1. The set $\{|\phi_1\rangle, |\phi_2\rangle\}$ is an orthonormal basis set for a 2-dimensional Hilbert space. The states $|W\rangle$, $|\theta_1\rangle$ and $|\theta_2\rangle$ are defined as

$$|W\rangle = \alpha\,|\phi_1\rangle + i\alpha\,|\phi_2\rangle\ ,$$
$$|\theta_1\rangle = \frac{i}{\sqrt{3}}\,|\phi_1\rangle - \frac{\sqrt{2}}{\sqrt{3}}\,|\phi_2\rangle\ , \quad |\theta_2\rangle = \frac{1}{\sqrt{2}}\,|\phi_1\rangle + \frac{i}{\sqrt{2}}\,|\phi_2\rangle\ .$$

(a) The state $|W\rangle$ is normalized. The real and imaginary parts of the constant α are equal. Find α.

[6 marks]

(b) Using the representation

$$|\phi_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}\ , \qquad |\phi_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}\ ,$$

express the operator $\hat{M} = |\theta_1\rangle\langle\theta_2|$ as a matrix.

[5 marks]

(c) Find out and explain whether or not $\hat{M} = |\theta_1\rangle\langle\theta_2|$ is hermitian. Explain whether the operator $\hat{M}$ can represent a physical observable.

[6 marks]

(d) The observable B is represented by the operator $\hat{B} = |\theta_2\rangle\langle\theta_2|$. Calculate the uncertainty of the observable B in the state $|\phi_1\rangle$.

[10 marks]

(e) If B is measured, what are the possible answers that can be obtained?

[8 marks]

(f) If the system Hamiltonian is

$$\hat{H} \;=\; F\,|\phi_1\rangle\langle\phi_1| \;+\; G\,|\phi_2\rangle\langle\phi_2| \;=\; \begin{pmatrix} F & 0 \\ 0 & G \end{pmatrix}$$

and the system is in the state $|\theta_1\rangle$ at time $t = 0$, find the state at any later time t. Here F and G are real constants.

[15 marks]

2. Consider a particle of mass m in one dimension, subject to the potential

$$V(x) \;=\; -\lambda\delta(x)\;.$$

Here λ is a positive constant and $\delta(x)$ is the Dirac delta function.

We will consider stationary solutions of the time-independent Schroedinger equation.

(a) Explain why the derivative of the stationary solution, $\psi'(x)$, need not be continuous at $x = 0$.

[3 marks]

(b) Derive the boundary conditions

$$\psi_R'(0) - \psi_L'(0) \;=\; -\frac{2m\lambda}{\hbar^2}\psi_L(0) \;=\; -\frac{2m\lambda}{\hbar^2}\psi_R(0)$$

where $\psi_L(x)$ and $\psi_R(x)$ are the wavefunctions on the left half-line and right half-line respectively.

Hint: you might consider integrating the Schroedinger equation from $-\epsilon$ to $+\epsilon$, and then taking the limit $\epsilon \to 0$.

[12 marks]

(c) This system has a single bound state at some negative energy, $E < 0$. This eigenfunction has the form

$$\psi(x) \;=\; \begin{cases} A_1e^{\alpha x} \;+\; A_2e^{-\alpha x} & \text{for} \quad x < 0 \\ A_3e^{\alpha x} \;+\; A_4e^{-\alpha x} & \text{for} \quad x > 0 \end{cases}$$

where α is a positive constant.

Explain which of these terms should be dropped, and why.

Derive the relationship between α and E.

[10 marks]

(d) Use the boundary conditions and normalization to determine α and the normalization constants A_i, in terms of λ. Assume A_1 to be real and positive.

[15 marks]

(e) Calculate the expectation value of momentum in the bound state.

[10 marks]

_____*_____

SAMPLE ANSWERS

_____*_____

1. Question 1.

   The set $\{|\phi_1\rangle, |\phi_2\rangle\}$ is an orthonormal basis set for a 2-dimensional Hilbert space. The states $|W\rangle$, $|\theta_1\rangle$ and $|\theta_2\rangle$ are defined as

$$|W\rangle = \alpha\,|\phi_1\rangle + i\alpha\,|\phi_2\rangle\ ,$$
$$|\theta_1\rangle = \frac{i}{\sqrt{3}}\,|\phi_1\rangle - \frac{\sqrt{2}}{\sqrt{3}}\,|\phi_2\rangle\ , \quad |\theta_2\rangle = \frac{1}{\sqrt{2}}\,|\phi_1\rangle + \frac{i}{\sqrt{2}}\,|\phi_2\rangle\ .$$

   (a) Question 1(a)

   The state $|W\rangle$ is normalized. The real and imaginary parts of the constant α are equal. Find α.

   [6 marks]

   [Sample Answer:]

$$|\alpha|^2 + |i\alpha|^2 = 1 \quad \Longrightarrow |\alpha|^2 = \frac{1}{2} \quad \Longrightarrow |\alpha| = \frac{1}{\sqrt{2}}$$

   Since the real and imaginary parts of α are equal, we can write

$$\alpha = b + ib$$

   where b is a real number. Then $|\alpha|^2 = b^2 + b^2 = 2b^2$. Hence

$$2b^2 = \frac{1}{2} \quad \Longrightarrow b = \pm\frac{1}{2}$$

   Therefore we have

$$\text{either} \quad \alpha = \frac{1}{2} + \frac{i}{2} \quad \text{or} \quad \alpha = -\frac{1}{2} - \frac{i}{2}$$

-=-=-=-= * =-=-=-=-

(b) Question 1(b)

Using the representation

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

express the operator $\hat{M} = |\theta_1\rangle\langle\theta_2|$ as a matrix.

[5 marks]

[Sample Answer:]

$$|\theta_1\rangle = \frac{i}{\sqrt{3}}|\phi_1\rangle - \frac{\sqrt{2}}{\sqrt{3}}|\phi_2\rangle = \begin{pmatrix} \frac{i}{\sqrt{3}} \\ -\frac{\sqrt{2}}{\sqrt{3}} \end{pmatrix}$$

$$|\theta_2\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{i}{\sqrt{2}}|\phi_2\rangle = \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix}$$

$$\hat{M} = |\theta_1\rangle\langle\theta_2| = \begin{pmatrix} \frac{i}{\sqrt{3}} \\ -\frac{\sqrt{2}}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & -i/\sqrt{2} \end{pmatrix} = \begin{pmatrix} \frac{i}{\sqrt{6}} & +\frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{3}} & \frac{i}{\sqrt{3}} \end{pmatrix}$$

$$= \frac{1}{\sqrt{6}} \begin{pmatrix} i & +1 \\ -\sqrt{2} & i\sqrt{2} \end{pmatrix}$$

-=-=-=-= * =-=-=-=-

(c) Question 1(c)

Find out and explain whether or not $\hat{M} = |\theta_1\rangle\langle\theta_2|$ is hermitian.

Explain whether the operator $\hat{M}$ can represent a physical observable.

[6 marks]

[Sample Answer:]

$$\hat{M}^\dagger = \begin{pmatrix} -\frac{i}{\sqrt{6}} & -\frac{1}{\sqrt{3}} \\ +\frac{1}{\sqrt{6}} & -\frac{i}{\sqrt{3}} \end{pmatrix} \neq \hat{M}$$

Hence not hermitian.

Physical observables are represented by hermitian operators (measured values need to be real). Hence $\hat{M}$ cannot represent a physical observable.

-=-=-=-= * =-=-=-=-

(d) Question 1(d)

The observable B is represented by the operator $\hat{B} = |\theta_2\rangle\langle\theta_2|$. Calculate the uncertainty of the observable B in the state $|\phi_1\rangle$.

[10 marks]

[Sample Answer:]

$$|\theta_2\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{i}{\sqrt{2}}|\phi_2\rangle = \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix}$$

$$\hat{B} = |\theta_2\rangle\langle\theta_2| = \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & -i/\sqrt{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$$

$$\hat{B}^2 = \frac{1}{4}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 2 & -2i \\ 2i & 2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} = \hat{B}$$

In the state $|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$,

$$\langle B\rangle = \langle\theta_1|\,\hat{B}\,|\theta_1\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix}\hat{B}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = B_{11} = \frac{1}{2}$$

and

$$\langle B^2\rangle = \langle B\rangle = \frac{1}{2}$$

so that

$$\langle B^2\rangle - \langle B\rangle^2 = \frac{1}{2} - \frac{1}{4} = \frac{1}{4}$$

The uncertainty is

$$\Delta B = \sqrt{\langle B^2\rangle - \langle B\rangle^2} = \frac{1}{2}$$

-=-=-=-= * =-=-=-=-

(e) Question 1(e)
If B is measured, what are the possible answers that can be obtained?

[8 marks]

[**Sample Answer:**]
The eigenvalues of the B matrix are the possible results of a measurement. Calculation shows the eigenvalues to be 0 and 1. These are the possible values.
The eigenvalue calculation might go as follows:

$$\begin{vmatrix} \frac{1}{2}-\lambda & \frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2}-\lambda \end{vmatrix} = 0 \quad \Longrightarrow \quad \left(\frac{1}{2}-\lambda\right)^2 - \frac{i}{2}\left(-\frac{i}{2}\right) = 0$$
$$\Longrightarrow \quad \frac{1}{4} + \lambda^2 - \lambda - \frac{1}{4} = 0$$
$$\Longrightarrow \quad \lambda^2 - \lambda = 0 \quad \Longrightarrow \quad \lambda = 0, 1$$

-=-=-=-= * =-=-=-=-

(f) Question 1(f)
If the system Hamiltonian is

$$\hat{H} = F\,|\phi_1\rangle\langle\phi_1| + G\,|\phi_2\rangle\langle\phi_2| = \begin{pmatrix} F & 0 \\ 0 & G \end{pmatrix}$$

and the system is in the state $|\theta_1\rangle$ at time $t = 0$, find the state at any later time t. Here F and G are real constants.

[15 marks]

[Sample Answer:]
Let's denote the system wavefunction components as $u(t)$ and $v(t)$, i.e., the wavefunction is

$$|\psi(t)\rangle = \begin{pmatrix} u(t) \\ v(t) \end{pmatrix}$$

Using the time-dependent Schroedinger equation, $\hat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$, we obtain

$$\begin{pmatrix} F & 0 \\ 0 & G \end{pmatrix}\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} \quad \Longrightarrow \quad \begin{cases} u'(t) = -\frac{iF}{\hbar}u(t) \\ v'(t) = -\frac{iG}{\hbar}v(t) \end{cases}$$

which can be solved to give

$$u(t) = u(0)\exp\left[-\frac{iF}{\hbar}t\right] \; ; \quad v(t) = v(0)\exp\left[-\frac{iG}{\hbar}t\right]$$

The state at $t = 0$ is $|\theta_1\rangle = \frac{i}{\sqrt{3}}|\phi_1\rangle - \frac{\sqrt{2}}{\sqrt{3}}|\phi_2\rangle$, i.e.,

$$\begin{pmatrix} u(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} i/\sqrt{3} \\ -\sqrt{2}/\sqrt{3} \end{pmatrix}$$

Therefore

$$u(t) = \frac{i}{\sqrt{3}}\exp\left[-\frac{iF}{\hbar}t\right] \; ; \quad v(t) = -\frac{\sqrt{2}}{\sqrt{3}}\exp\left[-\frac{iG}{\hbar}t\right]$$

so that the wavefunction at time t is

$$|\psi(t)\rangle = \begin{pmatrix} \frac{i}{\sqrt{3}}\exp\left[-\frac{iF}{\hbar}t\right] \\ -\frac{\sqrt{2}}{\sqrt{3}}\exp\left[-\frac{iG}{\hbar}t\right] \end{pmatrix} = \frac{i}{\sqrt{3}}e^{-iFt/\hbar}|\phi_1\rangle - \frac{\sqrt{2}}{\sqrt{3}}e^{-iGt/\hbar}|\phi_2\rangle$$

-=-=-=-= * =-=-=-=-

2. Question 2.

Consider a particle of mass m in one dimension, subject to the potential

$$V(x) \;=\; -\,\lambda\delta(x)\;.$$

Here λ is a positive constant and $\delta(x)$ is the Dirac delta function.

We will consider stationary solutions of the time-independent Schroedinger equation.

(a) Question 2(a)

Explain why the derivative of the stationary solution, $\psi'(x)$, need not be continuous at $x = 0$.

[3 marks]

[Sample Answer:]

The derivative needs to be continuous if the potential is everywhere finite. The potential here is $-\infty$ at $x = 0$, i.e., not finite everywhere. Hence the derivative $\psi'(x)$ does not need to be continuous.

-=-=-=-= * =-=-=-=-

(b) Question 2(b)

Derive the boundary conditions

$$\psi'_R(0) - \psi'_L(0) \;=\; -\,\frac{2m\lambda}{\hbar^2}\psi_L(0) \;=\; -\,\frac{2m\lambda}{\hbar^2}\psi_R(0)$$

where $\psi_L(x)$ and $\psi_R(x)$ are the wavefunctions on the left half-line and right half-line respectively.

Hint: you might consider integrating the Schroedinger equation from $-\epsilon$ to $+\epsilon$, and then taking the limit $\epsilon \to 0$.

[12 marks]

[Sample Answer:]

The second equality follows from the continuity of the wavefunction $\psi(x)$, which is continuous although its derivative is not: $\psi_L(0) =$

$\psi_R(0) = \psi(0)$. To obtain the eqation for the derivative discontinuity, we need the Schroedinger equation.

The Schroedinger equation is

$$-\frac{\hbar^2}{2m}\psi''(x) \; - \; \lambda\delta(x)\psi(x) = E\psi(x)$$
$$\implies \quad \psi''(x) \; = \; -\frac{2m\lambda}{\hbar^2}\delta(x)\psi(x) - -\frac{2mE}{\hbar^2}\psi(x)$$

Integrating both sides from $x = -\epsilon$ to $x = +\epsilon$, one obtains

$$\int_{-\epsilon}^{\epsilon}\psi''(x)dx \; = \; -\frac{2m\lambda}{\hbar^2}\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)dx - \frac{2mE}{\hbar^2}\int_{-\epsilon}^{\epsilon}\psi(x)dx$$

The first integral is equal to $\psi'(\epsilon) - \psi'(-\epsilon)$ because $\frac{d}{dx}\psi'(x) = \psi''(x)$. (Fundamental Theorem of Calculus.)

The second integral is $\psi(0)$ due to the definition of the Dirac delta function.

Since $\psi(x)$ is continuous, the last integral can be approximated for very small ϵ as $\psi(0)2\epsilon$, which is an infinitesimal quantity.

Thus we have

$$\psi'(\epsilon) - \psi'(-\epsilon) \; = \; -\frac{2m\lambda}{\hbar^2}\psi(0) \; - \; \frac{4mE}{\hbar^2}\psi(0)\epsilon$$

In the limit $\epsilon \to 0$, the last term vanishes, and also

$$\lim_{\epsilon\to 0}\psi'(\epsilon) = \psi_R(0) \, , \qquad \lim_{\epsilon\to 0}\psi'(-\epsilon) = \psi_L(0) \, .$$

Hence we obtain the boundary condition

$$\psi'_R(0) - \psi'_L(0) \; = \; -\frac{2m\lambda}{\hbar^2}\psi(0)$$

or

$$\psi'_R(0) - \psi'_L(0) \; = \; -\frac{2m\lambda}{\hbar^2}\psi_L(0) \; = \; -\frac{2m\lambda}{\hbar^2}\psi_R(0)$$

-=-=-=-= * =-=-=-=-

(c) Question 2(c)

This system has a single bound state at some negative energy, $E < 0$. This eigenfunction has the form

$$\psi(x) \;=\; \begin{cases} A_1 e^{\alpha x} \;+\; A_2 e^{-\alpha x} & \text{for} \quad x < 0 \\ A_3 e^{\alpha x} \;+\; A_4 e^{-\alpha x} & \text{for} \quad x > 0 \end{cases}$$

where α is a positive constant.

Explain which of these terms should be dropped, and why.

Derive the relationship between α and E.

[10 marks]

[**Sample Answer:**]

For $x < 0$, the term $e^{-\alpha x}$ blows up at large negative x, so that the wavefunction becomes impossible to normalize. Hence for normalizability, the term $A_2 e^{-\alpha x}$ should be dropped.

For the corresponding reason, the term $e^{+\alpha x}$ is not allowed in the $x > 0$ half-line. Hence the term $A_3 e^{\alpha x}$ should be dropped as well. The eigenfunction has the form

$$\psi(x) \;=\; \begin{cases} A_1 e^{\alpha x} & \text{for} \quad x < 0 \\ A_4 e^{-\alpha x} & \text{for} \quad x > 0 \end{cases}$$

To determine the constant α in terms of the energy, we need to consider the Schroedinger equation either for $x < 0$ or for $x > 0$, away from the problematic point $x = 0$.

Considering $x < 0$, the time-independent SE is

$$-\frac{\hbar^2}{2m}\psi''(x) \;=\; E\psi(x)$$

Using $\psi(x) = A_1 e^{\alpha x}$ gives

$$-\frac{\hbar^2}{2m}A_1(\alpha^2)e^{\alpha x} \;=\; EA_1 e^{\alpha x} \qquad \Longrightarrow \qquad \alpha \;=\; \sqrt{\frac{2m(-E)}{\hbar^2}}$$

Since E is negative, α is a real constant.

Can also express E in terms of α:

$$E \;=\; -\,\frac{\hbar^2\alpha^2}{2m}$$

-=-=-=-= * =-=-=-=-

(d) Question 2(d)

Use the boundary conditions and normalization to determine α and the normalization constants A_i, in terms of λ. Assume A_1 to be real and positive.

[15 marks]

[**Sample Answer:**]

The wavefunction is $\psi_L(x) = A_1 e^{\alpha x}$ on the left and $\psi_R(x) = A_4 e^{-\alpha x}$ on the right.

Continuity of the wavefunction:

$$\psi_L(0) = \psi_R(0) \qquad \Longrightarrow \qquad A_1 = A_4$$

Normalization:

$$\int_{-\infty}^{0} |\psi_L(x)|^2 \, dx \;+\; \int_{0}^{\infty} |\psi_R(x)|^2 \, dx \;=\; 1$$

$$\Longrightarrow \qquad |A_1|^2 \int_{-\infty}^{0} e^{2\alpha x} dx \;+\; |A_1|^2 \int_{0}^{\infty} e^{-2\alpha x} dx \;=\; 1$$

$$\Longrightarrow \qquad |A_1|^2 \frac{1}{2\alpha} \;+\; |A_1|^2 \frac{1}{2\alpha} \;=\; 1$$

$$\Longrightarrow \qquad |A_1|^2 \;=\; \alpha \;=\; \sqrt{-\frac{2mE}{\hbar^2}}$$

Discontinuity of ψ':

$$-\alpha A_1 - \alpha A_1 \;=\; -\frac{2m\lambda}{\hbar^2} A_1 \qquad \begin{cases} \text{using } \psi_L'(0) = A_1(\alpha)e^0 = \alpha A_1 \\ \text{and } \psi_R'(0) = A_4(-\alpha)e^0 = -\alpha A_1 \end{cases}$$

$$\Longrightarrow \quad \alpha \;=\; \frac{m\lambda}{\hbar^2} \qquad \Longrightarrow \qquad A_1 \;=\; \sqrt{\alpha} \;=\; \sqrt{\frac{m\lambda}{\hbar^2}}$$

(We could also calculate the energy, $E = -\frac{\hbar^2\alpha^2}{2m} = -\frac{m\lambda^2}{2\hbar^2}$, if we were asked to.)

-=-=-=-= * =-=-=-=-

(e) Question 2(e)
Calculate the expectation value of momentum in the bound state.

[10 marks]

[Sample Answer:]
The wavefunction of the bound state is $\psi_L(x) = A_1 e^{\alpha x}$ on the left and $\psi_R(x) = A_1 e^{-\alpha x}$ on the right. We will continue to treat A_1 as a real positive number, so the wavefunction is everywhere real.

The momentum operator is $\hat{p} = -i\hbar\frac{\partial}{\partial x}$; hence the expectation value of momentum in the state $\psi(x)$ is

$$\begin{aligned}\langle p\rangle &= \int_{-\infty}^{\infty} dx\psi^*(x)\hat{p}\psi(x) = \int_{-\infty}^{\infty} dx\psi^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)\\ &= -i\hbar\int_{-\infty}^{\infty} dx\psi(x)\psi'(x)\end{aligned}$$

We've used $\psi^*(x) = \psi(x)$ since the wavefunction is real.
Now we can use the expression for the wavefunction to calculate $\int dx\psi(x)\psi'(x)$. The problem is that there are different expressions for the negative half-line and positive half-line. Hence we split up the integral into two parts:

$$\begin{aligned}\int_{-\infty}^{\infty} dx\psi(x)\psi'(x) &= \int_{-\infty}^{0} dx\psi(x)\psi'(x) + \int_{0}^{\infty} dx\psi(x)\psi'(x)\\ &= \int_{-\infty}^{0} dx\psi_L(x)\psi_L'(x) + \int_{0}^{\infty} dx\psi_R(x)\psi_R'(x)\\ &= \int_{-\infty}^{0} dx\left(A_1e^{\alpha x}\right)\left(A_1\alpha e^{\alpha x}\right) + \int_{0}^{\infty} dx\left(A_1e^{-\alpha x}\right)\left(-A_1\alpha e^{-\alpha x}\right)\\ &= A_1^2\alpha\int_{-\infty}^{0} dx e^{2\alpha x} - A_1^2\alpha\int_{0}^{\infty} dx e^{-2\alpha x}\end{aligned}$$

The two integrals are equal, this can be seen by evaluating both or by a variable transformation:

$$\begin{aligned}\int_{x=-\infty}^{x=0} dx e^{2\alpha x} &= \int_{u=\infty}^{u=0} d(-u)e^{2\alpha(-u)} = \int_{u=\infty}^{u=0} d(-u)e^{2\alpha(-u)}\\ &= -\int_{\infty}^{0} du e^{-2\alpha u} + \int_{0}^{\infty} du e^{-2\alpha u} = \int_{0}^{\infty} dx e^{-2\alpha x}\end{aligned}$$

Hence the two integrals cancel, and we have

$$\langle p \rangle \;=\; -i\hbar \int_{-\infty}^{\infty} dx \psi(x)\psi'(x) \;=\; -i\hbar A_1^2 \alpha \times 0 \;=\; 0$$

-=-=-=-= * =-=-=-=-