

UNIVERSITY OF OSLO

FACULTY OF MATHEMATICS AND NATURAL SCIENCES

Solution to exam in: FYS3110, Quantum mechanics

Day of exam: Dec. 7. 2012

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

Problem 1

1.1 Definition of hermitian conjugate operator: $\langle\psi|O^\dagger|\psi\rangle = \langle\psi|O|\psi\rangle^*$. A hermitian operator is equal to its own conjugate: $O^\dagger = O$.

Properties (see Griffiths, chapter 3): Real eigenvalues. Eigenvalues correspond to measurement values, they should be real.

Eigenstates with different eigenvalues are orthogonal. Eigenstates are states for which the measurement value is the corresponding eigenvalue with 100% certainty. Physical states that for sure give different measurement values must be orthogonal.

Eigenstates span the Hilbert space¹. It must be possible to assign probabilities for getting a particular measurement value for *any* state. This means that it must be possible to write any state as a superposition of eigenstates. This is the spanning or completeness property.

1.2 The lowest energy is E_1 . There are 2 states with this energy, $|1, L\rangle$ and $|1, R\rangle$, or two orthogonal linear combinations of these two.

1.3 The hermitean conjugate operator is defined as:

$$\langle\psi|H'^\dagger|\psi\rangle = \langle\psi|H'|\psi\rangle^*$$

¹ The last property is not automatic for hermitian operators in an ∞ -dimensional Hilbert space.

for all states $|\psi\rangle$. Evaluating the right hand side with $H' = -\sum_{nm} (g_{nm}|n, L\rangle\langle m, R| + h_{nm}|n, R\rangle\langle m, L|)$ we get

$$\begin{aligned}
\langle\psi|H'|\psi\rangle^* &= -\left(\sum_{nm} (g_{nm}\langle\psi|n, L\rangle\langle m, R|\psi\rangle + h_{nm}\langle\psi|n, R\rangle\langle m, L|\psi\rangle)\right)^* \\
&= -\sum_{nm} (g_{nm}^*\langle\psi|m, R\rangle\langle n, L|\psi\rangle + h_{nm}^*\langle\psi|m, L\rangle\langle n, R|\psi\rangle) \\
&= -\sum_{nm} (h_{nm}^*\langle\psi|m, L\rangle\langle n, R|\psi\rangle + g_{nm}^*\langle\psi|m, R\rangle\langle n, L|\psi\rangle) \\
&= -\sum_{nm} (h_{mn}^*\langle\psi|n, L\rangle\langle m, R|\psi\rangle + g_{mn}^*\langle\psi|n, R\rangle\langle m, L|\psi\rangle) \\
&= \langle\psi|\left(-\sum_{nm} (h_{mn}^*|n, L\rangle\langle m, R| + g_{mn}^*|n, R\rangle\langle m, L|)\right)\psi\rangle
\end{aligned}$$

Therefore

$$H'^\dagger = -\sum_{nm} (h_{mn}^*|n, L\rangle\langle m, R| + g_{mn}^*|n, R\rangle\langle m, L|)$$

Hermiticity $H'^\dagger = H'$. Comparing the expression for H'^\dagger to that for H' we see that

$$\underline{g_{nm} = h_{mn}^*}$$

1.4 Normalization: $\langle\psi_k|\psi_k\rangle = A_k^2(1+k^2) = 1 \implies A_k = 1/\sqrt{1+k^2}$. The trial energy E_T is

$$\begin{aligned}
E_T &= \langle\psi_k|H_0 + H'|\psi_k\rangle \\
&= A_k^2((\langle 1, L| + k\langle 1, R|)(H_0 + H')(|1, L\rangle + k|1, R\rangle)) \\
&= A_k^2(\langle 1, L|H_0|1, L\rangle + k^2\langle 1, R|H_0|1, R\rangle - k\langle 1, L|H'|1, R\rangle - k\langle 1, R|H'|1, L\rangle) \\
&= A_k^2(E_1 + k^2E_1 - kg_{11} - kg_{11})
\end{aligned}$$

Inserting the expression for A_k we get

$$E_T = E_1 - \frac{2kg_{11}}{1+k^2}$$

We find the minimum by differentiating

$$\frac{\partial E_T}{\partial k} = -\frac{2g_{11}}{1+k^2} + \frac{4k^2g_{11}}{(1+k^2)^2} = 0$$

which implies

$$(1+k^2) = 2k^2 \implies k^2 = 1 \implies k = \pm 1$$

It is clear from the expression for E_T with g_{11} positive that $k = +1$ is a minimum while $k = -1$ is a maximum. Therefore the lowest upper bound on the ground state energy obtained from this class of trial states is

$$E_g \leq E_T^{min} = E_1 - \frac{2g_{11}}{1+1} = \underline{E_1 - g_{11}}$$

1.5 Both wells have width a . The left well is centered around $-a/2 - b = a/2 - (a+b)$ while the right well is centered around $a/2 + b$. For a well of width a centered around $a/2$ the wavefunctions are $\sqrt{2/a} \sin(n\pi x/a)$. We obtain the wavefunctions by translating an amount $-(a+b)$ and $+b$ respectively.

$$\psi_{n,L}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}(x + a + b)\right), \quad \psi_{n,R}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}(x - b)\right)$$

Using $\sin(n\pi(x + a + b)/a) = \sin(n\pi(x + b)/a + n\pi) = (-1)^n \sin(n\pi(x + b)/a)$ one can rewrite

$$\psi_{n,L}(x) = (-1)^n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}(x + b)\right) = e^{in\pi} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}(x + b)\right)$$

As eigenfunctions differing by a phase factor represent the same physical state it is in general possible to write

$$\underline{\psi_{n,L}(x) = e^{i\phi_{n,L} + in\pi} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}(x + b)\right)}, \quad \underline{\psi_{n,R}(x) = e^{i\phi_{n,R}} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}(x - b)\right)}$$

where $\phi_{n,L}$ and $\phi_{n,R}$ are arbitrary phase factors.

On changing $x \rightarrow -x$ we see that

$$\sin\left(\frac{n\pi}{a}(x + b)\right) \rightarrow \sin\left(\frac{n\pi}{a}(-x + b)\right) = -\sin\left(\frac{n\pi}{a}(x - b)\right)$$

thus the action of the reflection operator on the basis-states is

$$\begin{aligned} P\psi_{n,L}(x) &= \psi_{n,L}(-x) = -e^{i\phi_{n,L} + in\pi} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}(x - b)\right) = \underline{-e^{i(\phi_{n,L} + n\pi - \phi_{n,R})} \psi_{n,R}(x)} \\ P\psi_{n,R}(x) &= \underline{-e^{-i(\phi_{n,L} + n\pi - \phi_{n,R})} \psi_{n,L}(x)} \end{aligned}$$

Some common choices:

$$\begin{aligned} \phi_{n,L} = \phi_{n,R} = 0: & \quad P\psi_{n,L}(x) = (-1)^{n-1} \psi_{n,R}(x), & P\psi_{n,R}(x) &= (-1)^{n-1} \psi_{n,L}(x) \\ \phi_{n,L} = n\pi, \phi_{n,R} = 0: & \quad P\psi_{n,L}(x) = -\psi_{n,R}(x), & P\psi_{n,R}(x) &= -\psi_{n,L}(x) \\ \phi_{n,L} = (n-1)\pi, \phi_{n,R} = 0: & \quad P\psi_{n,L}(x) = \psi_{n,R}(x), & P\psi_{n,R}(x) &= \psi_{n,L}(x) \end{aligned}$$

1.6 The lowest energy level is twofold degenerate in the absence of H' . We know that P commutes with H . The eigenstates of P in the ground state manifold are $(|1, L\rangle \pm |1, R\rangle)/\sqrt{2}$ and have distinct eigenvalues (± 1) . Therefore they are the *good states* and the first order perturbative correction can be gotten by evaluating the expectation value of H' in these two states

$$\frac{1}{2} (\langle 1, L | \pm \langle 1, R |) H' (|1, L\rangle \pm |1, R\rangle) = \pm (-g_{11} - g_{11}^*)/2 = \mp g_{11}$$

for real g_{11} . Therefore the splitting is $2g_{11}$ and the two lowest energies are $E_1 \pm g_{11}$.

1.7 Three spin-1/2 non-interacting fermions are inserted into the potential. The Pauli principle dictates at most two spin-1/2 particles in each spatial state, therefore the lowest energy state is filled with two particles and the third goes into the next lowest level. Therefore

$$E = 2(E_1 - g_{11}) + E_1 + g_{11} = \underline{3E_1 - g_{11}}$$

The two fermions in the lowest level have a symmetric spatial wavefunction under the interchange of the particles, therefore their spins must combine to form an antisymmetric spin-0 singlet in order to obey the fermion condition that the total wavefunction is antisymmetric. Combining spin-0 with the spin-1/2 of the third spin, the total spin of the three particles becomes 1/2.

Problem 2.

2.1 The interaction of the two spin-1/2 particles can be written

$$\vec{S}_p \cdot \vec{S}_e = \frac{1}{2} (S_{\text{tot}}^2 - S_p^2 - S_e^2) = \frac{1}{2} \left(S_{\text{tot}}^2 - \frac{3\hbar^2}{4} - \frac{3\hbar^2}{4} \right) = \frac{1}{2} S_{\text{tot}}^2 - \frac{3\hbar^2}{4}.$$

For two spin-1/2 particles the total spin S_{tot} can be either 0 or 1. Thus

$$\begin{aligned} H_{fs} |S_{\text{tot}} = 1\rangle &= \frac{\kappa}{\hbar^2} \hbar^2 \left(\frac{1}{2} 2 \cdot 1 - \frac{3}{4} \right) |S_{\text{tot}} = 1\rangle = \frac{\kappa}{4} |S_{\text{tot}} = 1\rangle \\ H_{fs} |S_{\text{tot}} = 0\rangle &= \frac{\kappa}{\hbar^2} \hbar^2 \left(0 - \frac{3}{4} \right) |S_{\text{tot}} = 0\rangle = -\frac{3\kappa}{4} |S_{\text{tot}} = 0\rangle \end{aligned}$$

thus the energy difference is

$$E_{S_{\text{tot}}=1} - E_{S_{\text{tot}}=0} = \kappa \left(\frac{1}{4} - \left(-\frac{3}{4} \right) \right) = \underline{\kappa}$$

The triplet level $S_{tot} = 1$ is threefold degenerate, while the singlet $S_{tot} = 0$ is only one state.

2.2 The electric dipole interaction is

$$H_E = -E_0 \cos(\omega t) \hat{k} \cdot (-e) \vec{r}$$

and the electric dipole decay formula contains the electric dipole moment $\mathcal{P}_i = \langle \psi_f | (-e) r_i | \psi_i \rangle$ and reads

$$A = \frac{\omega_0^3}{3\pi\epsilon_0 \hbar c^3} (|\mathcal{P}_x|^2 + |\mathcal{P}_y|^2 + |\mathcal{P}_z|^2)$$

The expressions for the magnetic and electric dipole interactions have a similar structure which becomes clearer by writing

$$H_m = -E_0 \cos(\omega t) \hat{k} \cdot (\vec{\mu}_p + \vec{\mu}_e) \frac{B_0}{E_0}$$

Thus we see that the generalized formula becomes

$$A_m = \frac{\omega_0^3}{3\pi\epsilon_0 \hbar c^3} (|\mathcal{M}_x|^2 + |\mathcal{M}_y|^2 + |\mathcal{M}_z|^2)$$

where $\mathcal{M}_i = \langle \psi_f | \mu_{pi} + \mu_{ei} | \psi_i \rangle \frac{B_0}{E_0}$. The ratio of the amplitudes of the magnetic and electric fields can be derived from the information that $\epsilon_0 E^2 = \frac{1}{\mu_0} B^2$. With this the ratio of amplitudes is

$$\frac{B_0}{E_0} = \sqrt{\frac{B_0^2}{E_0^2}} = \sqrt{\epsilon_0 \mu_0} = \sqrt{\frac{1}{c^2}} = \frac{1}{c}.$$

Therefore

$$\mathcal{M}_i = \frac{1}{c} \langle \psi_f | \mu_{pi} + \mu_{ei} | \psi_i \rangle.$$

We choose to calculate the lifetime of the $S_{tot} = 1$, $m = 0$ triplet state

$$|1, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

where the first spin denotes the electron spin in the S_z -direction. The final state is the singlet state: $|0, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

$$\langle 0, 0 | \mu_e^z + \mu_p^z | 1, 0 \rangle = -\frac{eg_e}{2m} \langle 0, 0 | S_e^z | 1, 0 \rangle + \frac{eg_p}{2m} \langle 0, 0 | S_p^z | 1, 0 \rangle$$

Evaluating the matrix elements we find ($|s_e^z s_p^z\rangle$)

$$\begin{aligned} \langle 0, 0 | S_e^z | 1, 0 \rangle &= \langle 0, 0 | \frac{\hbar}{2} \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{\hbar}{2} \\ \langle 0, 0 | S_p^z | 1, 0 \rangle &= \langle 0, 0 | \frac{-\hbar}{2} \frac{1}{\sqrt{2}} (-|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = -\frac{\hbar}{2} \end{aligned}$$

Therefore

$$\mathcal{M}_z = -\frac{e\hbar g_e}{4mc} - \frac{e\hbar g_p}{4m_p c}$$

The other matrix elements \mathcal{M}_x and \mathcal{M}_y vanish. We then get the following expression for the transition probability

$$\begin{aligned} A_m &= \frac{\omega_0^3}{3\pi\epsilon_0\hbar c^3} \left(-\frac{e\hbar g_e}{4mc} - \frac{e\hbar g_p}{4m_p c} \right)^2 \\ &= \frac{(\hbar\omega_0)^3}{3\pi\epsilon_0\hbar^4 c^3} \left(\frac{e\hbar}{2mc} \right)^2 \left(\frac{g_e}{2} + \frac{g_p}{2} \frac{m}{m_p} \right)^2 \\ &= (\Delta E)^3 \frac{e^2}{4\pi\epsilon_0\hbar c} \frac{1}{3(mc^2)^2\hbar} \left(\frac{g_e}{2} + \frac{g_p}{2} \frac{m}{m_p} \right)^2 \end{aligned}$$

where we have used $\hbar\omega_0 = \Delta E$. Now use $m_p/m = 1836$, $g_e = 2.00$, $g_p = 5.59$, $\frac{e^2}{4\pi\epsilon_0\hbar c} = \alpha \approx 1/137$, $mc^2\alpha^2 = 2 \cdot 13.6\text{eV}$ and $\hbar = 6.582 \cdot 10^{-16}\text{eVs}$

$$\begin{aligned} A_m &= (\Delta E)^3 \frac{\alpha^5}{3 \cdot (2 \cdot 13.6\text{eV})^2\hbar} \left(1 + \frac{5.59}{2 \cdot 1836} \right)^2 \\ &= \frac{(5.88 \cdot 10^{-6}\text{eV})^3}{137^5 \cdot 3 \cdot 4 \cdot (13.6\text{eV})^2 \cdot 6.582 \cdot 10^{-16}\text{eVs}} \left(1 + \frac{5.59}{2 \cdot 1836} \right)^2 = 2.9 \cdot 10^{-15}\text{s}^{-1} \end{aligned}$$

The lifetime is

$$\tau = 1/A_m = 3.46 \cdot 10^{14}\text{s} \approx \underline{11\text{My}}$$

i.e. 11 million years (!).

——THE END