

UNIVERSITY OF OSLO

Faculty of Mathematics and Natural Sciences

Exam: FYS3110 – Quantum mechanics

Date and time: Dec. 13. 2022, 15:00-19:00 (4 hours on Inspira)

Problem 1

1a) (6 points) What is a quantum state? In your answer, explain how a quantum state is different from a classical state and how it is represented mathematically.

Solution:

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/probabilities 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 max score on this subproblem there must be correct and not misleading answers to 1) what a quantum state is, 2) how it is represented mathematically and 3) how it is different from at classical state.

1b) (6 points) Explain briefly in words what good states are, and why they are useful. Give an example.

Solution:

Good states is a concept in degenerate time-independent perturbation theory. Good states are unperturbed degenerate states that diagonalize the perturbation in the degenerate subspace. That is, when the good states are used as basis vectors the matrix of the perturbation in the degenerate subspace is diagonal. Note that good states are not necessarily eigenstates of the full Hamiltonian.

Good states are useful because one can read off the energy corrections directly as the diagonal matrix elements. I.e. one can use non-degenerate perturbation theory in terms of the good states.

An example of good states are the hydrogen $|nlm\rangle$ -states when the perturbation is the first relativistic correction to the kinetic energy. In that case the only angular dependence of the perturbation operator is as powers of L^2 , and since the nlm -states are eigenstates of L^2 , the perturbation matrix $\langle nl'm'|(p^2)^2|nlm\rangle \propto \delta_{l',l}\delta_{m',m}$ is diagonal. Other examples of good states treated in the lectures are: $|nljm_j\rangle$ in the hydrogen (weak-field) Zeeman effect, the $|nlmm_s\rangle$ states in the hydrogen strong-field Zeeman case (Paschen-Back effect), $|S_{tot}, M_{tot}\rangle$ of the proton and the electron spin for the hydrogen hyperfine-interaction, and $|nljm_j\rangle$ for the hydrogen spin-orbit interaction perturbation.

Grading:

To get full score on this subproblem there must be correct and not misleading answers to 1) what good states are, 2) why they are useful and 3) at least one example. For the example both the good states and the associated perturbation must be mentioned for full credit.

Problem 2

Grading:

All the multiple choice problems give 2 points for the correct answer, and 0 points for a wrong or no answer.

2a) (2 points) Consider the Coulomb problem (hydrogen) bound states $|nlm\rangle$. Compute

$$\sum_{l',m'} \langle nl'm'| (L_x^2 + L_y^2 + 2L_z^2) |nlm\rangle$$

The answer is ...

Solution:

$$\begin{aligned} \sum_{l',m'} \langle nl'm'| (L_x^2 + L_y^2 + 2L_z^2) |nlm\rangle &= \sum_{l',m'} \langle nl'm'| (L^2 + L_z^2) |nlm\rangle \\ &= \sum_{l',m'} \hbar^2 (l(l+1) + m^2) \delta_{l',l} \delta_{m',m} \\ &= \underline{\hbar^2 (l(l+1) + m^2)}. \end{aligned}$$

2b) (2 points) An operator K is written as

$$K = e^{iaG}$$

where G is a linear hermitian operator and a is a real number. For general (real) values of a , the operator K is ...

Solution:

Expanding the exponential gives

$$K = 1 + iaG + \frac{1}{2!}(iaG)^2 + \dots = \sum_{n=0}^{\infty} \frac{1}{n!} (iaG)^n$$

G is a linear operator, and so is any integer powers of G , thus K is linear. To check if K is hermitian or unitary, we form the hermitian conjugate of K .

$$\begin{aligned} K^\dagger &= 1 - iaG^\dagger + \frac{1}{2!}(-iaG^\dagger)^2 + \dots = \sum_{n=0}^{\infty} \frac{1}{n!} (-iaG^\dagger)^n \\ &= 1 - iaG + \frac{1}{2!}(-iaG)^2 + \dots = \sum_{n=0}^{\infty} \frac{1}{n!} (-iaG)^n = e^{-iaG} = K^{-1} \end{aligned}$$

where we used the hermiticity of G : $G^\dagger = G$. For general values of a we see that $K^\dagger \neq K$ and so K is in general not hermitian, however it is always unitary as $K^\dagger = K^{-1}$, and so the correct answer is linear and unitary.

2c) (2 points) What is the energy splitting induced when a proton with spin-1/2 at rest is placed in a magnetic field of 1T?

(Some properties of protons and electrons and constants: $g_p = 5.59$, $g_e = 2.0023$, $m_p = 1836m_e$, $\mu_B = \frac{e\hbar}{2m_e} = 5.788 \cdot 10^{-5} \text{eV/T}$.)

Select the nearest alternative...

Solution:

The proton is a spin-1/2 particle. When placed in a magnetic field it interacts with the field as

$$H = -g_p \frac{e}{2m_p} \vec{S} \cdot \vec{B}$$

Choosing the z-direction along the field, we find that the energy splitting between the states with $S^z = \pm \frac{1}{2}$ is

$$\Delta E = g_p \frac{e\hbar}{2m_p} B = g_p \frac{e\hbar}{2m_e} \frac{m_e}{m_p} B = g_p \mu_B \frac{m_e}{m_p} B = 5.59 \cdot 5.788 \cdot 10^{-5} \text{eV/T} \cdot \frac{1}{1836} \cdot 1 \text{T} = 1.76 \cdot 10^{-7} \text{eV}$$

So the nearest alternative is 10^{-7}eV .

2d) (2 points) A d-electron ($l = 2$) is in a state where its orbital angular momentum z-component is known to be $-\hbar$ and its spin-z component is known to be $+\hbar/2$. What is the probability that its total angular momentum is measured to be $5/2$?

Solution:

Using the Clebsch-Gordan table $2 \times 1/2$ we see that the indicated state state with $l = 2, m_l = -1$ and $s = 1/2, m_s = +1/2$ can be written

$$|2, -1\rangle \otimes |1/2, +1/2\rangle = \sqrt{\frac{2}{5}}|5/2, -1/2\rangle - \sqrt{\frac{3}{5}}|3/2, -1/2\rangle$$

The probability of measuring the total angular momentum to be $5/2$ is

$$P_{5/2} = |\langle 5/2, -1/2 | (|2, -1\rangle \otimes |1/2, +1/2\rangle)|^2 = \frac{2}{5}$$

Thus the correct alternative is $2/5$.

2e) (2 points) Two indistinguishable spin-0 bosons have each an orbital angular momentum of $l = 1$. What is the set of possible values for the total angular momentum of these bosons?

Solution:

The bosons are spinless particles with angular momentum 1. Adding the orbital angular momenta one find that they can combine to total values $L = 0, 1, 2$. The state of identical bosons must be symmetric under the interchange of the two bosons. Inspecting the Clebsch-Gordan table 1×1 we see that only the $L = 0$ and $L = 2$ states are symmetric. Thus the set of possible values is $\{0, 2\}$.

2f) (2 points) What is the value of the integral

$$\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta Y_1^{*0}(\theta, \phi) L_- Y_1^1(\theta, \phi).$$

Y_l^m are the usual spherical harmonics, and $L_- = L_x - iL_y$ where L_x and L_y are the x and y-components of the orbital angular momentum operator.

Solution:

The spherical harmonics are eigenfunctions of angular momentum. When applying L_- the m -quantum number is lowered. Properly normalized we have

$$L_- Y_l^m = \hbar \sqrt{l(l+1) - m(m-1)} Y_l^{m-1}$$

Inserting $l = 1$ and $m = 1$ we see that $L_- Y_1^1 = \sqrt{2}\hbar Y_1^0$. The spherical harmonics are orthonormal functions and so

$$\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta Y_1^{*0}(\theta, \phi) L_- Y_1^1(\theta, \phi) = \sqrt{2}\hbar \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta Y_1^{0*}(\theta, \phi) Y_1^1(\theta, \phi) = \underline{\sqrt{2}\hbar}$$

2g) (2 points) A charged particle is moving in a 3D harmonic oscillator potential. When the energy of the particle is $\hbar\omega(2 + 3/2)$ there are in all 6 degenerate states. What is the maximum ratio of lifetimes for these 6 states computed in the electric dipole approximation. (maximum ratio of lifetimes = longest lifetime/shortest lifetime) Use results from first-order time-independent perturbation theory in the electric-dipole approximation. (Hint: The lifetime of a state $|i\rangle$ is the inverse sum of spontaneous transition rates out of state $|i\rangle$)

Solution:

The six degenerate states with energy $\hbar\omega(2 + 3/2)$ are $|200\rangle, |020\rangle, |002\rangle, |110\rangle, |010\rangle$, and $|011\rangle$. The inverse lifetime of a state $|i\rangle$ is the sum of spontaneous transition rates

$$\tau_i^{-1} = \sum_f R_{fi}$$

where the spontaneous transition rates in the electric dipole approximation is

$$R_{fi} = \frac{4\omega_0^3}{3c^3\hbar\epsilon_0} |D_{fi}|^2.$$

Here $\hbar\omega_0 > 0$ is the energy difference between the initial and the final states, and the dipole matrix-elements are

$$|D_{fi}|^2 = q^2 (|\langle f|x|i\rangle|^2 + |\langle f|y|i\rangle|^2 + |\langle f|z|i\rangle|^2).$$

For a decay to occur $|D_{fi}|^2$ must be non-zero. Since $x \propto a_x^\dagger + a_x$ etc. the non-zero matrix elements occur only for transitions to final states where one of the quantum numbers is decreased by one from the initial state. This lowers the energy by $\hbar\omega$ thus all the decays have the same ω_0 . Let us first consider the state $|200\rangle$ ($|020\rangle$ and $|002\rangle$ are similar). The $|200\rangle$ can only decay to $|100\rangle$. The spontaneous decay rate is proportional to

$$R_{100,200} \propto |\langle 100 | (a_x^\dagger + a_x) | 200 \rangle|^2 = (\sqrt{2})^2 = 2.$$

Then consider $|110\rangle$ ($|011\rangle$ and $|101\rangle$ are similar). The state $|110\rangle$ can decay to $|010\rangle$ or $|100\rangle$:

$$R_{010,110} \propto |\langle 010 | (a_x^\dagger + a_x) | 110 \rangle|^2 = (\sqrt{1})^2 = 1,$$

$$R_{100,110} \propto |\langle 100 | (a_y^\dagger + a_y) | 110 \rangle|^2 = (\sqrt{1})^2 = 1.$$

Thus the sum of the decay rates is the same for $|200\rangle$ as for $|110\rangle$ (and also for the other states). Thus all lifetimes are equal, meaning that all lifetime ratios, and therefore also the maximum one, is 1.

Problem 3

3a) (6 points) A one dimensional harmonic oscillator with Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}kx^2$ is at time $t = 0$ in an equal-amplitude superposition of its two lowest energy eigenstates $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Then at time $t = 0$ the oscillator stiffness k is suddenly increased an amount α before it relaxes back to its original value, that is the stiffness can be written as $k(t) = k + \alpha e^{-\gamma t}$ for $t > 0$. α and γ are real positive numbers with units of force per length and inverse time respectively. Use first order time-dependent perturbation theory to calculate the probability of finding the oscillator in the energy eigenstate $|2\rangle$ at time $t \rightarrow \infty$.

Solution:

The equation for the $n = 2$ probability amplitude a_2 is to first order in perturbation theory

$$a_2(\infty) = a_2(0) + \frac{1}{i\hbar} \sum_k \int_0^\infty dt' \langle 2|H^1|k\rangle e^{i(E_2 - E_k)t/\hbar} a_k(0) \quad (1)$$

Now $a_0(0) = a_1(0) = 1/\sqrt{2}$, and $a_2(0) = 0$. Thus

$$a_2(\infty) = \frac{1}{i\hbar} \frac{1}{\sqrt{2}} \int_0^\infty dt' \left(\langle 2|H^1|0\rangle e^{i(E_2 - E_0)t/\hbar} + \langle 2|H^1|1\rangle e^{i(E_2 - E_1)t/\hbar} \right)$$

where the energy differences are $E_2 - E_0 = 2\hbar\omega$ and $E_2 - E_1 = \hbar\omega$.

The perturbation is $H^1(t) = \frac{1}{2}\alpha x^2 e^{-\gamma t} = \alpha \frac{\hbar}{4m\omega} (a + a^\dagger)^2 e^{-\gamma t}$, and so the matrix elements are

$$\begin{aligned} \langle 2|H^1|0\rangle &= \frac{\alpha\hbar}{4m\omega} \langle 2|(a + a^\dagger)^2|0\rangle e^{-\gamma t} = \frac{\alpha\hbar}{4m\omega} \langle 2|a^\dagger a^\dagger|0\rangle e^{-\gamma t} = \frac{\alpha\hbar}{4m\omega} \sqrt{2} e^{-\gamma t}, \\ \langle 2|H^1|1\rangle &= \frac{\alpha\hbar}{4m\omega} \langle 2|(a + a^\dagger)^2|1\rangle e^{-\gamma t} = 0. \end{aligned}$$

Thus only the $k = 0$ term in the sum is non-zero:

$$\begin{aligned} a_2(\infty) &= \frac{1}{i\hbar} \frac{1}{\sqrt{2}} \int_0^\infty dt' e^{i2\omega t'} \frac{\alpha\hbar}{4m\omega} e^{-\gamma t'} \sqrt{2} = \frac{1}{i\hbar} \frac{\alpha\hbar}{4m\omega} \int_0^\infty dt' e^{(i2\omega - \gamma)t'} \\ &= \frac{1}{i\hbar} \frac{\alpha\hbar}{4m\omega} \frac{e^{(i2\omega - \gamma)\infty} - 1}{i2\omega - \gamma} = \frac{\alpha}{4m\omega} \frac{i}{i2\omega - \gamma}. \end{aligned}$$

Taking the modulus square of this we get

$$P_2(\infty) = |a_2(\infty)|^2 = \frac{\alpha^2}{16m^2\omega^2} \frac{1}{(i2\omega - \gamma)(-i2\omega - \gamma)} = \frac{\alpha^2}{16m^2\omega^2} \frac{1}{(4\omega^2 + \gamma^2)}.$$

Grading:

Up to 2 points for writing down Eq. (1) correctly including the sum over k . Up to 2 points

for getting the matrix elements and inserting the energies correctly, and up to 2 points for calculating the integrals and getting the final answer.

3b) (6 points) Use the variational principle with the normalized trial function $\psi(x) = (\frac{2\lambda}{\pi})^{1/4} e^{-\lambda x^2}$ to show that a particle moving in a one dimensional potential $V(x)$ which is *negative* for all x and where $V(|x| \rightarrow \infty) \rightarrow 0$, will have at least one bound state.

Solution:

The variational principle for a normalized trial wave function is

$$E_0 \leq \int_{-\infty}^{\infty} dx \psi^*(x) \left(\frac{p^2}{2m} + V(x) \right) \psi(x) = \left(\frac{2\lambda}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx e^{-\lambda x^2} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) e^{-\lambda x^2}$$

The second derivative is

$$e^{-\lambda x^2} \frac{\partial^2}{\partial x^2} e^{-\lambda x^2} = e^{-\lambda x^2} \frac{\partial}{\partial x} \left(-2\lambda x e^{-\lambda x^2} \right) = (-2\lambda + 4\lambda^2 x^2) e^{-2\lambda x^2},$$

and therefore the integrals involving the kinetic energy are

$$-\frac{\hbar^2}{2m} \left(\frac{2\lambda}{\pi} \right)^{1/2} \left[-2\lambda \underbrace{\int_{-\infty}^{\infty} dx e^{-2\lambda x^2}}_{\left(\frac{\pi}{2\lambda} \right)^{1/2}} + 4\lambda^2 \underbrace{\int_{-\infty}^{\infty} dx x^2 e^{-2\lambda x^2}}_{\frac{\sqrt{\pi}}{2(2\lambda)^{3/2}}} \right] = \frac{\hbar^2}{2m} (2\lambda - \lambda) = \frac{\hbar^2 \lambda}{2m}$$

where we used Rottmann for the second integral. We therefore get

$$E_0 \leq \frac{\hbar^2}{2m} \lambda + \left(\frac{2\lambda}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx V(x) e^{-2\lambda x^2} \quad (2)$$

For $\lambda \rightarrow 0$ the right hand side approaches 0. To find the behavior of the right hand side for very small but finite λ we can expand the exponential function in the integrand. We then get

$$E_0 \leq \left(\frac{2\lambda}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx V(x) + \frac{\hbar^2}{2m} \lambda + \mathcal{O}(\lambda^{3/2})$$

Now we note that the integral in the first term is always negative since $V(x) < 0$ for all x . Thus if the first term is bigger in magnitude than the others the right hand side will be negative. For small enough, but finite values of λ this will happen as the first term goes as $\sqrt{\lambda}$ while the rest of the terms is of the order λ or bigger. For small enough λ we have $\sqrt{\lambda} \gg \lambda$. Thus there exists a value of λ for which the trial energy is negative, and therefore also E_0 .

More formally we can also proceed by seeking the minimum of the right hand side. To do that we differentiate w.r.t. λ and equate to zero. Differentiating gives an equation for the minimal λ -value; λ_0 :

$$\frac{\hbar^2}{2m} + \left(\frac{2\lambda_0}{\pi}\right)^{-1/2} \frac{1}{\pi} \int_{-\infty}^{\infty} dx V(x) e^{-2\lambda_0 x^2} - \left(\frac{2\lambda_0}{\pi}\right)^{1/2} 2\lambda_0 \int_{-\infty}^{\infty} dx V(x) x^2 e^{-2\lambda_0 x^2} = 0$$

which can be reshuffled into

$$\left(\frac{2\lambda_0}{\pi}\right)^{-1/2} \frac{1}{\pi} \int_{-\infty}^{\infty} dx V(x) e^{-2\lambda_0 x^2} = -\frac{\hbar^2}{2m} + \left(\frac{2\lambda_0}{\pi}\right)^{1/2} 2\lambda_0 \int_{-\infty}^{\infty} dx V(x) x^2 e^{-2\lambda_0 x^2}$$

Multiplying both sides by $2\lambda_0$ gives

$$\left(\frac{2\lambda_0}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx V(x) e^{-2\lambda_0 x^2} = -\frac{\hbar^2}{2m} 2\lambda_0 + \left(\frac{2\lambda_0}{\pi}\right)^{1/2} (2\lambda_0)^2 \int_{-\infty}^{\infty} dx V(x) x^2 e^{-2\lambda_0 x^2}$$

Now we insert this into the original inequality using $\lambda = \lambda_0$ and get

$$E_0 \leq \underbrace{\frac{\hbar^2}{2m} \lambda_0 - \frac{\hbar^2}{2m} 2\lambda_0}_{-\frac{\hbar^2 \lambda_0}{2m}} + \left(\frac{2\lambda_0}{\pi}\right)^{1/2} (2\lambda_0)^2 \int_{-\infty}^{\infty} dx V(x) x^2 e^{-2\lambda_0 x^2}$$

The integral in the last term is negative because $V < 0$, and therefore the right hand side is negative, implying that the upper bound on the ground state energy is negative: The potential admits at least one bound state.

Grading:

Up to 4 points for getting the trial energy Eq. (2) correctly, and up to 2 points for arguing correctly that the trial energy implies the existence of at least one bound state.

Problem 4

4a) (6 points) Use time-independent perturbation theory to find an estimate correct to order a_0/ξ for the ground state energy of the hamiltonian

$$H = \frac{\vec{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0} \frac{e^{-r/\xi}}{r}$$

where ξ is a large real positive number with units of length. a_0 is the Bohr radius.

Solution:

This problem can be solved very quickly by expanding the exponential function to first order

$$H = \frac{\vec{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} + \frac{e^2}{4\pi\epsilon_0} \frac{1}{\xi}.$$

Terms that involve $(1/\xi)^2$ and higher are neglected. By dimensional analysis they will eventually give a contribution $\mathcal{O}((a_0/\xi)^2)$. The truncated Hamiltonian is as for a particle in a Coulomb potential plus a constant term. Thus all energy levels will be shifted by the same amount. Therefore the energy of the ground state correct to $\mathcal{O}(a_0/\xi)$ will be

$$E_{gs} = E_1 + \frac{e^2}{4\pi\epsilon_0} \frac{a_0}{\xi} = E_1 - 2E_1 \frac{a_0}{\xi} = E_1 \left(1 - 2\frac{a_0}{\xi}\right).$$

It is also possible to solve this problem by rewriting the Hamiltonian as

$$H = \underbrace{\frac{\vec{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}}_{H^0} + \underbrace{\frac{e^2}{4\pi\epsilon_0 r} \left(1 - e^{-r/\xi}\right)}_{H^1}$$

The ground state of the Coulomb problem is non-degenerate, so the first order energy correction is

$$E_{100}^1 = \langle 100 | H^1 | 100 \rangle = \int d^3r \psi_{100}^*(r) \frac{e^2}{4\pi\epsilon_0 r} \left(1 - e^{-r/\xi}\right) \psi_{100}(r). \quad (3)$$

Using the Coulomb problem ground state wave function $\psi_{100}(r) = \frac{1}{a_0^{3/2}\pi^{1/2}} e^{-r/a_0}$ the integrals becomes

$$\begin{aligned} E_{100}^1 &= \frac{e^2}{4\pi\epsilon_0} \frac{1}{\pi a_0^3} 4\pi \int_0^\infty dr r^2 \frac{1}{r} \left(1 - e^{-r/\xi}\right) e^{-2r/a_0} = \frac{e^2}{4\pi\epsilon_0} \frac{4}{a_0^3} \left(\int_0^\infty dr r e^{-2r/a_0} - \int_0^\infty dr r e^{-r(\frac{2}{a_0} + \frac{1}{\xi})} \right) \\ &= \underbrace{\frac{e^2}{4\pi\epsilon_0 a_0}}_{-2E_1} \frac{4}{a_0^2} \left[\left(\frac{a_0}{2}\right)^2 \underbrace{\int_0^\infty dx x e^{-x}}_1 - \left(\frac{2}{a_0} + \frac{1}{\xi}\right)^{-2} \underbrace{\int_0^\infty dx x e^{-x}}_1 \right] \\ &= -2E_1 \frac{4}{a_0^2} \left[\left(\frac{a_0}{2}\right)^2 - \left(\frac{a_0}{2}\right)^2 \left(1 + \frac{a_0}{2\xi}\right)^{-2} \right] = -2E_1 \left[1 - \left(1 + \frac{a_0}{2\xi}\right)^{-2} \right] \\ &\approx -2E_1 \left[1 - \left(1 - 2\frac{a_0}{2\xi}\right) \right] = -2E_1 \frac{a_0}{\xi} \end{aligned}$$

The integral can be done either using partial integration, or differentiating under the integral of $e^{-\lambda x}$, or by looking up in Rottmann: Bestimmt integral 135) setting a=1 and b=0. Adding this to the Coulomb problem ground state energy, we get

$$E = E_1 - 2E_1 \frac{a_0}{\xi} = E_1 \left(1 - 2\frac{a_0}{\xi}\right).$$

which is the same as above.

Grading:

Just stating the perturbation formalism without connecting it concretely to this problem is awarded only half a point. Although mathematically possible, it does not make much

physical sense to perturb around the free particle solution in this problem. Such attempts are awarded at most 3 points *if carried out to completion*. Partial credit of 3 points are awarded for writing down the correct expression Eq. (3) including the correct hydrogen ground state wave functions. Full score is given if one arrives at the correct result in a convincing way.

4b) (6 points) A hamiltonian operator is written $H = A + bB$ where b is a real-valued parameter and A and B are hermitian operators not dependent on the parameter b . This hamiltonian H has a non-degenerate ground state with an energy $E_{gs}(b)$ which is a function of b . Show that $\frac{\partial^2 E_{gs}}{\partial b^2}|_{b=b_0} \leq 0$ for any real value of b_0 .

Solution:

First write $b = \delta + b_0$ where $\delta = b - b_0$. Then the Hamiltonian is $H = A + (\delta + b_0) B = A + b_0 B + \delta B$. Now we can treat this using perturbation theory with $H^0 = A + b_0 B$ and $H^1 = \delta B$. Perturbation theory about b_0 gives generally

$$E_{gs}(b) = E_{gs}(b_0) + G_1(b_0)\delta + G_2(b_0)\delta^2 + \mathcal{O}(\delta^3)$$

where the G 's are coefficients of the perturbation expansion. Differentiating this twice with respect to b (δ) gives

$$\frac{\partial^2 E_{gs}}{\partial b^2} = 2G_2(b_0) + \mathcal{O}(\delta),$$

and when inserting $b = b_0$, which implies $\delta = 0$, we get

$$\frac{\partial^2 E_{gs}}{\partial b^2}|_{b=b_0} = 2G_2(b_0).$$

$G_2(b_0)$ is the second order perturbative correction to the ground state and is for a non-degenerate ground state

$$G_2(b_0) = \sum_{m \neq gs} \frac{|\langle m|B|0\rangle|^2}{E_{gs} - E_m}$$

where the states and energies are those of the unperturbed hamiltonian $H^0 = A + b_0 B$. Now the numerator is always positive or zero, but since the ground state is the lowest energy and is non-degenerate; $E_{gs} < E_m$, the denominator is always negative, and therefore $G_2(b_0)$ is less than or equal to zero for any value of b_0 , and we have proved the inequality.

It is also possible to obtain this answer using the Feynman-Hellman theorem that gives an expression for the first derivative of the ground state energy. The so obtained expression must then be differentiated again to get the second derivative and it must be recognized that the kets also depend on b . First-order non-degenerate perturbation theory for the (derivative of the) kets can then be used to give exactly the same expression as above.

Grading:

For full score one has to shown in a convincing way that the inequality holds for all values of b_0 , not just for $b_0 = 0$. If the proof is restricted only to $b_0 = 0$ a maximum of 4 points

is awarded. Note that differentiating a (variational) inequality makes no sense, as differentiating both sides of an inequality does not imply that the inequality still holds. Such approaches are fundamentally flawed and give no credit. The ground state of a Hamiltonian depends implicitly on its parameters, here b . Thus it is wrong to assert that $E_{gs} = \alpha + b\beta$, where α and β are independent of b . Such approaches give also no credit.