

Answers exam Kwantumfysica 2, June 21, 2012

Exercise 1

(a) Explain what is the purpose or use of the addition of angular momentum and give the definition of a "good" quantum number.

Addition of angular momentum is useful when individual angular momenta are not conserved, i.e. when they are coupled. E.g. if the Hamiltonian contains a $J_1 \cdot J_2$ term, then $[H, J_{iz}] \neq 0$, in other words, $d\langle J_{iz} \rangle / dt \neq 0$. Only the total angular momentum ($J = J_1 + J_2$) will be conserved in general. The purpose is to obtain a C.S.C.O.

A "good" quantum number is an eigenvalue of a constant of motion. An operator Q is a constant of motion if it satisfies $[H, Q] = 0$ and $\partial Q / \partial t = 0$. The Hamiltonian and the constants of motion form a C.S.C.O. that can be diagonalized simultaneously. Stationary states can then be labelled by means of "good" quantum numbers in a time-independent way.

(b) Use the table below to write down the Clebsch-Gordan decomposition of the state $|j_1, j_2; j, m\rangle = |2, 1; 1, 0\rangle$ in terms of the product states $|j_1, j_2; m_1, m_2\rangle$ and verify the convention $\langle j_1, j_2; j_1, j - j_1 | j, j \rangle > 0$.

Table 1: Clebsch-Gordan coefficients $\langle j_1, 1; m_1, m_2 | j, m \rangle$

j	$m_2 = 1$	$m_2 = 0$	$m_2 = -1$
$j_1 + 1$	$\left[\frac{(j_1+m)(j_1+m+1)}{(2j_1+1)(2j_1+2)} \right]^{\frac{1}{2}}$	$\left[\frac{(j_1-m+1)(j_1+m+1)}{(2j_1+1)(j_1+1)} \right]^{\frac{1}{2}}$	$\left[\frac{(j_1-m)(j_1-m+1)}{(2j_1+1)(2j_1+2)} \right]^{\frac{1}{2}}$
j_1	$-\left[\frac{(j_1+m)(j_1-m+1)}{2j_1(j_1+1)} \right]^{\frac{1}{2}}$	$\frac{m}{[j_1(j_1+1)]^{\frac{1}{2}}}$	$\left[\frac{(j_1-m)(j_1+m+1)}{2j_1(j_1+1)} \right]^{\frac{1}{2}}$
$j_1 - 1$	$\left[\frac{(j_1-m)(j_1-m+1)}{2j_1(2j_1+1)} \right]^{\frac{1}{2}}$	$-\left[\frac{(j_1-m)(j_1+m)}{j_1(2j_1+1)} \right]^{\frac{1}{2}}$	$\left[\frac{(j_1+m)(j_1+m+1)}{2j_1(2j_1+1)} \right]^{\frac{1}{2}}$

For the state $|j_1, j_2; j, m\rangle = |2, 1; 1, 0\rangle$, one has $j = j_1 - 1$, which means one has to use the bottom row of the table. This yields:

$$|2, 1; 1, 0\rangle = \sqrt{\frac{3}{10}} |2, 1; -1, 1\rangle - \sqrt{\frac{4}{10}} |2, 1; 0, 0\rangle + \sqrt{\frac{3}{10}} |2, 1; 1, -1\rangle$$

(c) In case of a constant, uniform external electric field one has to calculate the matrix elements $\langle nlm|z|n'l'm'\rangle$. Show that rotational invariance implies that for $\Delta m = m' - m \neq 0$ these matrix elements vanish. Show that the behavior under parity transformations demands that for even $l + l'$ these matrix elements vanish. Write down which matrix elements are nonzero for $n = 2, n' = 1$.

In case of a constant, uniform external electric field taken along the z -axis, the system is invariant under rotations around the z -axis. One has $[L_z, z] = 0$, which implies

$$\langle nlm|[L_z, z]|n'l'm'\rangle = 0 \Rightarrow \Delta m \langle nlm|z|n'l'm'\rangle = 0$$

Hence, for $\Delta m \neq 0$: $\langle nlm|z|n'l'm'\rangle = 0$.

Under a parity transformation $\vec{r} \rightarrow -\vec{r}$: $\psi_{nlm} \rightarrow (-1)^l \psi_{nlm}$ and $z \rightarrow -z$. Hence,

$$\langle nlm|z|n'l'm'\rangle = \int d^3r \psi_{nlm}^*(\vec{r}) z \psi_{n'l'm'}(\vec{r})$$

is only nonvanishing if $(-1)^{l+l'+1} = 1$, i.e. when $l + l'$ is odd.

For $n = 2, n' = 1$, the only nonvanishing matrix element is then $\langle 210|z|100\rangle$.

(d) Explain why j is not a good quantum number in case of a constant, uniform external magnetic field and discuss what is the consequence for the time dependence of a state that has a given j at $t = 0$?

In case of a constant, uniform external magnetic field along the z -axis, the Zeeman term in the Hamiltonian is proportional to $L_z + 2S_z$, which does not commute with J^2 . Therefore, $[H, J^2] \neq 0$, which means j is not a good quantum number. This implies that $d\langle J^2 \rangle / dt \neq 0$. A state of given j at $t = 0$ may thus change into a mixture of states with different j values for $t > 0$.

Exercise 2

(a) Construct the solutions of the Schrödinger equation for the infinite square well potential,

$$V(x) = \begin{cases} 0 & -a \leq x \leq a \\ \infty & \text{elsewhere} \end{cases}$$

and give the allowed energies.

Solutions of the Schrödinger equation can be written in the form $A \sin(kx) + B \cos(kx)$. In this case they must satisfy $\psi(\pm a) = 0$, which leads to:

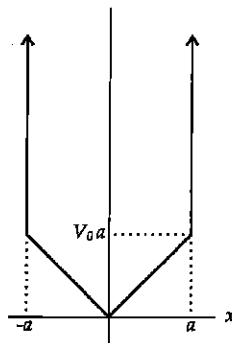
$$\psi_n(x) = A \sin k_n x, \quad \text{with } k_n = \frac{n\pi}{2a}, \quad \text{for } n = 2, 4, \dots$$

$$\psi_n(x) = B \cos k_n x, \quad \text{with } k_n = \frac{n\pi}{2a}, \quad \text{for } n = 1, 3, \dots$$

The normalization is then $A = B = 1/\sqrt{a}$. One could also have taken:

$$\psi_n(x) = A \sin k_n(x - a), \quad \text{with } k_n = \frac{n\pi}{2a}, \quad \text{for } n = 1, 2, 3, \dots$$

The allowed energies are $E_n = \hbar^2 k_n^2 / (2m) = \hbar^2 n^2 \pi^2 / (8ma^2)$.



Next consider the case $V(x) + V_0|x|$ for constant V_0 (see figure).

(b) Calculate in first order perturbation theory the correction to the ground state energy due to the addition of the potential $V_0|x|$ to $V(x)$. Give the condition(s) for which this perturbative result is valid.

Unperturbed ground state: $\psi_1^{(0)}(x) = (1/\sqrt{a}) \cos(\pi x/(2a))$. The first order correction to the ground state:

$$E_1^{(1)} = \langle \psi_1^{(0)} | V_0|x| | \psi_1^{(0)} \rangle = \frac{V_0}{a} \int_{-a}^a dx |x| \cos^2\left(\frac{\pi x}{2a}\right) \\ = \frac{2V_0}{a} \int_0^a dx x \cos^2\left(\frac{\pi x}{2a}\right).$$

Using for instance that $2 \cos^2(\alpha) = 1 + \cos(2\alpha)$ and integrating by parts, yields:

$$E_1^{(1)} = \frac{V_0 a}{2} \left(1 - \frac{4}{\pi^2}\right)$$

This result is valid as long as V_0 is small enough, such that the correction is much smaller than $E_1^{(0)}$.

(c) Obtain an upper bound to the ground state energy for the potential $V(x) + V_0|x|$ using the following normalized trial function,

$$\psi_T(x) = \sqrt{\frac{15}{16a^3}} (a^2 - x^2),$$

and show that it is larger than the perturbative result. Argue whether this is expected or not.

Although there is no parameter to vary, from the variational method we know that for any trial wave function one obtains an upper bound to the exact ground state energy:

$$E[\psi_T] = \langle \psi_T | H | \psi_T \rangle = \int_{-a}^a \psi_T(x)^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0|x| \right) \psi_T(x) dx \geq E_0.$$

A straightforward calculation yields:

$$E[\psi_T] = \frac{\hbar^2}{ma^2} \frac{5}{4} + \frac{5}{16} V_0 a,$$

which is larger than the perturbative result for all a and V_0 . Since the perturbative result is not the exact result, this was not necessarily expected.

(d) Give an example of a trial function that would give an upper bound on the first excited state for $V(x) + V_0|x|$.

Only a trial function for the first excited state that is orthogonal to the true ground state will yield an upper bound on the first excited state energy. Since the true ground state is even under $x \rightarrow -x$, any odd trial function will do, e.g. $\phi_T(x) \sim (a^2 - x^2)x$.

(e) Obtain the first two leading terms in $V_0 a/E$ for the allowed energies using the WKB method, assuming the ground state energy E_{gs} to be larger than $V_0 a$. Recall that $(1-x)^{3/2} = 1 - 3x/2 + 3x^2/8 + \dots$

Since $E_{gs} > V_0 a$, one can use the WKB result: $\int_{-a}^a p(x) dx = n\pi\hbar$, with $p(x) = \sqrt{2m(E - V_0|x|)}$.

$$\int_{-a}^a p(x) dx = 2 \int_0^a \sqrt{2m(E - V_0 x)} = \frac{4}{3} \sqrt{2mE} \frac{E}{V_0} \left(1 - \left(1 - \frac{V_0 a}{E}\right)^{3/2}\right).$$

Upon Taylor expanding one finds:

$$n\pi\hbar \approx \frac{4}{3} \sqrt{2mE} \frac{E}{V_0} \left(\frac{3}{2} \frac{V_0 a}{E} - \frac{3}{8} \frac{V_0^2 a^2}{E^2}\right),$$

which, upon taking the square and dropping the V_0^2 term, yields:

$$n^2 \pi^2 \hbar^2 \approx 8ma^2 \left(E - \frac{1}{2} V_0 a\right),$$

i.e.

$$E \approx \frac{n^2 \pi^2 \hbar^2}{8ma^2} + \frac{1}{2} V_0 a,$$

a result that is larger than the first order perturbative result, but can be smaller than the answer obtained with the trial function in (c) if V_0 is small enough.

Exercise 3

Consider the Hamiltonian $H = H_0 + H'$, where the states $\psi_n^{(0)}$ form an orthonormal set of eigenstates of H_0 with energies $E_n^{(0)}$, i.e. $H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$. H' is a perturbation acting from time $t_0 = 0$.

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

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

the coefficients satisfy

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

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

Plugging $\psi(t)$ into the Schrödinger equation $i\hbar d\psi(t)/dt = (H_0 + H'(t))\psi(t)$ and taking the inner product with the state $\psi_n^{(0)}$ ($\langle \psi_n^{(0)} | \psi(t) \rangle = c_n(t) \exp(-iE_n^{(0)}t/\hbar)$) yields the answer.

(b) Consider the particular case of a two-level system consisting of states a and b , with $H' = \theta(t)V$, where V is an \tilde{r} -independent, t -independent potential. What is the probability that the system is in state b for $t > 0$ if for $t < 0$ it is in state a ?

Since H' does not couple the states a and b , i.e. $H'_{ab} = 0$, the probability to be in state b for $t > 0$ is zero. One can also calculate this explicitly by solving the relevant exact equations:

$$\begin{aligned} i\hbar \dot{c}_a(t) &= H'_{aa} c_a(t), \\ i\hbar \dot{c}_b(t) &= H'_{bb} c_b(t). \end{aligned}$$

In this case both equations can be solved as follows:

$$\frac{d \ln c_i(t)}{dt} = -i\theta(t)V/\hbar \Rightarrow c_i(t) = c_i(0) \exp(-iVt/\hbar) \text{ for } t \geq 0.$$

Under the boundary conditions $c_a(0) = 1, c_b(0) = 0$, this yields $|c_a(t)|^2 = 1$ and $|c_b(t)|^2 = 0$, as expected.

(c) Derive the same probability in first-order time-dependent perturbation theory for an \tilde{r} -dependent, t -independent potential V .

Now $H'_{ab} \neq 0$ in general, hence one has in first order perturbation theory (for which $c_n^{(0)}(t) = \delta_{na}$):

$$\dot{c}_b^{(1)} = \frac{1}{i\hbar} \sum_{n=a,b} H'_{mn} c_n^{(0)}(t) e^{i(E_m^{(0)} - E_n^{(0)})t/\hbar} = \frac{1}{i\hbar} H'_{ba} e^{i(E_b^{(0)} - E_a^{(0)})t/\hbar}.$$

This yields:

$$c_b^{(1)} = \frac{1}{i\hbar} V_{ba} \int_0^t dt' e^{i\omega_{ba}t'} = \frac{-2iV_{ba}}{\hbar\omega_{ba}} e^{i\omega_{ba}t'/2} \sin(\omega_{ba}t'/2).$$

Hence,

$$|c_b^{(1)}|^2 = \frac{4|V_{ba}|^2}{\hbar^2\omega_{ba}^2} \sin^2(\omega_{ba}t/2).$$

(d) Show for the two cases in (b) and (c) whether the average energy is conserved or not.

For $H = H_0 + \theta(t)V$:

$$\langle H \rangle(t) = \sum_n |c_n(t)|^2 E_n^{(0)} + \theta(t) \sum_{n,m} c_n^*(t) c_m(t) V_{nm} e^{i\omega_{nm}t}$$

Case (b): $\langle H \rangle(t) = E_a^{(0)} + \theta(t)V_{aa}$, hence $\langle \dot{H} \rangle \neq 0$, but only at $t = 0$.

Case (c): there is an oscillation between states a and b , so the average energy is not conserved (note that this is not a question about the time-averaged energy).