

UNIVERSITY OF OSLO

Faculty of Mathematics and Natural Sciences

Solution to exam in: FYS3110, Quantum mechanics

Day of exam: Nov. 28., 2016 (4 hours exam)

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

Problem 1

Consider a quantum system described by the following Hamiltonian on a three-dimensional Hilbert space with an orthonormal basis $\{|1\rangle, |2\rangle, |3\rangle\}$, where $g \ll 1$ is a small parameter

$$H = -|1\rangle\langle 1| + |3\rangle\langle 3| + g(|1\rangle\langle 2| + |2\rangle\langle 1|) + 2g(|1\rangle\langle 3| + |3\rangle\langle 1|)$$

1.1 The unperturbed ($g = 0$) Hamiltonian is $H = -|1\rangle\langle 1| + 0|2\rangle\langle 2| + |3\rangle\langle 3|$ from which we can just read off the unperturbed energy and eigenstates:

Energy eigenvalue	Energy eigenstate
-1	$ 1\rangle$
0	$ 2\rangle$
1	$ 3\rangle$

1.2 The perturbation is $H^1 = g(|1\rangle\langle 2| + |2\rangle\langle 1|) + 2g(|1\rangle\langle 3| + |3\rangle\langle 1|)$. And from 1.1 the unperturbed ground state is $|1\rangle$ with energy -1 and is not degenerate. We can use first order non-degenerate perturbation theory:

$$|1^1\rangle = \sum_{i \neq 1} \frac{\langle i | H^1 | 1 \rangle}{E_1^0 - E_i^0} |i\rangle$$

The matrix elements are $\langle 2 | H^1 | 1 \rangle = g$ and $\langle 3 | H^1 | 1 \rangle = 2g$. Thus

$$|1^1\rangle = \frac{g}{-1 - 0} |2\rangle + \frac{2g}{-1 - 1} |3\rangle$$

thus correct to first order in g , the ground state is $|gs\rangle = c(|1\rangle - g|2\rangle - g|3\rangle)$ where $c = \frac{1}{\sqrt{1+2g^2}}$. Note, that $c = 1 + \mathcal{O}(g^2)$, thus specifying the answer as $c = 1$ is also ok up to

$\mathcal{O}(g)$.

1.3 $E_{trial} = \frac{\langle gs|H|gs\rangle}{\langle gs|gs\rangle}$. Lets compute $H|gs\rangle$

$$\begin{aligned} H|gs\rangle &= cH(|1\rangle - g|2\rangle - g|3\rangle) = c(-1|1\rangle + g|2\rangle + 2g|3\rangle - g^2|1\rangle - 2g^2|1\rangle - g|3\rangle) \\ &= c(-(1+3g^2)|1\rangle + g|2\rangle + g|3\rangle) \end{aligned}$$

This gives $E_{trial} = \langle gs|H|gs\rangle = |c|^2 [-(1+3g^2) - 2g^2] = \underline{\underline{\frac{-1-5g^2}{1+2g^2}}}$

Now lets compute the perturbation theory result: First order gives $E_{gs}^1 = \langle 1|H^1|1\rangle = 0$. The second order perturbation theory result is gotten from $E_{gs}^2 = \langle 1|H^1|1^1\rangle = \langle 1|H^1(-g|2\rangle - g|3\rangle) = -g^2 - 2g^2 = -3g^2$ which implies that the ground state energy correct up to order g^2 is

$$\underline{\underline{E_{gs} = -1 - 3g^2}}$$

Expanding the variational result $E_{trial} = \frac{-1-5g^2}{1+2g^2} = -\frac{1+5g^2}{1+2g^2} = -(1+5g^2)(1-2g^2) + \mathcal{O}(g^4) = \underline{\underline{-1 - 3g^2 + \mathcal{O}(g^4)}}$ which agrees with the variational estimate up to $\mathcal{O}(g^2)$.

Problem 2

2.1 The condition that $\hat{A}\hat{B}$ is hermitian is $(\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}$. Using the fact that the left hand side is $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A}$ where the last equality follows from the fact that $\hat{A}$ and $\hat{B}$ both are hermitian, we see that $\hat{B}\hat{A} = \hat{A}\hat{B}$ and therefore $\underline{\underline{[\hat{A}, \hat{B}] = 0}}$.

The fact that $\hat{A}$ and $\hat{B}$ commutes means that a common complete set of eigenstates for the two operators can be constructed. Since the spectrum of $\hat{A}$ is non-degenerate, this set is unique and is the set of eigenstates of $\hat{A}$. The same arguments that was used for the commutator between $\hat{A}$ and $\hat{B}$ can be used with $\hat{C}$ replacing $\hat{B}$, thus $[\hat{A}, \hat{C}] = 0$. and so one can find a common complete set of states that are simultaneously eigenstates for both $\hat{A}$ and $\hat{C}$. Since the set of eigenstates of $\hat{A}$ is unique (it is non-degenerate) this set must also eigenstates of $\hat{C}$. The same argument holds for eigenstates of $\hat{B}$. Thus the set of eigenstates of $\hat{A}$ is also eigenstates for $\hat{B}$ and $\hat{C}$. Lets label this set $|\eta_n\rangle$ and name the eigenvalues of operators $\hat{B}$ and $\hat{C}$ for b_n and c_n respectively. Then $[\hat{B}, \hat{C}]|\eta_n\rangle = \hat{B}\hat{C}|\eta_n\rangle - \hat{C}\hat{B}|\eta_n\rangle = (b_n c_n - c_n b_n)|\eta_n\rangle = 0$. This holds for all $|\eta_n\rangle$ and their linear combinations, thus $\underline{\underline{[\hat{B}, \hat{C}] = 0}}$.

This last commutator can be used to calculate the matrix element: $0 = \langle \psi_1 | [\hat{B}, \hat{C}] | \psi_2 \rangle = \langle \psi_1 | \hat{B} \hat{C} | \psi_2 \rangle - \langle \psi_1 | \hat{C} \hat{B} | \psi_2 \rangle = \langle \psi_2 | \hat{C}^\dagger \hat{B}^\dagger | \psi_1 \rangle^* - \langle \psi_1 | \hat{C} \hat{B} | \psi_2 \rangle = \langle \psi_2 | \hat{C} \hat{B} | \psi_1 \rangle^* - \langle \psi_1 | \hat{C} \hat{B} | \psi_2 \rangle = (b_1^* - b_2) \langle \psi_2 | \hat{C} | \psi_1 \rangle = (b_1 - b_2) \langle \psi_2 | \hat{C} | \psi_1 \rangle$ where we have used that $\hat{B}$ has real eigenvalues as it is a hermitian operator. (One can arrive at this expression more quickly by acting with $\hat{B}$ to the left in the first term, and to the right in the second term.) For $b_1 \neq b_2 \implies \langle \psi_2 | \hat{C} | \psi_1 \rangle = 0$.

Another way of proving this last fact is to consider the eigenstates of $\hat{B}$ in terms of the $|\eta_i\rangle$'s. The operator $\hat{B}$ may have a degenerate spectrum (several b_i 's might be equal to each other), thus $|\psi_1\rangle = \sum_i g_{1i} |\eta_i\rangle$ where g_{1i} 's are only non-zero for states with identical values of b_i . Likewise $|\psi_2\rangle = \sum_j g_{2j} |\eta_j\rangle$ where g_{2j} are non-zero only for those states with identical eigenvalue b_j . Thus the two sums goes over *different* states. Therefore since the $|\eta\rangle$ are also eigenstates for $\hat{C}$ we can write

$$\langle \psi_1 | \hat{C} | \psi_2 \rangle = \sum_{ij} g_{1i}^* g_{2j} \langle \eta_i | \hat{C} | \eta_j \rangle = \sum_{ij} g_{1i}^* g_{2j} c_j \langle \eta_i | \eta_j \rangle = 0$$

where the last inequality follows from the orthogonality of the $|\eta_i\rangle$ states which is a consequence of the fact that $\hat{A}$ is hermitian and has a non-degenerate spectrum.

Problem 3

3.1 The total angular momentum before the decay is $j = 1/2$ since the neutron is a spin-1/2 particle. When the decay products both have spin-1/2, the total spin after the decay will be either 0 or 1, and since the relative orbital angular momentum also only can take integer values, the total angular momentum will take an *integer* value. Thus it is not possible to get a total angular momentum value of $j = 1/2$ as it is a half-integer. Therefore the decay of a neutron into a proton and an electron is not allowed even though such a process conserves electric charge. In fact a neutron decays not into two but three particles, a proton, an electron and an antineutrino which also carries spin-1/2. The third spin-1/2 makes it possible to construct a total $j = 1/2$ state.

3.2 The initial state of particle X is $|\frac{3}{2}, \frac{3}{2}\rangle$. X decays into a spin-1/2 particle A and a spin-0 particle B with relative orbital angular momentum l . The total angular momentum is conserved and is 3/2 before the decay. Adding the spin and orbital angular momentum after the decay the total angular momentum can take the two values $\{l + 1/2, |l - 1/2|\}$

which must be equal to $3/2$. This gives two possible values of l : $\underline{l = 1}$ or $\underline{l = 2}$. For $l = 1$ the z-component of the relative angular momentum can maximally be $+\hbar$, thus the spin-z component of particle A must necessarily be $+\hbar/2$. Thus the probability is $\underline{1}$ for $l = 1$. This answer can also be gotten by examining the Clebsch-Gordan table $1 \times 1/2$.

For $l = 2$ we must write the $|\frac{3}{2}, \frac{3}{2}\rangle$ as a combination of $l = 2$ and $s_A = 1/2$ states. For this we need the Clebsch-Gordan table $2 \times 1/2$. From this table we see that

$$|\frac{3}{2}, +\frac{3}{2}\rangle = \sqrt{\frac{4}{5}}|2, +2\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle - \sqrt{\frac{1}{5}}|2, +1\rangle \otimes |\frac{1}{2}, +\frac{1}{2}\rangle$$

and the probability of measuring particle A's spin component to be $+\frac{\hbar}{2}$ is therefore $\underline{1/5}$. which is obtained formally as $P_{+\frac{\hbar}{2}} = \sum_{m=-2}^2 |(\langle 2, m| \otimes \langle \frac{1}{2}, +\frac{1}{2}|) |\frac{3}{2}, \frac{3}{2}\rangle|^2$.

Problem 4

4.1 The Hamiltonian is $H = -\frac{\hbar^2 \partial^2}{2m \partial x^2}$ and gives $E_k = \frac{\hbar^2 k^2}{2m}$ when it acts on the given energy eigenfunctions. The periodic boundary condition implies a quantization of the values of k . $e^{ik(x+L)} = e^{ikx} \implies e^{ikL} = 1 \implies k = \frac{2\pi}{L}z$ where z is an integer. Therefore the allowed energy eigenvalues are $\underline{E_z = \frac{\hbar^2 z^2}{2m}}$ with $z \in 0, \pm 1, \pm 2, \dots$. The energy eigenvalue 0 is not degenerate, but the other levels are twofold degenerate as z and $-z$ correspond to different states, but gives the same energy eigenvalue.

4.2 For the $k = 0$ state we can use non-degenerate perturbation theory. We get $E_0^1 = \langle 0|H^1|0\rangle = \int_0^L dx \frac{1}{\sqrt{L}} V_0 \cos(2\pi x/a) \frac{1}{\sqrt{L}} = 0$. For $k \neq 0$ we must use degenerate perturbation theory. For a given value k we must also calculate the matrix elements to the degenerate state $|-k\rangle$. Lets consider in general the matrix element $\langle k'|H^1|k\rangle$

$$\begin{aligned} \langle k'|H^1|k\rangle &= \int_0^L dx \frac{e^{ik'x}}{\sqrt{L}} V_0 \cos\left(\frac{2\pi}{a}x\right) \frac{e^{-ikx}}{\sqrt{L}} = \frac{V_0}{2L} \int_0^L dx e^{i(k'-k)x} (e^{-i2\pi x/a} + e^{i2\pi x/a}) \\ &= \frac{V_0}{2L} \int_0^L dx \left(e^{i\frac{2\pi}{L}(z'-z+N)x} + e^{i\frac{2\pi}{L}(z'-z-N)x} \right) \end{aligned}$$

where we have used $k = 2\pi z/L$ and $a = L/N$. Note that $z' - z \pm N$ are integers. The integral can be simplified by introducing $u = 2\pi x/L$. For any integer m we have

$$\frac{1}{L} \int_0^L dx e^{i\frac{2\pi}{L}mx} = \frac{1}{2\pi} \int_0^{2\pi} du e^{imu} = \frac{1}{2\pi} \int_0^{2\pi} du (\cos mu + i \sin mu) = \delta_{m,0}$$

because for $m \neq 0$ the function oscillates for m full periods over the integration interval. For $m = 0$ the sine term is zero and the cosine is 1. A more straightforward way of doing

the integral is

$$\frac{1}{2\pi} \int_0^{2\pi} du e^{imu} = \frac{1}{2\pi im} (e^{i2\pi m} - 1)$$

which is 0 for $m \neq 0$. For $m = 0$ one gets a $0/0$ -expression which can be dealt with using L'Hopitals rule or by taking the limit as $m \rightarrow 0$ which is easiest done by replacing $e^{im\theta}$ by its Taylor-expansion around $m = 0$. $\lim_{m \rightarrow 0} \frac{1}{2\pi im} (e^{i2\pi m} - 1) = \lim_{m \rightarrow 0} \frac{1+2\pi im+\dots-1}{2\pi im} = 1$.

With this result for the integral the matrix elements are

$$\langle z' | H^1 | z \rangle = \frac{V_0}{2} (\delta_{z', z-N} + \delta_{z', z+N})$$

Degenerate perturbation theory. Lets consider $z > 0$ and construct the matrix elements in the degenerate subspace (the W -matrix)

$$\begin{aligned} \langle -z | H^1 | -z \rangle &= 0 \\ \langle -z | H^1 | z \rangle &= \frac{V_0}{2} (\delta_{2z, N} + \delta_{2z, -N}) = \frac{V_0}{2} \delta_{2z, N} \\ \langle z | H^1 | -z \rangle &= \frac{V_0}{2} (\delta_{-2z, N} + \delta_{2z, N}) = \frac{V_0}{2} \delta_{2z, N} \\ \langle z | H^1 | z \rangle &= 0 \end{aligned}$$

For $N \neq 2z$ this matrix will be zero and the first order correction to the energy will also be 0. The only non-zero correction comes when $N = 2z$. The energy corrections for this particular value $z = N/2$ which corresponds to $k = \frac{2\pi}{L} \frac{N}{2} = \frac{\pi}{a}$ (and $k = -\frac{\pi}{a}$) are thus given by

$$\det \begin{pmatrix} -E^1 & V_0/2 \\ V_0/2 & -E^1 \end{pmatrix} = 0 \implies (E^1)^2 - \left(\frac{V_0}{2}\right)^2 = 0 \implies \underline{E^1 = \pm \frac{V_0}{2}}$$

A more elegant way of solving this problem which do not require any integrals is to realize that

$$H^1 |k\rangle = V_0 \cos\left(\frac{2\pi}{a}x\right) \frac{1}{\sqrt{L}} e^{ikx} = \frac{V_0}{2} \frac{1}{\sqrt{L}} \left(e^{i(k-\frac{2\pi}{a})x} + e^{i(k+\frac{2\pi}{a})x} \right) = \frac{V_0}{2} \left(|k - \frac{2\pi}{a}\rangle + |k + \frac{2\pi}{a}\rangle \right).$$

From which it follows that the matrix elements are $\langle k' | H^1 | k \rangle = \frac{V_0}{2} \delta_{k', k \pm \frac{2\pi}{a}}$. It is now easy to write down the W -matrix of the perturbation in the degenerate subspace. The diagonal elements are always 0 because $k' = k$ gives 0. The offdiagonal elements are obtained by setting $k' = -k$ where we get a contribution $V_0/2$ only for $k = \pm \frac{\pi}{a}$. This gives exactly the W -matrix above. Strictly speaking the integer $N = L/a$ needs to be an even number in this problem for $k = \pi/a$ to be possible. This is because $k = \frac{2\pi z}{Na} = \frac{\pi}{a} \implies 2z = N$.

4.3

First order perturbation theory gives

$$\begin{aligned} a_{k'}(\infty) &= \frac{1}{i\hbar} \int_0^\infty dt \langle k' | V_0(t) \cos\left(\frac{2\pi}{a}x\right) | k \rangle e^{i(E_{k'} - E_k)t/\hbar} \\ &= \frac{g}{i\hbar} \langle k' | \cos\left(\frac{2\pi}{a}x\right) | k \rangle \int_0^\infty dt e^{-\alpha t} e^{i(E_{k'} - E_k)t/\hbar} \end{aligned}$$

Writing $k = \frac{2\pi}{L}z$ the matrix element $\langle k' | \cos(\frac{2\pi}{a}x) | k \rangle$ is just the one calculated in 4.2. The time integral is simple. We get

$$a_{k'}(\infty) = \frac{g}{2i\hbar} \left(\delta_{k', k - \frac{2\pi}{a}} + \delta_{k', k + \frac{2\pi}{a}} \right) \frac{-1}{i(E_{k'} - E_k)/\hbar - \alpha}$$

where $E_k = \frac{\hbar^2 k^2}{2m}$. Thus we see that there can only be transitions to states k' 's that differ from k by $\pm 2\pi$. The transition probabilities are

$$P_{k \rightarrow k \pm \frac{2\pi}{a}} = |a_{k \pm \frac{2\pi}{a}}(\infty)|^2 = \frac{1}{4} |g|^2 \frac{1}{\hbar^2 \alpha^2 + (E_{k \pm \frac{2\pi}{a}} - E_k)^2}$$

One can also simplify (?) $E_{k \pm \frac{2\pi}{a}} - E_k = \frac{\hbar^2}{2m} \left(\left(k \pm \frac{2\pi}{a}\right)^2 - k^2 \right) = \frac{\hbar^2}{2m} \left(\left(\frac{2\pi}{a}\right)^2 \pm \frac{4\pi}{a}k \right)$

We see that the transition probability decreases with the increasing energy difference between the states $|E_{k \pm \frac{2\pi}{a}} - E_k|$, thus an energy difference of zero implies maximal transition probability. This happens for $k = \pm \frac{\pi}{a}$ as the states $k' = \mp \frac{\pi}{a}$ differ by exactly $\mp \frac{2\pi}{a}$ from k and have the same energy. Therefore transitions are most likely to happen when the particle is in the states given by $k = \pm \frac{\pi}{a}$ which transitions into states $k' = \mp \frac{\pi}{a}$.

– THE END –