QTC, NWI-MOL112, exercises week 6

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Question 1: Two-fold symmetry in 1-D

The derivative operator has odd parity. If we define

$$y = -x \tag{1}$$

then

$$\frac{\partial}{\partial y} = \frac{\partial x}{\partial y}\frac{\partial}{\partial x} = -\frac{\partial}{\partial x}. \tag{2}$$

More formal we could write

$$\hat{\imath}\frac{\partial}{\partial x}\hat{\imath}^\dagger = -\frac{\partial}{\partial x}, \tag{3}$$

where $\hat{\imath}$ is the inversion operator defined by

$$\hat{\imath}x\hat{\imath}^\dagger = -x. \tag{4}$$

1a. Show that Eq. (3) is correct by applying it to an arbitrary function $f(x)$.

1b. What is the parity of the linear momentum operator $\hat{p}_x$?

The kinetic energy operator in 1-D is given by

$$\hat{T} = -\frac{\hat{p}^2}{2\mu}.$$

1c. What is the parity of this kinetic energy operator?

The 1-D harmonic oscillator is given by

$$\hat{H} = \hat{T} + V(x) = -\frac{\hat{p}^2}{2\mu} + \frac{1}{2}kx^2.$$

1d. Show that this Hamiltonian commutes with $\hat{\imath}$.

1e. What is the parity of Hermite polynomial $H_0(x)$ (see exercise first week)

1f. What is the parity of Hermite polynomial $H_1(x)$?

1g. Use the recursion relation for Hermite polynomials to find the parity of $H_n(x)$ for $n = 0, 1, 2, \ldots$.

1h. What is the parity of harmonic oscillator eigenfunction $\phi_n(x)$, for $n = 0, 1, \ldots$?

1i. What is the parity of Legendre polynomial $P_L(z)$, for $L = 0, 1, 2, \ldots$? (Use the recursion relations in Chapter 8).

Question 2: Parity of spherical harmonics

In 3D, the inversion operator is defined by

$$\hat{\imath}\boldsymbol{r}\hat{\imath}^\dagger = -\boldsymbol{r}. \tag{5}$$

2a. What is the parity of the linear momentum operator in 3D, $\hat{\boldsymbol{p}}$?

2b. What is the parity of angular momentum operator $\hat{\boldsymbol{l}}$?

2c. Derive the transformation of spherical polar angles (θ, ϕ) under inversion,

$$\hat{\imath}\theta\hat{\imath}^\dagger = \pi - \theta \tag{6}$$
$$\hat{\imath}\phi\hat{\imath}^\dagger = \phi + \pi. \tag{7}$$

2d. What is the parity of the Racah normalized spherical harmonic $C_{L,0}(\theta, \phi)$? (Use the result for the Legendre polynomials).

2e. What is the parity of angular momentum ladder operators $\hat{l}_\pm$?

2f. Show that the parity of Racah normalized spherical harmonic $C_{L,M}(\theta,\phi)$ is the same as the parity of $C_{L,0}(\theta,\phi)$?

2g. What is the parity of spherical harmonic $Y_{j,m_j}(\theta,\phi)$?

The space-fixed z-component of the dipole operator for a diatomic molecule is

$$\hat{\mu}_z = \mu_0(r)\cos\theta,$$

where θ is the angle between the Jacobi vector of $\boldsymbol{r}$ of the diatomic molecule and the z-axis, and $\mu_0(r)$ is the dipole moment in the molecule fixed frame as a function of the distance r between the two atoms.

2h. Compute the expectation value of the dipole operator for a diatomic molecule with rotational wave function $Y_{jm_j}(\theta,\phi)$,

$$\mu_z = \langle jm_j|\hat{\mu}_z|jm_j\rangle.$$

(Hint: use the parity of the operator and of the rotational wave function.)

The *transition dipole moment* between two rotational states is defined by

$$\mu_{f,i} = \langle j_f m_f|\hat{\mu}_z|j_i m_i\rangle, \tag{8}$$

where j_i and m_i are the rotational quantum numbers of the initial state, and j_f and m_f are the rotational quantum numbers of the final state.

2i. Give the selection rule for this matrix element derived from considering inversion symmetry

2j. Use Eq. (8.50) of the lecture notes, to show that the transition dipole moment between two rotational wave functions is zero when $|j_i - j_f| > 1$.

2k. The most abundant molecule in the universe is H_2. Why is it so hard for astromers to observe rotational transitions in H_2?

The coupled angular momentum wave function for an atom-homonuclear diatom system H_2-He is denoted by $|(jl)JM\rangle$, where j is the rotational quantum number for the diatom, l is associated with the rotation on the atom around the center-of-mass, and J and M are the total angular momentum quantum numbers (see Chapter 8).

2l. Find the expression for the parity of the wave function, i.e., evaluate

$$\hat{\imath}|(jl)JM\rangle = ?$$

2m. The operator $\hat{P}_{1,2}$ permutes the two hydrogen atoms. What is the eigenvalue of $|(jl)JM\rangle$ with respect to this operators? In other words, evaluate

$$\hat{P}_{1,2}|(jl)JM\rangle$$

2n. What is the speedup in a variational calculation when both inversion and permutation symmetry are used?

Question 3: Matrix representations of symmetry operators in $\mathbb{R}^3$

3a. Find the 3×3 matix representation $\boldsymbol{E}$ of the inversion operator $\hat{\imath}$ defined by

$$\hat{\imath}\boldsymbol{r} = -\boldsymbol{r},$$

where $\boldsymbol{r}$ is a column vector with three elements. In other words, find the matrix $\boldsymbol{E}$ such that

$$\boldsymbol{E}\boldsymbol{r} = -\boldsymbol{r}.$$

3b. Find the matrix representation $\boldsymbol{S}_{xz}$ of $\hat{\sigma}_{xz}$, reflection in the xz-plane.

The reflection operator can be written as the product of inversion and rotation. For the matrix representation we can write:

$$\boldsymbol{S}_{xz} = \boldsymbol{I}\boldsymbol{E}.$$

3c. Find the rotation matrix $\boldsymbol{R}$.

The matrix $\boldsymbol{R}$ represents some rotation around a vector $\hat{\boldsymbol{n}}$ over an angle ϕ: $\hat{R}(\hat{\boldsymbol{n}},\phi)$.

3d. Determine the vector $\hat{\boldsymbol{n}}$ and the angle ϕ.