

Homework sheet 3 – Due 03/02/2025

Problem 1: Compatible and incompatible observables, Dynamics of spin-1 system [1 + 2 + 2 + 1 + 2 + 2 = 10 points]

Consider a spin-1 using $|1, m\rangle$ as an orthonormal eigenbasis of \hat{L}^2, \hat{L}_z

$$|1, 1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1, 0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1, -1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

In this basis we introduce the Hamiltonian H and two further operators A, B

$$H = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad A = a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad B = b \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (\omega_0, a, b \in \mathbb{R}). \quad (1)$$

- a) Expand H in terms of \hat{L}_i, \hat{N}_{ij} and $\mathbf{1}_{3 \times 3}$, where \hat{N}_{ij} are quadrupole operators introduced on sheet 2, exercise 3.
- b) Show that H and A correspond to a complete set of compatible observables. Determine their shared eigenbasis and express H, A in this basis.
- c) Let the system be prepared in the state $|\psi_0\rangle = \frac{1}{\sqrt{2}} |1, 1\rangle + \frac{1}{2} |1, 0\rangle + \frac{1}{2} |1, -1\rangle$.
 - Determine the probabilities of the system being in angular momentum state $|1, 1\rangle, |1, 0\rangle, |1, -1\rangle$.
 - Determine the energy expectation value and standard deviation.
- d) Instead of measuring H we now measure A . Which results do you obtain with which probability?
- e) Calculate $|\psi(t)\rangle = e^{-iHt/\hbar} |\psi_0\rangle$ as well as expectation values $\langle A \rangle(t), \langle B \rangle(t)$. Are they both time dependent? If no, why?
- f) Determine the probability of measuring B in eigenvalue $-b$ at time t . Sketch your result.

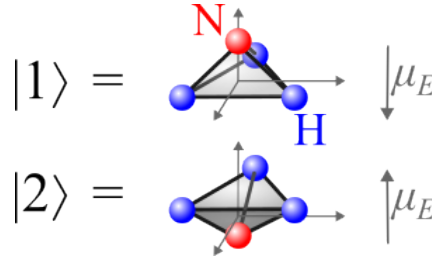


Figure 1: Graphical representation of the two most relevant quantum states of the Ammonia molecule. Since nitrogen is more electronegative than hydrogen, the squished tetrahedra have a net dipole moment.

Problem 2: Rabi oscillations in a circular field [2 + 5 + 3 = 10 points]

Consider a spin-1/2 particle in a magnetic field such that $|\uparrow\rangle$ has energy $\hbar\omega_0/2$ and $|\downarrow\rangle$ has energy $-\hbar\omega_0/2$. The system is initialized in the ground state.

At time t a magnetic field $B_1(\cos(\omega t), \sin(\omega t), 0)^T$ is switched on (as in the lecture course, use the notation $\omega_1 = g\mu_B B_1/\hbar$).

a) Write down the Hamiltonian in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis.

b) Find the time dependent wave function using the Ansatz $|\psi(t)\rangle = \begin{pmatrix} Ae^{-i(\Omega+\omega)t/2} \\ Be^{-i(\Omega-\omega)t/2} \end{pmatrix}$.

Hint: Use the notations $\nu = \sqrt{(\omega_0 - \omega)^2 + \omega_1^2}$ and $\theta = \arctan(\omega_1/[\omega_0 - \omega])$.

c) Calculate the time and θ dependent probability for the system to be in $|\uparrow\rangle$ state. What is the smallest field strength B_1 (i.e. smallest θ) to drive transitions from $|\downarrow\rangle$ to $|\uparrow\rangle$? What is the minimal time t needed to obtain such a transition?

Problem 3: Ammonia molecule and energy-time uncertainty [1 + 1 + 1 + 2 + 4 + 1 = 10 points]

The Ammonia molecule NH_3 has the shape of a flattened tetrahedron. While it has a multitude of quantum states (vibrational modes and quantum states of the electrons inside the molecule), the main, low lying states of relevance for this exercise are the two orientations of the tetrahedron (cf. Fig. 1):

$$|1\rangle = |\text{N above H-triangle}\rangle; |2\rangle = |\text{N below H-triangle}\rangle \quad (2)$$

The Hamiltonian in the basis $\{|1\rangle, |2\rangle\}$ is given by $\hat{H} = \hat{H}_0 + \delta\hat{H}$,

$$\hat{H}_0 = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix} \quad (3)$$

$$\delta\hat{H} = -\mathcal{E}\hat{\mu}_E. \quad (4)$$

Here \hat{H}_0 is the Hamiltonian in the absence of an external electric field \mathcal{E} and experimentally it is known that $0 < A \sim 10^{-4}eV$. The perturbation $\delta\hat{H}$ stems from an electric field \mathcal{E} coupling to the electric dipole operator

$$\hat{\mu}_E = -\mu_e \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mu_e > 0. \quad (5)$$

For problems a)-d) consider only \hat{H}_0 , i.e. the molecule in the absence of a field.

- a) Calculate the expectation value of \hat{H}_0 in the quantum state when the N atom resides above the H-triangle.
- b) Calculate the expectation value of the electric dipole operator $\hat{\mu}_E$ for the states $|1\rangle$ and $|2\rangle$.
- c) Determine eigenvalues and eigenstates of Eq. (3). Where is the nitrogen atom in the ground state: above or below the H-triangle? What is the ground state expectation value of a electric dipole operator?
- d) Assuming the system is initialized in the quantum state when the N atom resides above the H-triangle, calculate the probability $p_{\text{above}}(t)$ to find the N atom above the H triangle at time t . Similarly, calculate the time-dependent probability $p_{\text{below}}(t)$ to find N below the H triangle. Does the N atom stick to its initial position? Note that there is no force exerted on it!

Comment: Quantum mechanical particles can "tunnel" between different positions. We will get back to this at the very end of the lecture course (part III).

- e) Heisenberg-uncertainty for energy and time.

The Schrödinger equation relates $i\hbar\frac{d}{dt}$ to energy (i.e. the Hamiltonian \hat{H}).

- i) Show that $[i\hbar\frac{d}{dt}, t] = i\hbar$ by showing that for any state $|\psi(t)\rangle$

$$[i\hbar\frac{d}{dt}, t] |\psi(t)\rangle = i\hbar |\psi(t)\rangle. \quad (6)$$

Hint: Differential operators act on everything to their right. Use the chain rule.

ii) By analogy to the general Heisenberg uncertainty formula $\langle \Delta \hat{A}^2 \rangle \langle \Delta \hat{B}^2 \rangle \geq |\langle [A, B] \rangle|^2/4$ motivate the energy-time uncertainty relation

$$\Delta E \Delta t \geq \frac{\hbar}{2}, \quad (7)$$

where $\Delta E^2 = \langle \psi | (\hat{H} - \langle \hat{H} \rangle)^2 | \psi \rangle$ for given state $|\psi\rangle$.

Comment: The role of time in quantum mechanics is different from the role of observables – it is simply a parameter in the Schrödinger equation. In this sense, the notion of a Heisenberg uncertainty-relation for energy and time is conceptually distinct from the one for two non-commuting observables. The notion of uncertainty Δt is not defined in the same way as for operators. Instead, as we will do in iii), it can only be inferred indirectly from, e.g., the oscillation time.

iii) Compare the energy uncertainty in state $|1\rangle$ with the time period of one oscillation in $p_{\text{above}}(t)$ for time evolution initialized as $|\psi(0)\rangle = |1\rangle$?

iv) What is the energy uncertainty of the ground state? What is the time period for quantum oscillations $p_{\text{above}}(t), p_{\text{below}}(t)$ when the system is initialized in the ground state? Discuss the Heisenberg bound.

f) We now include the electric field \mathcal{E} and calculate the groundstate energy. Expand in \mathcal{E} and compare to the result for the ground state energy as obtained from perturbation theory.

Problem 4: Perturbation theory [5 + 5 = 10 points.]

Solve the Hamiltonian

$$\hat{H} = B \left[\hat{L}_z + \frac{\gamma}{\hbar} (\{\hat{L}_z, \hat{L}_y\} + \hat{L}_x^2) \right] \quad (8)$$

for $\hat{L}_{x,y,z}$ representing spin-3/2 particles perturbatively in γ .

Hint: Feel free to use Mathematica or other software.

a) Calculate eigenvalues to $\mathcal{O}(\gamma^2)$ and sketch the solution.

b) Calculate corrections to the eigenvectors to $\mathcal{O}(\gamma)$ keeping only the correction terms $|\psi^{(1)}\rangle$ which are orthogonal to unperturbed states $|\psi^{(0)}\rangle$. Does the particle in the ground state for $B > 0$ have non-vanishing probability to be in $m = 3/2, m = 1/2, m = -1/2$ states?