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Höhere Quantenmechanik
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# Exercise sheet 2

(Submission date: Until 02.05.2022 12:00)

## Exercise 1: particle in a ring *(7 Points)*

Consider a particle in two dimensions which is confined to a ring of radius $R$ by an infinite potential. In polar coordinates, the Hamiltonian can be written as

$$\mathbf{H}_0 = -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial\theta^2},$$

where $\theta$ is the polar angle. This can be thought of as a minimal model for a molecule like benzene.

(i) Find the eigenvalues $E_n$ and eigenfunctions $\Psi_n(\theta)$ of the above Hamiltonian. Is the ground state degenerate? And the first excited state? *(2 Points)*

(ii) Suppose the system is perturbed by $\mathbf{V} = \lambda x = \lambda R\cos(\theta)$, which mimics the electric potential generated by a dipolar molecule. Compute the first- and second-order corrections to the ground state energy due to the perturbation $\mathbf{V}$. *(2 Points)*

(iii) Compute the first-order correction to the ground state wave function due to the perturbation $\mathbf{V}$. *(1 Point)*

(iv) We now consider the perturbation $\mathbf{V}_m = A\cos(m\theta)$, which depends on the integer number $m \in \mathbb{Z}$. Using perturbation theory, compute the first-order correction to the energy of the first excited states of $\mathbf{H}_0$ and the corresponding eigenfunctions. For which values of $m$ is the degeneracy lifted by the perturbation $\mathbf{V}_m$? *(2 Points)*

## Exercise 2: ferromagnetic spins *(6 Points)*

Consider a system of two spin-$\frac{1}{2}$ particles described by the Hamiltonian $\mathbf{H}_0 = -J\vec{\mathbf{S}}_1\cdot\vec{\mathbf{S}}_2$ $(J > 0)$, where $\vec{\mathbf{S}}_1 = (\mathbf{S}_1^x, \mathbf{S}_1^y, \mathbf{S}_1^z)$ and $\vec{\mathbf{S}}_2 = (\mathbf{S}_2^x, \mathbf{S}_2^y, \mathbf{S}_2^z)$ are the spin operators for particles 1 and 2, respectively.

(i) Find the eigenvalues and eigenfunctions of $\mathbf{H}_0$. *(3 Points)*
*Hint: use* $\vec{\mathbf{S}}_{tot} = \vec{\mathbf{S}}_1 + \vec{\mathbf{S}}_2$ *to rewrite* $\mathbf{H}_0$ *in a convenient form.*

(ii) Calculate the first-order energy correction to the ground state energy due to the perturbation $\mathbf{V} = \lambda[(\mathbf{S}_{tot}^x)^2 - (\mathbf{S}_{tot}^y)^2]$ and the corresponding zeroth-order eigenvectors. Is the degeneracy fully lifted? *(3 Points)*
*Hint: use the ladder operators; remember that* $S^{\pm}|s,m\rangle = \hbar\sqrt{(s\mp m)(s\pm m+1)}|s,m\pm1\rangle$.

## Exercise 3: spin-orbit coupling *(7 Points)*

This *spin-orbit coupling* is a relativistic interaction that can be described by a Hamiltonian of the form $\mathbf{H}_{soc} \propto \vec{\mathbf{L}} \cdot \vec{\mathbf{S}}$. In this exercise, we take the Hamiltonian of the hydrogen atom, $\mathbf{H}_0$, and we perturb it by the addition of the spin-orbit coupling $\mathbf{H}_{soc}$.

(i) For the non-relativistic solution of the hydrogen problem, one usually utilizes the conserved quantities

$$\vec{\mathbf{L}}^2, \mathbf{L}_z, \mathbf{S}_z, \vec{\mathbf{S}}^2 \quad \text{(quantum numbers } l, m_l, m_s, s) \tag{1}$$

to write the eigenfunctions. Alternatively one can use the basis of the eigenfunctions of

$$\vec{\mathbf{L}}^2, \vec{\mathbf{J}}^2, \mathbf{J}_z, \vec{\mathbf{S}}^2 \quad \text{(quantum numbers } l, j, m_j, s), \tag{2}$$

where $\vec{\mathbf{J}} = \vec{\mathbf{L}} + \vec{\mathbf{S}}$ is total angular momentum.

Evaluate the commutators of the operators in Eqs. (1) and (2) with the $\vec{\mathbf{L}} \cdot \vec{\mathbf{S}}$ term from $\mathbf{H}_{soc}$. You should find that the quantities (1) are not anymore conserved, but those in Eq. (2) are. *(2 Points)*

(ii) For the hydrogen atom, spin-orbit coupling can be described by

$$\mathbf{H}_{soc} = \frac{1}{2}\left(\frac{1}{m^2c^2}\right)\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{\vec{\mathbf{L}} \cdot \vec{\mathbf{S}}}{r^3}, \tag{3}$$

where $m$ and $e$ are the mass and the charge of the electron, and $c$ is the speed of light. Treat $\mathbf{H}_{soc}$ as the pertubation to $\mathbf{H}_0 = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$. Find the first-order pertubation-theory correction to the energies of the hydrogen eigenfunctions $|n, l, j, m_j\rangle$. *(5 Points)*

*Hint: You can use:*

$$\langle n, l | r^{-3} | n, l \rangle = \frac{1}{a_0^3} \frac{1}{n^3\, l(l+\frac{1}{2})(l+1)}, \tag{4}$$

*where* $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ *is the Bohr radius.*