Excercises Angular Momentum Theory

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Excercise 1: Rotation, inversion, and reflection in $\mathbb{R}^3$

1a. The inversion operator is defined by

$$\hat{i}\boldsymbol{x} = -\boldsymbol{x}.$$

Give the matrix representation of $\hat{i}$ in $\mathbb{R}^3$.

1b. The operator $\hat{R}_x(\pi)$ is a rotation around the $\boldsymbol{x}$-axis over an angle of π radians. Give its matrix representation in $\mathbb{R}^3$.

1c. Also give the matrix representations of $\hat{R}_y(\pi)$ and $\hat{R}_z(\pi)$.

1d. The product of the inversion operator and any of these rotation operators gives a reflection. Multiply the matrix representation of the operators to determine which reflection planes correspond to $\hat{i}\hat{R}_x$, $\hat{i}\hat{R}_y$, and $\hat{i}\hat{R}_z$.

Excercise 2: One-photon transitions

The intensity of a one-photon transition from an initial state Ψ_i to a final state Ψ_f is proportional to the square of the matrix element

$$\mu_{fi} = \langle \Psi_f | \boldsymbol{e} \cdot \boldsymbol{\mu} | \Psi_i \rangle$$

where $\boldsymbol{e}$ is the polarization vector of the light and $\boldsymbol{\mu}$ is the dipole operator. The dipole operator in a space fixed frame is defined by

$$\boldsymbol{\mu}^{SF} = \sum_i q_i \boldsymbol{r}_i^{SF},$$

where i runs over all electrons and nuclei of the molecule, q_i are the charges and $\boldsymbol{r}_i$ are the coordinates of the particles. The space-fixed spherical components of the dipole operator are defined by

$$\mu_m^{SF} = R_{1,m}(\boldsymbol{\mu}^{SF}), \quad m = 1, 0, -1$$

where $R_{1,m}$ are regular harmonics of rank 1.

A body-fixed frame $\boldsymbol{R}(\alpha, \beta, \gamma)$ relates body-fixed (BF) and space-fixed coordinates through

$$\boldsymbol{r}^{SF} = \boldsymbol{R}(\alpha, \beta, \gamma)\boldsymbol{r}^{BF},$$

where α, β, and γ are zyz-Euler angles.

A body-fixed frame can be defined for a diatomic molecule by taking β, and α to be the polar angles of the diatomic axis and setting $\gamma = 0$.

The body-fixed components of the dipole operator are also defined by

$$\boldsymbol{\mu}^{SF} = \boldsymbol{R}(\alpha, \beta, \gamma)\boldsymbol{\mu}^{BF}$$

2a. Substitute this expression for $\boldsymbol{\mu}^{SF}$ into the definition of the spherical components μ_m^{SF}.

2b. Use Wigner's convention to move the rotation matrix $\boldsymbol{R}(\alpha, \beta, 0)$ out of the argument of the rank-1 regular harmonics.

2c. Use the rotational properties of the regular harmonics to write the result as a sum over products of rotation matrices and the body-fixed spherical components of the dipole operator

$$\mu_m^{BF} \equiv R_{1,m}(\boldsymbol{\mu}^{BF})$$

Electronic-rotational wave funcions of diatomic molecules may be written as

$$|LM\rangle = \Phi_{electronic}^{BF} Y_{LM}(\beta, \alpha)$$

2d. Compute the matrix elements

$$\mu_{L_1 M_1; L_2 M_2} = \langle L_1 M_1 | \mu_m^{SF} | L_2 M_2 \rangle$$

2e. Use the symmetry properties of Clebsch-Gordan coefficients to determine the rotational selectrion rules for one-photon transitions induced by linearly polarized light (only e_0^{SF} is nonzero, so transitions are determined by matrix elements of μ_0^{SF})

2f. Idem for circularly polarized light.