle = \langle 1 | (2a^\dagger a + 1) | 1 \rangle = 3 \quad (14)$$

where we used $[a, a^\dagger] = 1$. Now, what about the higher order even terms $\left(\frac{x}{a}\right)^p$, with $p \in \{6, 8, 10, \dots\}$? They will give a contribution that is proportional to $D \left(\frac{E_R}{D}\right)^{p/4}$ which depends on the ratio E_R/D whenever $p \neq 4$. For instance the $p = 6$ term goes as $D \left(\frac{E_R}{D}\right)^{3/2} = E_R \sqrt{\frac{E_R}{D}} < E_R$ for $E_R \ll D$. Thus the only term in first order perturbation theory that gives a result which is proportional to the recoil energy alone is $p = 4$. Therefore first order perturbation theory gives

$$E_0^1 = \frac{7}{16} E_R + \dots \quad (15)$$

where $\dots$ are other terms not directly proportional to E_R .

Grading: 1 point is given for writing down the general 1st order perturbation formula. Then additional points (up to 4) are given for how far one gets towards the correct result. Finally 1 point is given for justifying why the extra terms in perturbation do not give contributions that are proportional to E_R alone.

4c)(6 points) Second order perturbation theory will also give an energy correction to the ground state energy which is proportional to the recoil energy E_R alone. The second order energy correction is given by

$$E_0^2 = \sum_{m \neq 0} \frac{|\langle m | H^1 | 0 \rangle|^2}{E_0^0 - E_m^0} \quad (16)$$

where $E_m^0 = D + 2\sqrt{DE_R} \left(m + \frac{1}{2}\right)$. From this it becomes clear that the energy denominator will be proportional to $\sqrt{DE_R}$. The numerator contains an infinite sum squared of matrix elements. This is difficult to handle explicitly. However, we not going for the full answer. Instead things simplify considerably when we realize that only the first term squared, coming from x^3 will give a term proportional to $E_R\sqrt{DE_R}$ which is what is needed to get an answer which is proportional to E_r alone. This can be seen from

$$\langle m | D \left(\frac{x}{a}\right)^3 | 0 \rangle = D \left(\frac{1}{\sqrt{2}}\right)^3 \left(\frac{E_R}{D}\right)^{3/4} \langle m | (a^\dagger + a)^3 | 0 \rangle = \frac{1}{2^{3/2}} E_R^{3/4} D^{1/4} \langle m | (a^\dagger + a)^3 | 0 \rangle \quad (17)$$

The matrix element is can be calculated from

$$(a^\dagger + a)^3 | 0 \rangle = (a^\dagger + a)^2 | 1 \rangle = (a^\dagger + a) \left(\sqrt{2} | 2 \rangle + | 0 \rangle \right) = \sqrt{6} | 3 \rangle + 3 | 1 \rangle \quad (18)$$

which gives

$$\langle m | (a^\dagger + a)^3 | 0 \rangle = \sqrt{6} \delta_{m,3} + 3 \delta_{m,1} \quad (19)$$

Altogether this gives

$$E_0^2 = \frac{1}{2^3} \frac{E_R^{3/2} D^{1/2}}{2 D^{1/2} E_R^{1/2}} \left(\frac{3^2}{0-1} + \frac{\sqrt{6}^2}{0-3} \right) + \dots = -\frac{E_R}{16} (9+2) + \dots = -\frac{11}{16} E_R + \dots \quad (20)$$

where $\dots$ are other terms not directly proportional to E_R alone. The fact that other terms in the matrix elements do not contribute becomes clear from considering the general product of matrix elements

$$\langle 0 | D \left(\frac{x}{a}\right)^{p_1} | m \rangle \langle m | D \left(\frac{x}{a}\right)^{p_2} | 0 \rangle = D^2 \left(\frac{E_R}{D}\right)^{(p_1+p_2)/4} \times c \quad (21)$$

where c is a pure numerical factor that depends on m, p_1 and p_2 . Dividing by the energy denominator which goes as $\sqrt{DE_R}$ times a number, we see that the contribution of this p_1, p_2 term is

$$\Delta E \sim \frac{D^2 \left(\frac{E_R}{D}\right)^{(p_1+p_2)/4}}{D^{1/2} E_R^{1/2}} \quad (22)$$

and from this it follows that only $p_1 = p_2 = 3$ gives $\Delta E \sim E_R$.

Grading: 1 point is given for writing down the general 2nd order perturbation formula. Then additional points (up to 4) are given for how far one gets towards the correct result. Finally 1 point is given for justifying why the extra terms in perturbation do not give contributions that are proportional to E_R alone.

Not asked for: The Morse potential was treated exactly in the midterm exam problem 1.4. If we add together the perturbative contributions proportional to E_R from first and second order perturbation theory we find $\frac{7}{16}E_R - \frac{11}{16}E_R = -\frac{E_R}{4}$. From the midterm exam, problem 1.4, the exact ground state energy of this potential was found to be $E_{gs}/E_R = -s^2/4$. Using $\left(\frac{s+1}{2}\right)^2 = \frac{D}{E_R}$ we get

$$E_{gs} = -\frac{E_R}{4} \left(2\sqrt{\frac{D}{E_R}} - 1 \right)^2 \quad (23)$$

multiplying this out we get

$$E_{gs} = -\frac{E_R}{4} \left(4\frac{D}{E_R} - 4\sqrt{\frac{D}{E_R}} + 1 \right) = -D + \sqrt{E_R D} - \frac{E_R}{4} \quad (24)$$

Thus we see that perturbation theory to second order keeping only the term proportional to E_R alone in fact gives the exact result!