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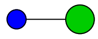
Problem 1: Electrical dipole transitions in polar molecules (Oral)

Learning objective

We derive selection rules for dipolar transitions in polar molecules and calculate transition matrix elements, using the Wigner-Eckart theorem.

Due to their asymmetric structure, heteronuclear molecules  have an electric dipole moment **d** along their symmetry axis. In this exercise, we are only concerned with the rotational degree of freedom of such molecules, which is described by the angular momentum **J**. The dynamics of such a "rigid rotor" is governed by $H_{\text{rot}} = B \cdot \mathbf{J}^2/\hbar^2$ (why? **spherically symmetrical, isotropic**). Thus, the states $|J, M\rangle$ are eigenstates of H_{rot} with energy $BJ(J+1)$ and degeneracy $2J+1$. The rotational constant $B/\hbar$ is typically of the order of the GHz. Consequently, it is possible to drive microwave transitions between different $|J, M\rangle$ states. In this exercise, we calculate the matrix elements of possible transitions. Electrical dipole transitions are only allowed if the matrix element $\langle J', M'|\,\mathbf{d}\,|J, M\rangle$ is different from zero.

a) First we describe the dipole operator **d** in a spherical basis with components d_q, where $q = 0, \pm 1$. The components are given by $d_0 = d\cos(\theta)$ and $d_\pm = \mp d\, e^{\pm i\phi}\sin(\theta)/\sqrt{2}$. They are proportional to spherical harmonics $d_q \propto Y_1^q$.

   Apply the Wigner-Eckart Theorem for the dipole matrix elements in the spherical representation $\langle J', M'|\, d_q\,|J, M\rangle$. What is the rank of the tensor d_q? Which selection rules for $\Delta J \equiv J' - J$ and $\Delta M \equiv M' - M$ can you derive directly from the Clebsch-Gordan coefficients?

b) Use a parity argument to show why $\Delta J = 0$ transitions are not allowed. To do this, use the above matrix elements and make use of the parity of the spherical harmonics involved.

c) We have now derived the selection rules $\Delta J = \pm 1$ with $\Delta M = q = 0, \pm 1$. We would like to simplify the dipole matrix elements. The Wigner-Eckart theorem allows us to choose q as well as M and M' freely to determine $\langle J'||d||J\rangle$. In order to do this, solve the equation for this term and choose $M = J$ and $q = 1$ to explicitely compute $\langle J+1||d||J\rangle$. How can you use this result to determine the matrix elements for $\Delta J = -1$?

   Hint: The appearing Clebsch-Gordan coefficient couples two "stretched states" (i.e. those states with $M = J$) to a final state which is also stretched. Think about a general property of such Clebsch-Gordan coefficient. The spherical harmonics for these states are given by equation

$$Y_J^J(\theta,\phi) = \frac{(-1)^J}{2^J J!}\sqrt{\frac{(2J+1)!}{4\pi}}\sin^J(\theta)e^{iJ\phi}.$$

   For odd n we have:

$$\int_0^\pi \mathrm{d}\theta\, \sin(\theta)^n = \frac{(\frac{n-1}{2})!(\frac{n+1}{2})!}{(n+1)!}2^{n+1}.$$

The final result for $\Delta J = +1$ should be

$$\langle J+1, M+q|\, d_q \,|J, M\rangle = d\sqrt{\frac{J+1}{2J+3}}\,\langle J, M; 1, q|J+1, M+q\rangle$$

d) As a simple application we consider a polar molecule in the ground state $|0,0\rangle$. First, compute the dipole moment for the ground state $\langle 00|\,\mathbf{d}\,|00\rangle$. A dipole moment can be induced by an external electric field $\mathbf{E} = E\mathbf{e_z}$ (static). To get an approximate value for this dipole moment, we treat the coupling of the dipole moment to the electric field $H_{\mathrm{E}} = -\mathbf{d}\cdot\mathbf{E} = -d_0 E$ as a perturbation (that is, $dE/B \ll 1$). Compute the induced dipole moment (component in z-direction) $\left\langle \widehat{00}\right| d_0 \left|\widehat{00}\right\rangle$ using the above matrix elements, where $\left|\widehat{00}\right\rangle$ stands for the ground state in first order perturbation theory.

Hint: The only appearing Clebsch-Gordan coefficient is again trivial in this case. What happens in general if one of the two angular momenta in the coupling is zero?

Problem 2: Squeezed states (Written)

Learning objective

In Problem Set 6, we studied coherent states. The quantum state of the harmonic oscillator, that minimizes the uncertainty relation with the uncertainty equally distributed between the non-commuting observables Q and P, is such a coherent state. In this exercise, we study *squeezed states*, for which the uncertainty of one of the observables is smaller than for the coherent state. To respect the uncertainty principle, the uncertainty of the other observable must be larger than for the coherent state. Squeezed states of light are an example of non-classical light.

For the harmonic oscillator with frequency ω, coherent states obey

$$\langle \Delta Q^2\rangle \;=\; \frac{\hbar}{2\omega} \quad \text{and} \quad \langle \Delta P^2\rangle \;=\; \frac{\hbar\omega}{2} \tag{1}$$

and thus squeezed states fulfill

$$\langle \Delta Q^2\rangle \;\leq\; \frac{\hbar}{2\omega} \quad \text{or} \quad \langle \Delta P^2\rangle \;\leq\; \frac{\hbar\omega}{2}\,. \tag{2}$$

We define the squeeze operator $S(\epsilon)$ as

$$S(\epsilon) = \exp\left(\frac{\epsilon^*}{2}\,a^2 - \frac{\epsilon}{2}\left(a^\dagger\right)^2\right)\,. \tag{3}$$

a) Write the operators Q and P in terms of the creation and annihilation operators of the harmonic oscillator and prove that coherent states satisfy equation (1).

b) Derive the following relations for $S(\epsilon)$ with $\epsilon = r\,\exp(i\phi)$, where r is an arbitrary radius and ϕ an arbitrary phase:

$$S^\dagger(\epsilon) \;=\; S^{-1}(\epsilon) = S(-\epsilon)\,, \tag{4}$$

$$S^\dagger(\epsilon)\;a\,S(\epsilon) \;=\; a\,\cosh(r) - a^\dagger\,e^{i\phi}\,\sinh(r)\,, \tag{5}$$

$$S^\dagger(\epsilon)\;a^\dagger\,S(\epsilon) \;=\; a^\dagger\,\cosh(r) - a\,e^{-i\phi}\,\sinh(r)\,. \tag{6}$$

c) Verify that the states $|\alpha\,,\,\epsilon\rangle = D(\alpha)\; S(\epsilon)\; |0\rangle$ are squeezed states. Here, $D(\alpha)$ is the displacement operator as introduced in Problem Set 6, Problem 3b).

Problem 3: Probability current in the presence of an electromagnetic field (Oral and Bonus)

Learning objective

We consider spinless particles in a classical electromagnetic field and derive the probability current.

In Gaussian units, the considered Hamiltonian reads in second quantization

$$H = H_{kin} + H_{ext} + H_{int} + H_{em}\ , \tag{7}$$

with the kinetic energy term in the presence of an electromagnetic field

$$H_{kin} = \frac{1}{2m}\int \mathrm{d}^3x\ \psi^\dagger(\mathbf{x})\left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)^2\psi(\mathbf{x})\ , \tag{8}$$

the interaction with an external potential

$$H_{ext} = \int \mathrm{d}^3x\ U(\mathbf{x})\psi^\dagger(\mathbf{x})\psi(\mathbf{x})\ , \tag{9}$$

the two-body interaction

$$H_{int} = \frac{1}{2}\int \mathrm{d}^3x\ \mathrm{d}^3y\ \psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{y})V(\mathbf{x}-\mathbf{y})\psi(\mathbf{y})\psi(\mathbf{x})\ , \tag{10}$$

and the energy of the electromagnetic field

$$H_{em} = \int \mathrm{d}^3x\ \frac{E_\perp^2 + B^2}{8\pi}\ . \tag{11}$$

Calculate the probability current. Start by calculating the time evolution of the particle density operator $\rho = \psi^\dagger(\mathbf{x})\psi(\mathbf{x})$, using the Heisenberg equation $\partial_t\rho = \frac{i}{\hbar}[H,\rho]$. Think about which terms of the Hamiltonian actually contribute to the commutator $[H,\rho]$ and use $[\psi(\mathbf{x}),\psi^\dagger(\mathbf{y})] = \delta(\mathbf{x}-\mathbf{y})$ to evaluate the remaining expressions. Bring the equation in the form of the continuity equation $\partial_t\rho + \nabla\mathbf{j} = 0$ and read off the probability current $\mathbf{j}$.