PHYS30201 Mathematical Fundamentals of Quantum Mechanics **Examples 1**

The questions on this sheet are revision of vector spaces.

Notation: In 3D, the position vector is written $\mathbf{r} = x\,\mathbf{e}_x + y\,\mathbf{e}_y + z\,\mathbf{e}_z$, and the corresponding operator is $\hat{\mathbf{x}} = \hat{x}\,\mathbf{e}_x + \hat{y}\,\mathbf{e}_y + \hat{z}\,\mathbf{e}_z$. Also, $\hat{p}_x$, $\hat{p}_y$ and $\hat{p}_z$ are the Cartesian components of the momentum operator $\hat{\mathbf{p}}$. In 1D, $\hat{p}_x$ is usually just written $\hat{p}$. Also, we often define $\{\hat{x}_1, \hat{x}_2, \hat{x}_3\} \equiv \{\hat{x}, \hat{y}, \hat{z}\}$.

1. Let $\{|n\rangle\}$ be an orthonormal basis for an N-dimensional complex vector space. Let a_n be the nth coordinate of $|a\rangle$ in this basis, and b_n that of $|b\rangle$, so that $|a\rangle = \sum_n a_n|n\rangle$ and $|b\rangle = \sum_n b_n|n\rangle$. $\hat{A}$, $\hat{B}$ etc are operators in the space. Prove the following (being careful not to confuse your free and dummy indices):

   i) $a_n = \langle n|a\rangle$ and $b_n^* = \langle b|n\rangle$

   ii) $\langle b|a\rangle = \sum_n b_n^* a_n = \langle a|b\rangle^*$

   iii) $\sum_n |n\rangle\langle n| = \hat{I}$
   [*Hint: show that, acting on an arbitrary ket* $|a\rangle$*, this operator returns* $|a\rangle$ *again.*]

   iv) $\langle b|\hat{A}|a\rangle = \sum_{nm} b_n^* A_{nm} a_m$, where $A_{nm} = \langle n|\hat{A}|m\rangle$

   v) $\sum_{nm} |n\rangle A_{nm}\langle m| = \hat{A}$
   [*Hint: consider its matrix element between an arbitrary bra and ket,* $\langle b|$ *and* $|a\rangle$*.*]

   vi) $\langle n|\hat{B}\hat{A}|m\rangle = \sum_k B_{nk}A_{km}$
   [*Hint: insert the identity operator between* $\hat{B}$ *and* $\hat{A}$*, and be careful with your indices.*]

   vii) The adjoint $\hat{A}^\dagger$ of an operator $\hat{A}$ is defined by $\langle b|\hat{A}^\dagger|a\rangle = \langle a|\hat{A}|b\rangle^*$ for all $\langle b|$ and $|a\rangle$. Show that the matrix representing $\hat{A}^\dagger$ is the Hermitan conjugate of the one representing $\hat{A}$.

   viii) If $\hat{A}$ is Hermitian, show that $\langle a|\hat{A}^2|a\rangle \geq 0$ for all $|a\rangle$.

2. The set $\{|1\rangle, |2\rangle, |3\rangle\}$ is an orthonormal basis for a 3D vector space. An operator $\hat{G}$ acts on vectors in this vector space and has the following effects on the basis vectors:

$$\begin{aligned} \hat{G}|1\rangle &= |1\rangle + |2\rangle \\ \hat{G}|2\rangle &= -|1\rangle + |2\rangle \\ \hat{G}|3\rangle &= 0 \end{aligned}$$

   For the vector $|\psi\rangle = C\big(|1\rangle + 2\mathrm{i}|2\rangle + (1+\mathrm{i})|3\rangle\big)$ in this space:

   i) Find a value for the constant C that normalises $|\psi\rangle$.

   ii) Write down the column vectors representing $|\psi\rangle$ and $\hat{G}|\psi\rangle$ in this basis.

   iii) Write down the matrix representation of $\hat{G}$ in this basis. Check that the representations of the operator and vectors are related in the same way as the abstract operator and vectors.

3. Find the eigenvalues and eigenvectors of the matrices

$$\text{i)}\ \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \text{ii)}\ \begin{pmatrix} a & b \\ b & a \end{pmatrix} \quad \text{iii)}\ \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \text{iv)}\ \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \quad \text{v)}\ \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix},$$

where θ is real. Say whether each matrix is Hermitian or unitary, and comment on how the properties of your results relate to the nature of the matrix.

4.i) Find the eigenvalues and eigenvectors of the matrix $\mathbf{M} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$. Verify that the matrix $\mathbf{S}$ of normalised eigenvectors is unitary (or equivalently that the eigenvectors are orthogonal) and that $\mathbf{S}^\dagger\mathbf{M}\mathbf{S}$ is diagonal. What are the diagonal elements of $\mathbf{S}^\dagger\mathbf{M}\mathbf{S}$?

ii) Find the eigenvalues and eigenvectors of the matrix $\mathbf{N} = \begin{pmatrix} 5 & 0 & 1 \\ 0 & 6 & 0 \\ 1 & 0 & 5 \end{pmatrix}$.

[*Hint:* $(0,1,0)^\top$ *is obviously one of them, and the other two must be orthogonal to it, with the form* $(u,0,v)^\top$*, so in fact you only need to consider* $\begin{pmatrix} 5 & 1 \\ 1 & 5 \end{pmatrix}$ *to find* $(u,v)^\top$*.*]

iii) Verify that $\mathbf{M}$ and $\mathbf{N}$ commute. If, as is likely, you have not obtained the same set of eigenvectors for both, explain why the theorem that commuting matrices possess a common set of eigenvectors is not violated.

5. For $\boldsymbol{\Omega} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, show that $\mathrm{e}^{\mathrm{i}a\boldsymbol{\Omega}} = \cos a\,\mathbf{I} + \mathrm{i}\sin a\,\boldsymbol{\Omega}$. [*Hint: recall that functions of operators and matrices are defined through their power series.*]

6. Consider the set of orthogonal normalised vectors $\{|n\rangle\}$ whose position-space representations are $\phi_n(x) = N_n H_n(x)\mathrm{e}^{-x^2/2}$, where H_n is the nth Hermite polynomial,

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2, \quad H_3(x) = 8x^3 - 12x,$$

and the normalisation constants are $N_0 = 1/\sqrt[4]{\pi}$, $N_1 = N_0/\sqrt{2}$, $N_2 = N_0/\sqrt{8}$, $N_3 = N_0/\sqrt{48}$. Note that $|0\rangle$ is not the zero vector!

[*You should work in position space for this question. Once we have covered creation and annihilation operators in the lectures, you can come back and use them to check your answers.*]

i) Verify that $|1\rangle$ is normalised.

ii) Verify that $\langle 0|2\rangle = 0$.

iii) For the function $f(x) = x^2\mathrm{e}^{-x^2/2}$, find the first four coefficients, $f_0, ..f_3$, of its expansion in this basis, $f(x) = \sum_{n=0}^{\infty} f_n\phi_n(x)$.

iv) Find the matrix elements $\langle 1|\hat{p}|0\rangle$ and $\langle 2|\hat{p}^2|0\rangle$.

v) Show that, if we write $\psi(x) \equiv h(x)\mathrm{e}^{-x^2/2}$, the first of the following two differential eigenvalue equations implies the second:

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + x^2\psi = \mathcal{E}\psi \quad \Rightarrow \quad \frac{\mathrm{d}^2 h}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}h}{\mathrm{d}x} + (\mathcal{E}-1)h = 0$$

Hence verify that the square-integrable solutions $\psi(x)$ of the first equation are obtained when $h(x)$ is a Hermite polynomial, with the allowed values of $\mathcal{E}$ being the positive odd integers.

7. Let $|\phi\rangle$ and $|\psi\rangle$ be possible states of a quantum mechanical particle in 1D, moving in a potential $V(x)$. Write down position-space representations of the following expressions:

(i) $\langle x|\psi\rangle$ (ii) $\langle\phi|\psi\rangle$ (iii) $\langle\phi|\hat{x}|\psi\rangle$ (iv) $\langle x|\hat{p}|\psi\rangle$ (v) $\langle p|\psi\rangle$ (vi) $\langle\psi|\hat{H}|\psi\rangle$

Specify which of these are numbers and which are functions.

Similarly, for a particle in 3D, write down position-space representations of the following:

(vii) $\langle\mathbf{r}|\psi\rangle$ (viii) $\langle\phi|\psi\rangle$ (ix) $\langle\phi|\hat{\mathbf{x}}|\psi\rangle$ (x) $\langle\mathbf{r}|\hat{\mathbf{p}}|\psi\rangle$ (xi) $\langle\mathbf{p}|\psi\rangle$ (xii) $\langle\psi|\hat{H}|\psi\rangle$

Specify which of these are scalars and which are vectors.

8. In this question, $\hat{A}$, $\hat{B}$ and $\hat{C}$ are arbitrary operators in any space. In parts (iii) and (iv) you should not use the differential representation of the position operator, but only the commutation relations $[\hat{p}_x, \hat{x}] = -\mathrm{i}\hbar$, $[\hat{x}, \hat{p}_y] = 0$, etc.

i) Show that $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$.

ii) If $[\hat{A}, \hat{B}] = c\hat{I}$, where c is a number, show that $[\hat{A}, \hat{B}^n] = cn\hat{B}^{n-1}$ and $[\hat{A}, \mathrm{e}^{\hat{B}}] = c\,\mathrm{e}^{\hat{B}}$.

iii) Let $Q(x)$ be a polynomial with derivative $R(x)$. Show that $[\hat{p}_x, Q(\hat{x})] = -\mathrm{i}\hbar R(\hat{x})$.

iv) Defining $\hat{L}_x = (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)$, show that

$$\text{(a) } [\hat{L}_x, \hat{x}] = [\hat{L}_x, \hat{p}_x] = 0; \qquad \text{(b) } [\hat{L}_x, \hat{y}] = \mathrm{i}\hbar\hat{z} \qquad \text{(c) } [\hat{L}_x, \hat{p}_z] = -\mathrm{i}\hbar\hat{p}_y.$$

v) Given a function of x, y and z, $V(\mathbf{r})$, show that in the position representation

$$[\hat{\mathbf{p}}, V(\hat{\mathbf{x}})] \underset{\mathbf{r}}{\longrightarrow} -\mathrm{i}\hbar\,\nabla V(\mathbf{r}).$$

[*Hint: Consider the commutator acting on some arbitrary state* $|f\rangle \underset{\mathbf{r}}{\longrightarrow} f(\mathbf{r})$.]

Hence, for a spherically symmetric function $V(\mathbf{r}) \equiv V(r)$, where $r = |\mathbf{r}|$, show that $[\hat{\mathbf{p}}, V(\hat{\mathbf{x}}))] \underset{\mathbf{r}}{\longrightarrow} -\mathrm{i}\,\hat{\mathbf{r}}\frac{\mathrm{d}V}{\mathrm{d}r}$ (where $\hat{\mathbf{r}} \equiv \mathbf{r}/r$ is the unit vector, not an operator!).

9. Write down expressions in both position and momentum representations for the particular eigenstate of momentum, $|\mathbf{p}_0\rangle$, where $\mathbf{p}_0 = \big(2\,\mathbf{e}_x - \mathbf{e}_z\big)\hbar/a$.

[*In the notation used in PHYS20672, the momentum eigenstate would be written* $|e_{\mathbf{p}_0}\rangle$.]