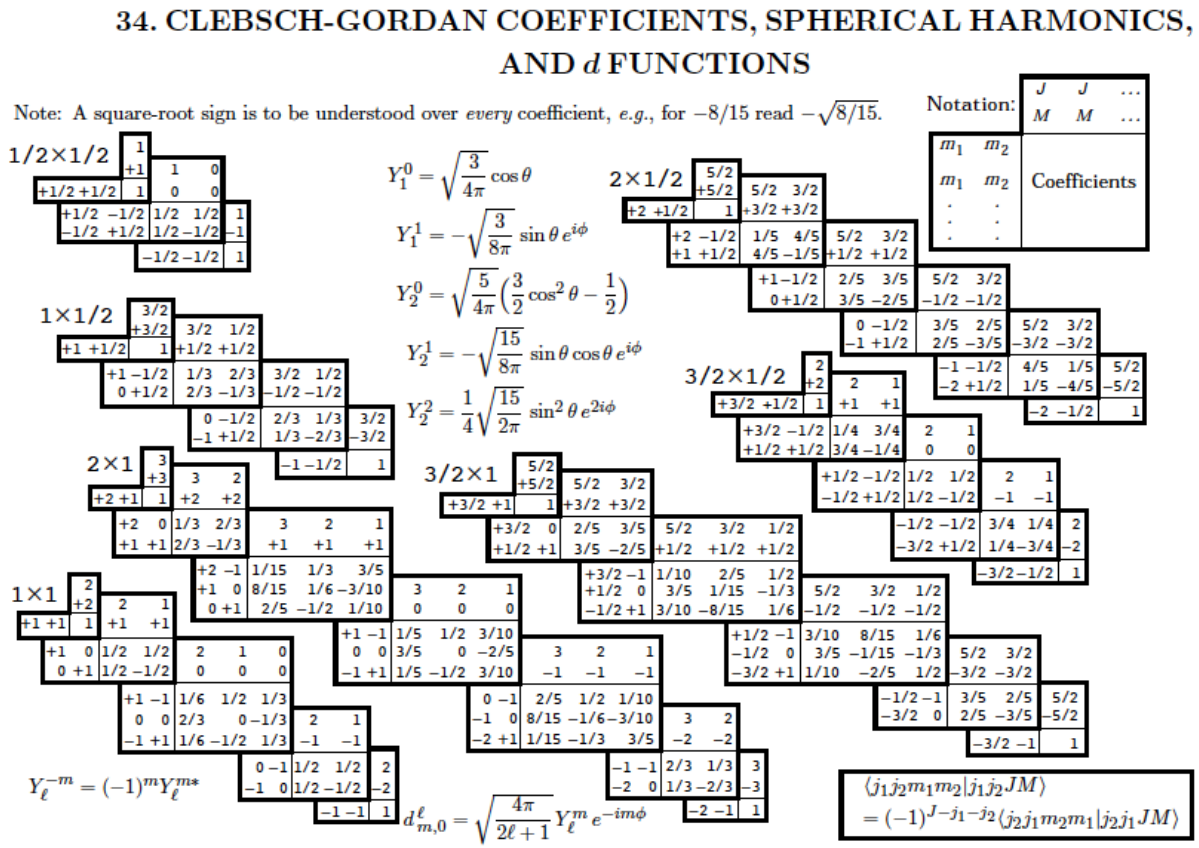
Answers exam Quantum Physics 2, 18 June 2014

Exercise 1

(a) Explain what are the properties of operators that are constants of motion and how they are used to describe stationary states.

> An operator Q is a constant of motion if it satisfies $[H, Q] = 0$ and $\partial Q/\partial t = 0$, such that $d\langle Q\rangle/dt = 0$. The Hamiltonian and constants of motion can be diagonalized simultaneously. As a consequence, stationary states can be specified by the eigenvalues of constants of motion, the so-called "good" quantum numbers, in a time-independent way.

(b) Use the table below to write down the Clebsch-Gordan decomposition of the state $|l, s; j, m_j\rangle = |1, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle$ and verify that acting with J_+ on the decomposition gives zero.



For the state $|l, s; j, m_j\rangle = |1, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle$, one reads off in the $1 \times 1/2$ part of the table for the Clebsch-Gordan coefficients in front of the states $|l, m_l\rangle|s, m_s\rangle$:

$$|1, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle = \sqrt{\frac{2}{3}}\,|1, 1\rangle|\frac{1}{2}, -\frac{1}{2}\rangle - \sqrt{\frac{1}{3}}\,|1, 0\rangle|\frac{1}{2}, \frac{1}{2}\rangle$$

Acting with $J_+ = L_+ + S_+$ on the decomposition yields for both terms a constant times the state $|1,1\rangle|\frac{1}{2},\frac{1}{2}\rangle$, which cancel when added:

$$\begin{aligned} J_+|1,\frac{1}{2};\frac{1}{2},\frac{1}{2}\rangle &= (L_+ + S_+)\left(\sqrt{\frac{2}{3}}\,|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle - \sqrt{\frac{1}{3}}\,|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle\right) \\ &= \left(\sqrt{\frac{2}{3}}\,\hbar - \sqrt{\frac{1}{3}}\,\hbar\sqrt{2}\right)|1,1\rangle|\frac{1}{2},\frac{1}{2}\rangle = 0 \end{aligned}$$

(c) In the calculation of the strong field Zeeman splitting, one can take into account the relativistic spin-orbit coupling effect as a perturbation. The first-order perturbative correction then involves the calculation of the matrix element $\langle l,s,m_l,m_s|\vec{L}\cdot\vec{S}\,|l,s,m_l,m_s\rangle$. Evaluate this matrix element and explain why one only has to consider such diagonal matrix elements, despite the degeneracy in some of the quantum numbers for the unperturbed system.

One way of arriving at the result is by writing

$$\vec{L}\cdot\vec{S} = \frac{1}{2}\left(L_+S_- + L_-S_+\right) + L_zS_z,$$

where only the last term contributes: $\langle l,s,m_l,m_s|\vec{L}\cdot\vec{S}\,|l,s,m_l,m_s\rangle = \langle l,s,m_l,m_s|L_zS_z|l,s,m_l,m_s\rangle = \hbar^2 m_l m_s$. Another way is given on page 280 of the book.

Off-diagonal elements in degenerate perturbation theory need to be considered, unless one can find operators that commute with both the unperturbed Hamiltonian and the perturbation, and having distinct eigenvalues (cf. the operator A on page 259/260 of the book). In this way one knows the eigenstates on which the perturbation will be diagonal. In the case of the strong magnetic field the C.S.C.O. of the unperturbed Hamiltonian is formed by $\vec{L}^2, L_z, \vec{S}^2, S_z$. The operators $\vec{L}^2$ and $\vec{S}^2$ also commute with $\vec{L}\cdot\vec{S}$, hence one only needs to consider matrix elements diagonal in l and s. The operators L_z and S_z do not commute with the spin-orbit term, so they cannot play the role of A, but there is no need for that. The unperturbed states are *nondegenerate* in m_l and m_s, due to the Zeeman term, see Eq. (6.79), except when $m_l + 2m_s = 0$. For instance, for $n = 2$ the states with $m_l = 1, m_s = -1/2$ and $m_l = -1, m_s = 1/2$ are degenerate. However, such two-fold degenerate states with nonzero m_l and $-m_l$ cannot be coupled by $L_\pm$, since $\Delta m_l \equiv m_l - (-m_l) \geq 2$ for $m_l \geq 1$. Considering exclusively diagonal matrix elements is therefore justified. Note that this issue has nothing to do with the perturbation lifting degeneracy.

(d) Consider a Hamiltonian H that commutes with the parity or reflection operator P : $x \to -x$. Show that $\langle\psi_a|H|\psi_b\rangle = 0$ whenever ψ_a is an even function of x and ψ_b is an odd function. Explain how this result helps to simplify degenerate perturbation theory calculations.

$[H,P] = 0$ implies $\langle\psi_a|[H,P]|\psi_b\rangle = 0$ which in turn implies $\langle P\psi_a|H|\psi_b\rangle = \langle\psi_a|H|P\psi_b\rangle$, hence for even ψ_a and odd ψ_b: $\langle\psi_a|H|\psi_b\rangle = -\langle\psi_a|H|\psi_b\rangle$. Therefore, $\langle\psi_a|H|\psi_b\rangle = 0$.

In degenerate perturbation theory off-diagonal matrix elements $\langle\psi_i|H'|\psi_j\rangle$ need to be considered for degenerate states ψ_i and ψ_j. Symmetry arguments can be used to identify the "good" linear combinations of ψ_i and ψ_j for which this matrix is automatically diagonal, like for the even and odd states if H commutes with the parity operator. P is another example of an operator A on page 259/260 of the book.

Exercise 2

Consider the one-dimensional harmonic oscillator as unperturbed system and introduce the perturbation

$$H'(x) = c\sqrt{b}\exp(-bx^2),$$

where b and c are positive constants.

(a) Calculate within perturbation theory the first-order correction to the ground state energy and determine for which values of c the result is valid when $b \gg m\omega/\hbar$.

The ground state wave function of the one-dimensional harmonic oscillator is given by

$$\psi_0^0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right).$$

The first-order correction to the ground state energy is given by:

$$E_0^1 = c\sqrt{b}\int_{-\infty}^{\infty} dx e^{-bx^2}(\psi_0^0(x))^2 = \frac{c\sqrt{b}}{\sqrt{1+\hbar b/(m\omega)}}.$$

Perturbation theory is valid if this correction is smaller than the unperturbed ground state energy $\hbar\omega/2$. In the limit $b \gg m\omega/\hbar$ the correction becomes $c\sqrt{m\omega/\hbar}$, hence:

$$c \ll \frac{\hbar^{3/2}}{2}\sqrt{\frac{\omega}{m}}.$$

Consider next the perturbation

$$H'(x) = c\,x\sqrt{b}\exp(-bx^2),$$

where b and c are positive constants.

(b) Show that in this case the first-order perturbative correction vanishes.

The first-order correction to the ground state energy is now given by:

$$E_0^1 = c\sqrt{b}\int_{-\infty}^{\infty} dx x e^{-bx^2}(\psi_0^0(x))^2 = 0,$$

due to symmetric integration of an odd integrand. In fact, $E_n^1 = 0$ for all n.

(c) Show that the second-order perturbative correction to the ground state energy is negative.

The second-order correction to the ground state energy is given by:

$$E_0^2 = \sum_{m \neq 0} \frac{|\langle \psi_m^0 | H' | \psi_0^0 \rangle|^2}{E_0^0 - E_m^0}.$$

The numerator is always positive and the denominator always negative ($E_m^0 > E_0^0 > 0$ for $m > 0$), so E_0^2 is negative.

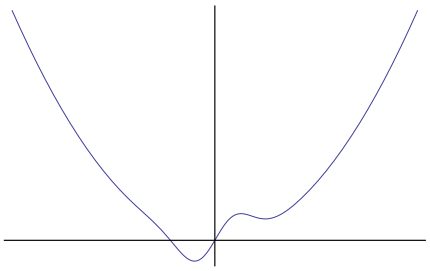
(d) Demonstrate using the variational principle that adding this perturbation H' can only decrease the energy of the ground state.

For all trial wave functions ψ_T it holds that

$$E[\psi_T] \equiv \frac{\langle \psi_T | H_0 + H' | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} \geq E_{g.s.},$$

where $E_{g.s.}$ denotes the true ground state energy. For $\psi_T = \psi_0^0$ one has $E[\psi_0^0] = \langle \psi_0^0 | H_0 | \psi_0^0 \rangle = E_0$, hence $E_{g.s.} \leq E_0$, where the equality only holds in the unperturbed case, i.e. when $c = 0$ such that $H' = 0$.

(e) Draw a picture of the potential including the perturbation H' and write down a trial wave function that might be expected to give a better upper bound on the ground state energy than the unperturbed ground state energy (motivate your choice).



As can be seen from the above illustration, the potential will be partly below zero for some negative x value, call it $x_{\min}$. A Gaussian centered around $x_{\min}$ may be expected to give a lower bound for instance, because it has larger probability at $x_{\min}$. Note that any purely even or purely odd trial wave function will yield zero expectation value of H' and will not lower the energy.

Exercise 3

Consider the Hamiltonian $H = H_0 + H'(t)$, where H' is a time-dependent perturbation that is nonzero for $t \geq 0$. Let $\psi_n^{(0)}$ be the orthonormal set of eigenstates of H_0 with energies $E_n^{(0)}$, i.e. $H_0 \, \psi_n^{(0)} = E_n^{(0)} \, \psi_n^{(0)}$.

(a) Show that with the following expansion on the states $\psi_n^{(0)}$

$$\psi(t) = \sum_n c_n(t) \, \psi_n^{(0)} \, e^{-i \, E_n^{(0)} t/\hbar},$$

the coefficients satisfy

$$\dot{c}_m(t) = \frac{1}{i\hbar} \sum_n c_n(t)\, e^{i\,(E_m^{(0)} - E_n^{(0)})t/\hbar}\, H'_{mn},$$

where $H'_{mn} = \langle \psi_m^{(0)} | H' | \psi_n^{(0)} \rangle$.

Plugging $\psi(t)$ into the Schrödinger equation $i\hbar d\psi(t)/dt = (H_0 + H'(t))\psi(t)$, taking the inner product with the state $\psi_m^{(0)}$ and exploiting orthonormality of the states $\psi_n^{(0)}$ yields the answer, like on p. 342 of the book, but now for an arbitrary number of states. Note that the sum over n includes m, since in general $(H')_{mm} \neq 0$.

(b) Consider the case where $H'(t) = V(r)\theta(t)$ for a two-level system consisting of states ψ_1 and ψ_2, such that $\langle \psi_i | V(r) | \psi_j \rangle \neq 0$ for $i \neq j$. Derive, to first nontrivial order in time-dependent perturbation theory, what is the probability to be in state ψ_2 as a function of time if the system is in state ψ_1 for $t < 0$.

In first order perturbation theory and for $c_n^{(0)}(t) = \delta_{n1}$:

$$\dot{c}_2^{(1)} = \frac{1}{i\hbar} \sum_{n=1}^{2} H'_{2n}\, c_n^{(0)}(t)\, e^{i\,(E_2^{(0)} - E_n^{(0)})t/\hbar} = \frac{1}{i\hbar} H'_{21}\, e^{i\,(E_2^{(0)} - E_1^{(0)})t/\hbar}.$$

This yields:

$$c_2^{(1)}(t) = \frac{1}{i\hbar} V_{21} \int_0^t dt' e^{i\,\omega_{21} t'} = \frac{-2iV_{21}}{\hbar\omega_{21}} e^{i\,\omega_{21} t/2} \sin\left(\frac{\omega_{21} t}{2}\right).$$

Hence, the probability to be in state ψ_2 for $t \geq 0$ is

$$|c_2^{(1)}(t)|^2 = \frac{4|V_{21}|^2}{\hbar^2 \omega_{21}^2} \sin^2\left(\frac{\omega_{21} t}{2}\right).$$