Question 1: Two-fold symmetry in 1-D

The derivative operator has odd parity. If we define

\[ y = -x \]  

then

\[ \frac{\partial}{\partial y} = \frac{\partial x}{\partial y} \frac{\partial}{\partial x} = -\frac{\partial}{\partial x}. \]  

More formal we could write

\[ \hat{i} \frac{\partial}{\partial x} \hat{i} = -\frac{\partial}{\partial x}, \]  

where \( \hat{i} \) is the inversion operator defined by

\[ \hat{i} x \hat{i} = -x. \]  

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

Answer: First, we define

\[ y \equiv -x \]  

\[ g(x) \equiv \hat{i} f(x) = f(\hat{i}x) = f(-x) = f(y), \]  

so

\[ \frac{\partial}{\partial x} g(x) = \frac{\partial x}{\partial y} \frac{\partial}{\partial y} f(y) = -f'(y) = f'(-x). \]  

and

\[ \hat{i} \frac{\partial}{\partial x} \hat{i} f(x) = \hat{i} \frac{\partial}{\partial x} g(x) = \hat{i} g'(x) = g'(\hat{i}x) = g'(-x) = -f'(x) \]  

so for any function \( f \),

\[ \hat{i} \frac{\partial}{\partial x} \hat{i} f = -\frac{\partial}{\partial x} f. \]  

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

Answer: \[ \hat{i} \hat{p}_x \hat{i} = \frac{\hbar}{i} \frac{\partial}{\partial x} \hat{i} = -\frac{\hbar}{i} \frac{\partial}{\partial x} = -\hat{p}_x \]  

so \( \hat{p}_x \) has odd parity.

The kinetic energy operator in 1-D is given by

\[ \hat{T} = \frac{\hat{p}_x^2}{2\mu}, \]  

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

Answer: \[ \hat{i} \hat{T} \hat{i} = -\frac{1}{2\mu} \hat{i} \hat{p}_x \hat{i} \hat{i} \hat{p}_x \hat{i} = -\frac{1}{2\mu} \hat{i} \hat{p}_x \hat{i} \hat{p}_x \hat{i} = -\frac{1}{2\mu} \hat{p}_x^2 = \hat{T}, \]  

so \( \hat{T} \) is invariant under inversion (even).
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 \( \hat{i} \).

**Answer:** From the transformation properties of \( x \) and \( \hat{p} \) in the previous question we have:

\[ \hat{i}x = -x\hat{i} \quad (14) \]
\[ \hat{i}\hat{p} = -\hat{p}\hat{i} \quad (15) \]

so we find

\[ \hat{i}x^2 = -ix^2 = x^2\hat{i} \quad (16) \]
\[ \hat{i}\hat{p}^2 = -\hat{p}^2\hat{i} \quad (17) \]

from which we get the commutators

\[ [\hat{i}, x^2] = 0 \quad (18) \]
\[ [\hat{i}, \hat{p}^2] = 0 \quad (19) \]

and so

\[ [\hat{i}, \hat{H}] = -\frac{1}{2\mu}[\hat{i}, \hat{p}^2] + \frac{1}{2}k[\hat{i}, x^2] = 0. \quad (20) \]

For the kinetic energy part we could also have used the result of the previous question.

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

**Answer:** Hermite polynomial \( H_0(x) = 1 \) has even parity.

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

**Answer:** Hermite polynomial \( H_1(x) = x \) has odd parity

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

**Answer:** The recursion relation is

\[ H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (21) \]

For \( n \leq 1 \) we found already that the parity is even if \( n \) is even and odd when \( n \) is odd. In the rhs of the recursion we see that if \( n \) is odd, the term with \( xH_n \) is even, and so is the term with \( H_{n-1} \), and hence \( H_{n+1} \) will also be even. If \( n \) is even we see that \( H_{n+1} \) will be odd.

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

**Answer:** The harmonic oscillator function \( \phi_n(x) \) is, apart from a normalization constant and a scaling of the coordinate equation to a Hermite polynomial times a Gaussian. The Gaussian \( e^{-x^2/2} \) is even, so \( \phi_n \) has the same parity as the Hermite polynomial \( H_n \), i.e., even for even \( n \) and odd for odd \( n \).

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

**Answer:** The parity of Legendre polynomial \( P_L \) is \((-1)^L\), i.e., even for even \( L \) and odd for odd \( L \). The derivation is analogous to the derivation of the parity of Hermite polynomials.
Question 2: Parity of spherical harmonics

In 3D, the inversion operator is defined by

$$\hat{r}i\hat{r}^\dagger = -\hat{r}.$$  \hspace{1cm} (22)

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

Answer: The transformation properties of the $y$ and $z$ component of $\hat{p}$ are the same as for the $x$ component, so

$$\hat{i}\hat{p}i^\dagger = -\hat{p}.$$ \hspace{1cm} (23)

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

Answer: First consider the $x$ component:

$$\hat{l}_x = y\hat{p}_z - z\hat{p}_y.$$ \hspace{1cm} (24)

Since both $y$ and $\hat{p}_z$ are odd, their product is even, and also $z\hat{p}_y$ is even, so $\hat{l}_x$ is even, and the other components can be shown to be even in the same way.

2c. Derive the transformation of spherical polar angles $(\theta, \phi)$ under inversion,

$$\hat{i}\theta i^\dagger = \pi - \theta$$

$$\hat{i}\phi i^\dagger = \phi + \pi.$$ \hspace{1cm} (25) \hspace{1cm} (26)

Answer: The spherical polar coordinates are defined by

$$r = r \begin{pmatrix} \cos \phi \sin \theta \\ \sin \phi \sin \theta \\ \cos \theta \end{pmatrix}.$$ \hspace{1cm} (27)

Inversion of $r$ gives

$$\hat{r}i\hat{r}^\dagger = -\hat{r}.$$ \hspace{1cm} (28)

First, consider the $z = r \cos \theta$ component. It must change sign when $\theta$ is transformed, but also, the range of $\theta$ must remain $[0, \pi]$, so we must have $\hat{i}\theta i^\dagger = \pi - \theta$, since $\cos(\pi - \theta) = -\cos \theta$. This transformation leaves $\sin \theta$ invariant, since $\sin(\pi - \theta) = \sin \theta$, so for the $x = r \cos \phi \sin \theta$ and $y = r \sin \phi \sin \theta$ to change sign, both $\cos \phi$ and $\sin \phi$ must change sign, which require $\hat{i}\phi i^\dagger = \phi + \pi$. Strictly speaking, since $\phi + \pi$ may be out of the range $[0, 2\pi]$, we should take the result modulo $2\pi$.

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

Answer: We can use

$$C_{L,0}(\theta, \phi) = P_L(\cos \theta),$$ \hspace{1cm} (29)

and the parity of Legendre polynomials $P_L$ is $(-1)^L$, so the transformed Racah normalized spherical harmonic is

$$\hat{i}C_{L,0}(\theta, \phi) = C_{L,0}(\pi - \theta, \phi + \pi)$$ \hspace{1cm} (30)

$$= P_L[\cos(\pi - \theta)]$$ \hspace{1cm} (31)

$$= P_L(\cos \theta)$$ \hspace{1cm} (32)

$$= (-1)^LP_L(\cos \theta)$$ \hspace{1cm} (33)

$$= (-1)^LC_{L,0}(\theta, \phi),$$ \hspace{1cm} (34)

so the parity of $C_{L,0}$ is $(-1)^L$ (even for even $L$, and odd for odd $L$).
2e. What is the parity of angular momentum ladder operators \( \hat{l}_\pm \)?

Answer: Angular momentum operators are invariant under inversion (see question 2b) and since \( \hat{l}_\pm = \hat{l}_z \pm i\hat{l}_y \), ladder operators are also invariant under inversion, i.e., they have even parity.

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

Answer: The ladder operator changes the \( M \) quantum number, e.g.,
\[
\hat{l}_+ C_{L,0}(\theta, \phi) = \hbar \sqrt{L(L+1) - M(M+1)} C_{L,1}(\theta, \phi)
\]
Since \( \hat{l}_+ \) is even, the parity of \( C_{L,1} \) is the same as the parity of \( C_{L,0} \). By repeatedly applying \( \hat{l}_+ \) or \( \hat{l}_- \), we can show that the \( M \) quantum number does not affect the parity, and the parity of \( C_{LM} \) is the same as for \( C_{L,0} \), i.e., \((-1)^L\).

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

Answer: Since normalization constants are invariant under inversion, the parity of spherical harmonics is the same as for Racah normalized spherical harmonics, i.e., \((-1)^j\).

The space-fixed \( z \)-component of the dipole operator for a diatomic molecule is
\[
\mu_z = \mu_0(r) \cos \theta,
\]
where \( \theta \) is the angle between the Jacobi vector of \( r \) 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.)

Answer: The dipole operator has odd parity, so
\[
\mu_z = \langle jm_j|\hat{\mu}_z|jm_j \rangle = \langle jm_j|\hat{i}^\dagger \hat{\mu}_z \hat{i}|jm_j \rangle = -\langle jm_j|\hat{i}^\dagger \hat{\mu}_z \hat{i}|jm_j \rangle
\]
We furthermore use the parity of spherical harmonics
\[
\hat{i}|jm_j \rangle = (-1)^l|jm_j \rangle.
\]
By taking the Hermitian conjugate on both sides of this equation, we also have
\[
\langle jm_j|\hat{i}^\dagger = (-1)^l \langle jm_j|
\]
so if we use Eqs. (39) and (40) in Eq. (38) we get
\[
\mu_z = -(-1)^l (-1)^l \langle jm_j|\hat{\mu}_z|jm_j \rangle = -\mu_z,
\]
so \( \mu_z = 0 \).

The transition dipole moment between two rotational states is defined by
\[
\mu_{f,i} = \langle j_f m_f |\mu_z| j_i m_i \rangle,
\]
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
Answer: Since the dipole operator is odd, the parity of initial and final state must be different, i.e., \( j_f - j_i \) must be odd.

2j. The most abundant molecule in the universe is \( \text{H}_2 \). Why is it so hard for astromers to observe rotational transitions in \( \text{H}_2 \)?

Answer: Electric dipole allowed transitions require the rotational quantum number to change by 1. However, \( \text{H}_2 \) is a homo-nuclear diatom, and the nuclear spin of a hydrogen atom is a half, so the rotational state can only go from odd to even if the nuclear wave function goes from odd to even. Since the coupling of the electric field to the nuclear spin is negligible, electric dipole transitions are forbidden. There are other mechanisms, electric quadrupole transitions, or magnetic dipole transitions, but they have an extremely low intensity.

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

Answer: The dipole operator is proportional to \( \cos \theta \), i.e., \( P_1(\cos \theta) \), or \( C_1,0(\cos \theta, \phi) \), so the matrix element of the dipole operator between to rotational states is a special case of Eq. (8.50) (see question 2i of week 5)

\[
\langle j_f m_f | C_{1,0} | j_i m_i \rangle = \sqrt{\frac{2 j_i + 1}{2 j_f + 1}} \langle 1, 0, j_i, m_i | j_f, m_f \rangle \langle 1, 0, j_i, 0 | j_f, 0 \rangle. \quad (43)
\]

The triangular conditions of Clebsch-Gordan coefficients require \( |j_i - j_f| \leq 1 \). The first Clebsch-Gordan coefficient on the rhs gives another selection rule: \( m_i = m_f \), this is because we only considered the \( z \) component of the dipole operator, which corresponds to light linearly polarized along the \( z \)-axis. The second Clebsch-Gordan coefficient, for which all the projection quantum numbers are zero, can only be nonzero when the sum of the angular momentum quantum numbers is even, i.e., when \( 1 + j_i + j_f \) is even. This gives the selection rule that \( j_i - j_f \) must be odd.

2l. Find the expression for the parity of the wave function, i.e., evaluate \( \hat{i} |(j)JM\rangle =? \)

Answer: We can write the coupled state as a linear combination of the uncoupled spherical harmonics \( |jm_j\rangle \) and \( |lm_l\rangle \), which have parities \((-1)^j \) and \((-1)^l \), respectively so

\[
\hat{i} |(j)JM\rangle = (-1)^{j+l} |(j)JM\rangle. \quad (44)
\]

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

\[
\hat{P}_{1,2} |(j)JM\rangle
\]

Answer: Since the wave function \( |(j)JM\rangle \) does not contain the nuclear spin part, we only get the rotational contribution from the permutation symmetry:

\[
\hat{P}_{1,2} |(j)JM\rangle = (-1)^j |(j)JM\rangle \quad (45)
\]

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 $3 \times 3$ matrix representation $E$ of the inversion operator $\hat{i}$ defined by

$$\hat{i} \mathbf{r} = -\mathbf{r},$$

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

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

Answer: The first column of the matrix representation is the image of the first basis vector, etc., so

$$E = \begin{bmatrix} i & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -i \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}. \quad (46)$$

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

Answer: Only the $y$-vector changes sign upon reflection in the $xz$-plane, so

$$S_{xz} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (47)$$

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

$$S_{xz} = RE.$$  

3c. Find the rotation matrix $R$.

Answer: 

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = R \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad (48)$$

so

$$R = S_{xz}E^{-1} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (49)$$

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

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

Answer: The $y$-basis vector is invariant, so this must be the rotation axis

$$\hat{n} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad (50)$$

and the $x$- and $z$-basis vectors change sign, so the angle must be $\phi = \pi$.  

Page 6 of 6