QM II: Übungszettel 8
(Abgabetermin: 10.06.2015)

Perturbation theory I (16 pts)

Consider two particles with spins $\hat{\vec{\mathbf{S}}}_1$, $\hat{\vec{\mathbf{S}}}_2$ that are fixed in space. The magnetic moment of spin 1 creates a magnetic field with which spin 2 interacts. The two particles are subjected to an external magnetic field, taken to be parallel to the z-axis, $\vec{B} = B_0\vec{e}_z$. The Hamiltonian then reads

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_0 + \hat{\mathbf{W}} = \omega_1 \hat{\mathbf{S}}_{1,z} + \omega_1 \hat{\mathbf{S}}_{2,z} + \frac{\mu_0}{4\pi}\frac{\gamma_1\gamma_2}{r^3}\left(\hat{\vec{\mathbf{S}}}_1 \cdot \hat{\vec{\mathbf{S}}}_2 - 3(\hat{\vec{\mathbf{S}}}_1 \cdot \vec{n})(\hat{\vec{\mathbf{S}}}_2 \cdot \vec{n})\right)$$

with $\omega_i = -\gamma_i B_0$ and $\gamma_{1/2}$ the gyromagnetic ratios. $r = |\vec{r}|$ denotes the distance between the two particles, and $\vec{n} = \vec{r}/r$.

(a) Take θ and ϕ to be the polar angles of $\vec{n}$. Show that the interaction term can be expressed in terms of second rank tensors as follows:

$$\begin{aligned}\hat{\mathbf{W}} = -\frac{\mu_0}{4\pi}\frac{\gamma_1\gamma_2}{r^3} \Big\{ & \left(3\cos^2\theta - 1\right)\hat{\mathbf{S}}_{1,z}\hat{\mathbf{S}}_{2,z} - \frac{1}{4}\left(3\cos^2\theta - 1\right)\left(\hat{\mathbf{S}}_{1,+}\hat{\mathbf{S}}_{2,-} + \hat{\mathbf{S}}_{1,+}\hat{\mathbf{S}}_{2,-}\right) \\ & + \frac{3}{2}\sin\theta\cos\theta e^{-i\phi}\left(\hat{\mathbf{S}}_{1,z}\hat{\mathbf{S}}_{2,+} + \hat{\mathbf{S}}_{1,+}\hat{\mathbf{S}}_{2,z}\right) + \frac{3}{2}\sin\theta\cos\theta e^{i\phi}\left(\hat{\mathbf{S}}_{1,z}\hat{\mathbf{S}}_{2,-} + \hat{\mathbf{S}}_{1,-}\hat{\mathbf{S}}_{2,z}\right) \\ & + \frac{3}{4}\sin^2\theta e^{-2i\phi}\hat{\mathbf{S}}_{1,+}\hat{\mathbf{S}}_{2,+} + \frac{3}{4}\sin^2\theta e^{2i\phi}\hat{\mathbf{S}}_{1,-}\hat{\mathbf{S}}_{2,-} \Big\}\end{aligned}$$

(b) Assume the gyromagnetic ratios to be different. Write down the eigenbasis of the unperturbed Hamiltonian and calculate the energy correction due to $\hat{\mathbf{W}}$ to first order. If you measure transitions between energy levels, how does the unperturbed spectrum look like? How the perturbed one?
Hint: Convince yourself that, to first order, energy corrections involve only diagonal matrix elements of $\hat{\mathbf{W}}$ (in the unperturbed eigenbasis). Show that only the first term in $\hat{\mathbf{W}}$ leads to non-zero diagonal matrix elements.

(c) Now take the gyromagnetic ratios to be equal. Write down the eigenbasis of the unperturbed Hamiltonian and calculate the energy correction due to $\hat{\mathbf{W}}$ to first order. If you measure transitions between energy levels, how does the unperturbed spectrum look like? How the perturbed one?
Hint: It is now only the second term in $\hat{\mathbf{W}}$ that leads to non-zero diagonal matrix elements. Show why this is the case.

Perturbation theory II (12 pts)

In a simple model, a diatomic molecule with permanent dipole moment $\hat{\vec{\mathbf{d}}}$ can be treated as a rigid rotor, $\hat{\mathbf{H}}_0 = -\frac{\hbar^2}{2I}\hat{\vec{\mathbf{L}}}^2$, where I is the moment of inertia and $B = \hbar^2/(2I)$ is referred to as rotational constant.

(a) Show that in any eigenstate of $\hat{\mathbf{H}}_0$, the expectation value of $\hat{\vec{\mathbf{d}}}$ is zero.

(b) A static electric field $\vec{E} = E_0\vec{e}_z$ interacts with the rotor's dipole moment, leading to a perturbation $\hat{\mathbf{H}}_1 = -\hat{\vec{\mathbf{d}}}\cdot\vec{E}$. Which eigenstates of $\hat{\mathbf{H}}_0$ are coupled by $\hat{\mathbf{H}}_1$? Calculate the energy corrections to second order and the perturbed wavefunctions to first order for $m = 0$. For what field strengths do you expect perturbation theory to be valid?

(c) *Optional: Show that the expectation value of $\hat{\vec{\mathbf{d}}}$ does not vanish for the perturbed states.*
This phenomenon of state-dependent dipole moments is at the basis of a proposal to use polar molecules for quantum information (DeMille, Phys. Rev. Lett. 88, 067901 (2002)).

Perturbation theory III (22 pts)

Consider two hydrogen atoms that are fixed in space with a distance R between them. The charge distribution of atom 1's electron creates an electrostatic potential at atom 2 with which the electron of atom 2 interacts. The charge distribution of each electron can be described by a multipole expansion. Since the atoms are neutral, the leading order term of the electrostatic interaction between the two hydrogen atoms is then given by the dipole-dipole term,

$$\hat{\mathbf{W}} = -\vec{\nabla}U \cdot \vec{d} = \frac{q^2}{4\pi\epsilon_0}\frac{1}{R^3}\left(\hat{\vec{\mathbf{r}}}_1 \cdot \hat{\vec{\mathbf{r}}}_2 - 3(\hat{\vec{\mathbf{r}}}_1 \cdot \vec{n})(\hat{\vec{\mathbf{r}}}_2 \cdot \vec{n})\right) ,$$

where $\vec{r}_i$ denotes the position of the electron with respect to the nucleus of atom i, and $\vec{n} = \vec{R}/R$. Choosing the z-axis parallel to $\vec{n}$, this simplifies to

$$\hat{\mathbf{W}} = \frac{q^2}{4\pi\epsilon_0}\frac{1}{R^3}\left(\hat{\mathbf{x}}_1\hat{\mathbf{x}}_2 + \hat{\mathbf{y}}_1\hat{\mathbf{y}}_2 - \hat{\mathbf{z}}_1\hat{\mathbf{z}}_2\right) .$$

The total Hamiltonian is given by

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \hat{\mathbf{W}} .$$

The ground state of the unperturbed Hamiltonian $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ is simply the product state of two hydrogen ground states with quantum numbers n_1, l_1, m_1, n_2, l_2, m_2.

(a) Show that the first order correction to the ground state energy is zero and calculate the second order correction. *Hint: You may approximate the numerator by* $2E_0 - E_{n_1'} - E_{n_2'}$ *by* $2E_0$. *Explain why this should be a good approximation.*

(b) Now assume that one of the hydrogen atoms is in the ground $1s$ state, whereas the other one is in $2p$. The corresponding eigenenergy of the unperturbed Hamiltonian is eight-fold degenerate. Show that the 8×8 matrix of $\hat{\mathbf{W}}$ in the eigenspace of this level can be broken up into four 2×2 matrices. Diagonalize one of the non-trivial 2×2 matrices. How does the interaction scale with R? Why is this scaling different from (a)? Is the interaction attractive or repulsive?

(c) Consider the time evolution of the state $n_1 = 0$, $l_1 = 0$, $m_1 = 0$, $n_2 = 1$, $l_2 = 1$, m_2 in the presence of the perturbation. Will the excitation stay on atom 2?