

1 Problem Set 7: Quantum Operators

1. Hermitian momentum operator

Show that the momentum operator is Hermitian.

The momentum operator can be expressed (in position basis) as

$$\hat{p} = i\hbar \frac{d}{dx} \quad (1)$$

Our task is to show that ¹

$$\langle \Psi' | \hat{p} | \Psi \rangle = \langle \Psi' | \hat{p} \Psi \rangle = \langle \hat{p} \Psi' | \Psi \rangle \quad (2)$$

Expanding operator application on ket,

$$\langle \Psi' | \hat{p} \Psi \rangle = \langle \Psi' | -i\hbar \frac{d\Psi}{dx} \rangle = \int_{-\infty}^{\infty} \Psi'^* \left(-i\hbar \frac{d\Psi}{dx} \right) dx \quad (3)$$

Expanding operator application on bra (dual vector),

$$\langle \hat{p} \Psi' | \Psi \rangle = \langle -i\hbar \frac{d\Psi'}{dx} | \Psi \rangle = \int_{-\infty}^{\infty} \Psi \left(i\hbar \frac{d\Psi'}{dx} \right) dx \quad (4)$$

Integration of parts gives us

$$\int_{-\infty}^{\infty} \Psi \left(i\hbar \frac{d\Psi'}{dx} \right) dx = i\hbar \left(\Psi \Psi' \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \Psi' \frac{d\Psi}{dx} dx \right) \quad (5)$$

where, of course, normalizability dictates that the wavefunctions must vanish at infinity. Inserting the constants back in to the integral, we get

$$\langle \hat{p} \Psi' | \Psi \rangle = \int_{-\infty}^{\infty} \Psi' \left(-i\hbar \frac{d\Psi}{dx} \right) dx \quad (6)$$

This is exactly the expression at Eq. (3). Hence, we see that

$$\langle \Psi' | \hat{p} \Psi \rangle = \langle \hat{p} \Psi' | \Psi \rangle \quad (7)$$

thus proving that the momentum operator is Hermitian. \square

¹Griffiths claimed that an equivalent proof is to use $\Psi' = \Psi$.

2. Hermitian Hamiltonian operator

Show that the Hamiltonian operator is Hermitian (potential is real).

The Hamiltonian operator can be expressed (in position basis) as

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(x) \quad (8)$$

Our task is to show that

$$\langle\Psi'|\hat{H}|\Psi\rangle = \langle\Psi'|\hat{H}\Psi\rangle = \langle\hat{H}\Psi'|\Psi\rangle \quad (9)$$

Operator application on bra gives us

$$\int_{-\infty}^{\infty} \Psi \left(-\frac{\hbar^2}{2m}\nabla^2\Psi' + V\Psi' \right)^* d\vec{r} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Psi \nabla^2\Psi'^* d\vec{r} + \int_{-\infty}^{\infty} \Psi V\Psi'^* d\vec{r} \quad (10)$$

Our task is to prove that we can switch the roles of Ψ' and Ψ'^* for the operator to be Hermitian. Observe that the second integral only has commuting scalar terms since potential is real. Hence, our only task is to prove the interchange of roles in the first integral. In cartesian coordinates, Laplacian is a linear combination of three spatial derivatives. If q_i is a cartesian coordinate,

$$-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Psi \sum_{i=1}^3 \frac{d^2\Psi'^*}{dq_i^2} d\vec{r} = -\frac{\hbar^2}{2m} \sum_{i=1}^3 \int_{-\infty}^{\infty} \Psi \frac{d^2\Psi'^*}{dq_i^2} d\vec{r} \quad (11)$$

By integration by parts similar to Eq. (5), the boundaries vanish and this gives us

$$-\frac{\hbar^2}{2m} \sum_{i=1}^3 \int_{-\infty}^{\infty} \Psi'^* \frac{d^2\Psi}{dq_i^2} d\vec{r} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Psi'^* \sum_{i=1}^3 \frac{d^2\Psi}{dq_i^2} d\vec{r} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Psi'^* \nabla^2\Psi d\vec{r} \quad (12)$$

We see that the roles of Ψ and Ψ'^* have been switched. Explicitly, the following equality holds

$$-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Psi \nabla^2\Psi'^* d\vec{r} + \int_{-\infty}^{\infty} \Psi V\Psi'^* d\vec{r} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Psi'^* \nabla^2\Psi d\vec{r} + \int_{-\infty}^{\infty} \Psi'^* V\Psi d\vec{r} \quad (13)$$

or

$$\langle\Psi'|\hat{H}\Psi\rangle = \langle\hat{H}\Psi'|\Psi\rangle \quad (14)$$

thus proving that the Hamiltonian operator, \hat{H} , is Hermitian. \square

3. Position and momentum operator in SHO basis

Find the matrix representation of position and momentum using harmonic oscillator orthonormal eigenfunction basis.

Recall that we have defined the raising and lowering ladder operators as

$$\hat{a}_+ = \sqrt{n+1}\Psi_{n+1} \quad \hat{a}_- = \sqrt{n}\Psi_{n-1} \quad (15)$$

where we can express the position and momentum operator as

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-) \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-) \quad (16)$$

Expressing it this way gives us the ticket to exploit orthonormality. Let $|n\rangle$ be the eigenfunction of Hamiltonian in an SHO potential that is expressible as

$$n(\xi) = \frac{m\omega^{1/4}}{\pi\hbar} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}; \quad \xi := \sqrt{\frac{m\omega}{\hbar}} x \quad (17)$$

We can find a closed form expression to generate the elements of the matrix representation in this basis. Denoting n' to be the n' 'th row and n to be the n th column, the matrix representation of ladder operators can be expressed as

$$\langle n | \hat{a}_+ | n' \rangle \quad \langle n | \hat{a}_- | n' \rangle \quad (18)$$

For the raising operator, the matrix elements can be expressed as

$$\langle n | \hat{a}_+ | n' \rangle = \sqrt{n'+1} \langle n | n'+1 \rangle = \sqrt{n'+1} \delta_{n(n'+1)} \quad (19)$$

For the lowering operator, the matrix elements can be expressed as

$$\langle n | \hat{a}_- | n' \rangle = \sqrt{n'} \langle n | n'-1 \rangle = \sqrt{n'} \delta_{n(n'-1)} \quad (20)$$

Note that n and n' must begin at the ground ($n, n'=0$) state. For convenience, we set the upperleft-most entry of the matrix to be the 0,0th entry. Hence, in matrix form, the ladder operators can be expressed as

$$\hat{a}_+ = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad \hat{a}_- = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad (21)$$

With these, one can easily express the position and momentum operator in matrix form

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(\begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} + \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \right) \quad (22)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad (23)$$

Similarly for momentum,

$$\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} \left(\begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} - \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \right) \quad (24)$$

$$= i\sqrt{\frac{\hbar m\omega}{2}} \begin{bmatrix} 0 & -\sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad (25)$$

More compactly (and completely), the matrix elements of position and momentum can be expressed as

$$x_{nn'} = \sqrt{\frac{\hbar(n'+1)}{2m\omega}} \delta_{n(n'+1)} + \sqrt{\frac{\hbar(n')}{2m\omega}} \delta_{n(n'-1)} \quad (26)$$

$$p_{nn'} = i\sqrt{\frac{\hbar m\omega(n'+1)}{2}} \delta_{n(n'+1)} - i\sqrt{\frac{\hbar m\omega(n')}{2}} \delta_{n(n'-1)} \quad (27)$$

4. Angular momentum in spherical harmonics basis

Find the matrix representation of y-component of angular momentum using spherical harmonics as basis.

We are tasked to express the y component of angular momentum using $m = -1, 0, 1$ spherical harmonics. To maintain the notion of ascending and descending the ladder using ladder operators and for convenience, we define the spherical harmonics as

$$|-1\rangle = |Y_1^{-1}\rangle \quad |0\rangle = |Y_1^0\rangle \quad |1\rangle = |Y_1^1\rangle \quad (28)$$

The ladder relations are expressed as

$$\hat{L}_+ |m\rangle = \hbar \sqrt{(l-m)(l+m+1)} |m+1\rangle \quad (29)$$

$$\hat{L}_- |m\rangle = \hbar \sqrt{(l+m)(l-m+1)} |m-1\rangle \quad (30)$$

With the given basis, we fix the value of l at $l = 1$. Then,

$$\hat{L}_+ |m\rangle = \hbar \sqrt{(1-m)(m+2)} |m+1\rangle \quad (31)$$

$$\hat{L}_- |m\rangle = \hbar \sqrt{(1+m)(-m+2)} |m-1\rangle \quad (32)$$

Recall that we can express that y-component of angular momentum in terms of ladders as

$$\hat{L}_y = \frac{1}{2i}(L_+ - L_-) \quad (33)$$

A three element basis set of spherical harmonics implies that we are dealing with a three-dimensional operator - a 3x3 square matrix. We define the matrix elements to have -1 as the lowest index of the matrix (upperleft-most has index $(-1, -1)$). Then, taking the matrix elements of the ladder operators

$$\langle m | \hat{L}_+ | m' \rangle = \hbar \sqrt{(1-m')(m'+2)} \langle m | m' + 1 \rangle = \hbar \sqrt{(1-m')(m'+2)} \delta_{m(m'+1)} \quad (34)$$

$$\langle m | \hat{L}_- | m' \rangle = \hbar \sqrt{(1+m')(-m'+2)} \langle m | m' - 1 \rangle = \hbar \sqrt{(1+m')(-m'+2)} \delta_{m(m'-1)} \quad (35)$$

Defining ordered tuples $\alpha = (m, m' + 1)$ and $\beta = (m, m' - 1)$, orthonormality tells us that the only non-zero entries are $\alpha = (0, 0)$ where $m = 0, m' = -1$ and $\alpha = (1, 1)$ where $m = 1, m' = 0$ for \hat{L}_+ and $\beta = (-1, -1)$ where $m = -1, m' = 0$ and $\beta = (0, 0)$ where $m = 0, m' = 1$ for \hat{L}_- . This gives us the matrix representations

$$\hat{L}_+ = \hbar \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix} \quad \hat{L}_- = \hbar \begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix} \quad (36)$$

From these, we can construct \hat{L}_y as

$$\hat{L}_y = \frac{1}{2i}(L_+ - L_-) = \frac{\hbar}{2i} \left(\begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix} - \begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix} \right) \quad (37)$$

or

$$\boxed{\hat{L}_y = \frac{\hbar}{2i} \begin{bmatrix} 0 & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}} \quad (38)$$

5. Spin in \hat{S}_z eigenspinor basis

Find the matrix representation of the y-component of spin using the spinor basis.

We are tasked to find the matrix representation of the y-component of spin using a two-dimensional spinor basis expressed as

$$\chi_+ = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \chi_- = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (39)$$

For spin, we have the following ladder operator relations

$$S_+ \chi_- = \hbar \chi_+ \quad (40)$$

$$S_- \chi_+ = \hbar \chi_- \quad (41)$$

$$S_+ \chi_+ = S_- \chi_- = 0 \quad (42)$$

Here, we have an additional condition for being eliminated at Eq. (42) we shall name as "overflow" condition. Finding the matrix representation of the ladder operators can be executed directly

$$\hat{S}_+ = \begin{bmatrix} \langle \chi_+ | \hat{S}_+ | \chi_+ \rangle & \langle \chi_+ | \hat{S}_+ | \chi_- \rangle \\ \langle \chi_- | \hat{S}_+ | \chi_+ \rangle & \langle \chi_- | \hat{S}_+ | \chi_- \rangle \end{bmatrix} \quad \hat{S}_- = \begin{bmatrix} \langle \chi_+ | \hat{S}_- | \chi_+ \rangle & \langle \chi_+ | \hat{S}_- | \chi_- \rangle \\ \langle \chi_- | \hat{S}_- | \chi_+ \rangle & \langle \chi_- | \hat{S}_- | \chi_- \rangle \end{bmatrix} \quad (43)$$

Due to orthonormality and overflow, three elements in each matrix gets reduced to zero. Hence.

$$\hat{S}_+ = \begin{bmatrix} 0 & \hbar \\ 0 & 0 \end{bmatrix} \quad \hat{S}_- = \begin{bmatrix} 0 & 0 \\ \hbar & 0 \end{bmatrix} \quad (44)$$

Expressing the y-component of spin as

$$\hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-) \quad (45)$$

we have

$$\hat{S}_y = \frac{1}{2i} \left(\begin{bmatrix} 0 & \hbar \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ \hbar & 0 \end{bmatrix} \right) \quad (46)$$

Hence, the matrix representation of the y-component of spin is

$$\boxed{\hat{S}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}} \quad (47)$$

Then, the possible values (eigenvalues) of S_y can be obtained from the characteristic polynomial

$$\lambda^2 - \frac{\hbar^2}{4} = 0 \iff \lambda = \pm \frac{\hbar}{2} \quad (48)$$

Finding the eigenspinors of S_y ,

$$\frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \pm \frac{\hbar}{2} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \iff -i\beta = \pm \alpha \quad (49)$$

This gives us the orthonormal eigenspinor of S_y

$$\boxed{\chi_+ = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}} \quad \boxed{\chi_- = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}} \quad (50)$$

6. Spin expectation and measurable values

Given spin state $\chi = A(2i, 3)^T$, find the expectation values of the three components of spin and find the allowable values of the x-component of spin.

Normalizing the spin state,

$$|\chi| = A^2(4 + 9) = 13A^2 = 1 \iff A = \frac{1}{\sqrt{13}} \quad (51)$$

Then, the normalized spin state is expressed as

$$\chi = \frac{1}{\sqrt{13}} \begin{bmatrix} 2i \\ 3 \end{bmatrix} \quad (52)$$

Recall the spin operators in the S_z eigenspinor basis are scaled Pauli spin matrices,

$$\hat{S}_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \hat{S}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (53)$$

Finding the expectation values of the three components of spin in the basis of S_z eigenspinor,

$$\langle \hat{S}_x \rangle = \langle \chi | \hat{S}_x | \chi \rangle = \frac{1}{\sqrt{13}} \begin{bmatrix} -2i \\ 3 \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{1}{\sqrt{13}} \begin{bmatrix} 2i \\ 3 \end{bmatrix} = \frac{\hbar}{26}(-6i + 6i) \quad (54)$$

$$\langle \hat{S}_y \rangle = \langle \chi | \hat{S}_y | \chi \rangle = \frac{1}{\sqrt{13}} \begin{bmatrix} -2i \\ 3 \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \frac{1}{\sqrt{13}} \begin{bmatrix} 2i \\ 3 \end{bmatrix} = \frac{\hbar}{26}(-6 - 6) \quad (55)$$

$$\langle \hat{S}_z \rangle = \langle \chi | \hat{S}_z | \chi \rangle = \frac{1}{\sqrt{13}} \begin{bmatrix} -2i \\ 3 \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \frac{1}{\sqrt{13}} \begin{bmatrix} 2i \\ 3 \end{bmatrix} = \frac{\hbar}{26}(4 + 9) \quad (56)$$

Hence, the expectation values of the three components of spin are,

$$\boxed{\langle S_x \rangle = 0} \quad \boxed{\langle S_y \rangle = -\frac{6\hbar}{13}} \quad \boxed{\langle S_z \rangle = \frac{\hbar}{2}} \quad (57)$$

Recall that the eigenspinors of L_x are

$$\chi_+^{(x)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \text{ with eigenvalue } +\frac{\hbar}{2}; \quad \chi_-^{(x)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \text{ with eigenvalue } -\frac{\hbar}{2} \quad (58)$$

Decomposing the spin state in the eigenspinor of L_x , we have

$$\chi = \langle \chi_+^{(x)} | \chi \rangle | \chi_+^{(x)} \rangle + \langle \chi_-^{(x)} | \chi \rangle | \chi_-^{(x)} \rangle \quad (59)$$

$$= \frac{1}{\sqrt{13}} \left(\begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} 2i \\ 3 \end{bmatrix} \right) \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} + \frac{1}{\sqrt{13}} \left(\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} 2i \\ 3 \end{bmatrix} \right) \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \quad (60)$$

$$= \frac{1}{\sqrt{26}}(2i + 3) \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} + \frac{1}{\sqrt{26}}(2i - 3) \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \quad (61)$$

Observe that squaring the coordinates in each basis gives us

$$|\langle \chi_+^{(x)} | \chi \rangle|^2 = \left| \frac{1}{\sqrt{26}}(2i + 3) \right|^2 = \frac{1}{2} \quad (62)$$

$$|\langle \chi_-^{(x)} | \chi \rangle|^2 = \left| \frac{1}{\sqrt{26}}(2i - 3) \right|^2 = \frac{1}{2} \quad (63)$$

Hence, the allowable values are

$$\boxed{+\frac{\hbar}{2} \quad \text{with probability } \frac{1}{2}} \quad \boxed{-\frac{\hbar}{2} \quad \text{with probability } \frac{1}{2}} \quad (64)$$