Quantum Theory. Problem Set 1

1.

(a) Consider a particle in a box. The Scrödinger equation in Dirac formalism is

$$\hat{H}|n\rangle = E_n|n\rangle,$$

where $\{|n\rangle, E_n\}$ are the nth eigenstate and eigenenergy respectively. We pass to coordinate representation by multiplying both sides of this equation by the position bra $\langle x|$ and using the continuous identity resolution

$$\int \mathrm{d}x'|x'\rangle\langle x'| = \hat{I}.$$

Then

$$\langle x|\hat{H}|n\rangle = \langle x|E_n|n\rangle,$$

where

$$\langle x|E_n|n\rangle = E_n\langle x|n\rangle \equiv E_n\psi_n(x),$$

and where

$$\begin{aligned}
\langle x|\hat{H}|n\rangle &= \langle x|\hat{H}\cdot\hat{I}|n\rangle \\
&= \int \mathrm{d}x'\langle x|\hat{H}|x'\rangle\langle x'|n\rangle \\
&= \int \mathrm{d}x' H(x,x')\delta(x-x')\psi_n(x') \\
&= H(x)\psi_n(x),
\end{aligned}$$

where

$$H(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

Finally, for the wavefunction in x representation, the Scroedinger equation can be written as

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi_n(x) = E_n\psi_n(x).$$

a.1) Solve for $V(x) = 0$. Try

$$\psi_n(x) = A_n\cos k_n x + B_n\sin k_n x,$$

and obtain

$$E_n = \frac{\hbar^2 k_n^2}{2m}.$$

a.2) Boundary conditions at $x = \pm a : \psi_n(\pm a) = 0$

$$\cos k_n a = 0 \Rightarrow k_n = \frac{(2n+1)\pi}{2a}, \qquad (n = 0, 1, 2, \ldots),$$

$$\sin k_n a = 0 \Rightarrow k_n = \frac{n\pi}{a} = \frac{(2n)\pi}{2a}, \qquad (n = 1, 2, \ldots).$$

a.3) Resumé:

$$k_n = \frac{n\pi}{2a}, \qquad E_n = \hbar^2 \left(\frac{n^2\pi^2}{8ma^2} \right), \qquad (n = 0, 1, 2, \ldots),$$

$$\psi_n(x) = \begin{cases} A_n \cos k_n x \ \ (n \text{ ODD}), \\ B_n \sin k_n x \ \ (n \text{ EVEN}). \end{cases}$$

a.4) Normalization:

$$\begin{aligned} A_n : \qquad 1 &= A_n^2 \int_{-a}^{a} \mathrm{d}x \cos^2 k_n x \\ &= \frac{A_n^2}{2} \int_{-a}^{a} \mathrm{d}x (1 + \cos 2k_n x) \\ &= \frac{A_n^2}{2} (2a) \Rightarrow A_n = \frac{1}{\sqrt{a}}. \end{aligned}$$

$$\begin{aligned} B_n : \qquad 1 &= B_n^2 \int_{-a}^{a} \mathrm{d}x \sin^2 k_n x \\ &= B_n^2 a \Rightarrow B_n = \frac{1}{\sqrt{a}}. \end{aligned}$$

Finally

$$\psi_n(x) = \begin{cases} \frac{1}{\sqrt{a}} \cos k_n x \ \ (n \text{ ODD}), \\ \frac{1}{\sqrt{a}} \sin k_n x \ \ (n \text{ EVEN}). \end{cases}$$

(b) It is given the wavefunction

$$\Phi(x) = N(a - |x|) = \begin{cases} N(a - x) \ \ x \geq 0, \\ N(a + x) \ \ x < 0. \end{cases}$$

b.1) Normalization:

$$
\begin{aligned}
N: \qquad 1 &= N^2 \int_{-a}^{a} \mathrm{d}x (a - |x|)^2 \\
&= N^2 \left[\int_{-a}^{0} \mathrm{d}x (a+x)^2 + \int_{0}^{a} \mathrm{d}x (a-x)^2 \right]
\end{aligned}
$$

substituting $x \to -x$ in the second integral produces

$$
1 = 2N^2 \int_{-a}^{0} \mathrm{d}x (a+x)^2 = 2N^2 \frac{a^3}{3} \Rightarrow N = \left(\frac{3}{2a^3} \right)^{1/2}.
$$

b.2) By definition

$$
\begin{aligned}
\langle n|\Phi\rangle &= \langle n|\hat{I}|\Phi\rangle \\
&= \int \mathrm{d}x' \langle n|x'\rangle\langle x'|\Phi\rangle \\
&= \int_{-a}^{a} \mathrm{d}x' \psi_n^*(x')\Phi(x')
\end{aligned}
$$

where

$$
\psi_n(x') \equiv \langle x'|n\rangle \Rightarrow \psi_n^*(x') = (\langle x'|n\rangle)^* = \langle n|x'\rangle,
$$

and

$$
\Phi(x) \equiv \langle x|\Phi\rangle.
$$

Then

$$
\begin{aligned}
\langle n|\Phi\rangle &= \int_{-a}^{a} \mathrm{d}x' \psi_n^*(x')\Phi(x') \\
&= 0, \qquad (n \text{ EVEN}),
\end{aligned}
$$

since $\Phi(x)$ is symmetric while $\sin k_n x$ is antisymmetric.

$$
\begin{aligned}
\langle n|\Phi\rangle &= \int_{-a}^{a} \mathrm{d}x' \psi_n^*(x')\Phi(x') \\
&= \frac{1}{\sqrt{a}} \left(\frac{3}{2a^3} \right)^{1/2} \int_{-a}^{a} \mathrm{d}x' \cos(k_n x')(a - |x|) \\
&= \frac{1}{\sqrt{a}} \left(\frac{3}{2a^3} \right)^{1/2} \frac{2}{k_n^2} \\
&= \sqrt{\frac{3}{2}} \left(\frac{8}{n^2\pi^2} \right), \qquad (n \text{ ODD})
\end{aligned}
$$

b.3) By definition

$$\langle x|\Phi\rangle = \Phi(x) = \left(\frac{3}{2a^3}\right)^{1/2}(a - |x|).$$

b.4) By definition

$$\langle x|x'\rangle = \delta(x - x').$$

2. Using the rules of bra-ket algebra, prove or evaluate the following:

a) $(XY)^\dagger = Y^\dagger X^\dagger$. The Hermitian adjoint of XY is defined by the correspondence:

$$XY|a\rangle \leftrightarrow \langle a|(XY)^\dagger\,.$$

However, we also have:

$$XY|a\rangle = X(Y|a\rangle) \leftrightarrow ((\langle a|Y^\dagger)X^\dagger = \langle a|Y^\dagger X^\dagger\,.$$

Therefore, $(XY)^\dagger = Y^\dagger X^\dagger$.

b) $\mathrm{tr}(XY) = \mathrm{tr}(YX)$.

$$\begin{aligned}
\mathrm{tr}(XY) &= \sum_{a'} \langle a'|\,XY\,|a'\rangle \\
&= \sum_{a'} \langle a'|\,XIY\,|a'\rangle \\
&= \sum_{a'} \langle a'|\,X\left(\sum_{a''} |a''\rangle\langle a''|\right)Y\,|a'\rangle \\
&= \sum_{a'}\sum_{a''} \langle a'|\,X\,|a''\rangle\langle a''|\,Y\,|a'\rangle \\
&= \sum_{a'}\sum_{a''} \langle a''|\,Y\,|a'\rangle\langle a'|\,X\,|a''\rangle \\
&= \sum_{a''} \langle a''|\,Y\left(\sum_{a'} |a'\rangle\langle a'|\right)X\,|a''\rangle \\
&= \sum_{a''} \langle a''|\,YX\,|a''\rangle \\
&= \mathrm{tr}(YX)\,,
\end{aligned}$$

where we used $I = \sum_{a'} |a'\rangle\langle a'| = \sum_{a''} |a''\rangle\langle a''|$.

c) $\sum_{a'} \Psi^*_{a'}(\mathbf{x}')\Psi_{a'}(\mathbf{x}'')$.

$$\begin{aligned}
\sum_{a'} \Psi^*_{a'}(\mathbf{x}')\Psi_{a'}(\mathbf{x}'') &= \sum_{a'} \langle \mathbf{x}' | \, a' \rangle^* \langle \mathbf{x}'' | \, a' \rangle \\
&= \sum_{a'} \langle a' | \, \mathbf{x}' \rangle \langle \mathbf{x}'' | \, a' \rangle \\
&= \sum_{a'} \langle \mathbf{x}'' | \, a' \rangle \langle a' | \, \mathbf{x}' \rangle \\
&= \langle \mathbf{x}'' | \left(\sum_{a'} |a'\rangle \langle a'| \right) |\mathbf{x}'\rangle \\
&= \langle \mathbf{x}'' | \, \mathbf{x}' \rangle \\
&= \delta(\mathbf{x}'' - \mathbf{x}') \,,
\end{aligned}$$

where δ is the Dirac δ-function.

3. Since

$$\langle + | + \rangle = 1 = \langle - | - \rangle, \qquad \langle + | - \rangle = 0,$$

we associate

$$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \qquad \langle +| \doteq \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad \langle -| \doteq \begin{pmatrix} 0 & 1 \end{pmatrix}.$$

Then

$$|+\rangle\langle +| \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad |+\rangle\langle -| \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

$$|-\rangle\langle +| \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad |-\rangle\langle -| \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then, for example

$$\begin{aligned}
\hat{S}_x &= \frac{\hbar}{2} \left(|+\rangle\langle -| + |-\rangle\langle +| \right) \\
&\doteq \frac{\hbar}{2} \left[\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right] \\
&\doteq \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\end{aligned}$$

In the same way one calculate

$$\hat{S}_y \doteq \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{S}_z \doteq \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Now that the matrix representation of the spin operators $\hat{S}_i$, $(i = x, y, z)$ is available, it is simple to calculate the required commutators just by multiplying matrices. For example

$$\begin{aligned}
[\hat{S}_x, \hat{S}_y] &= \hat{S}_x\hat{S}_y - \hat{S}_y\hat{S}_x \\
&= \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \left(\frac{\hbar}{2}\right)^2 \left[\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \right] \\
&= \left(\frac{\hbar}{2}\right)^2 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= \frac{\hbar^2}{4} 2i \left(\frac{2}{\hbar}\right) \left[\left(\frac{\hbar}{2}\right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \\
&= i\hbar\hat{S}_z.
\end{aligned}$$

The other cases can be worked exactly in the same way. We illustrate a single example for the anticommutator.

$$\begin{aligned}
\{\hat{S}_x, \hat{S}_y\} &= \hat{S}_x\hat{S}_y + \hat{S}_y\hat{S}_x \\
&= \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \left(\frac{\hbar}{2}\right)^2 \left[\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} + \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \right] \\
&= 0.
\end{aligned}$$

5.

a) Let us call the matrix J_z:

$$J_z = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

To find eigenvalues, solve $\det|\lambda I - J_z| = 0$, so $\lambda^2 - \lambda = 0, \Rightarrow \lambda = 0, \pm 1$. So, there is no degeneracy. To find the eigenvectors, let us write the generic eigenvector as $\vec{u}_\lambda = (x_1, x_2, x_3)$. Then

$$\begin{array}{lll}
\lambda = 0 \quad \Rightarrow & x_2 = 0,\ x_1 + x_3 = 0 & \Rightarrow \vec{u}_0 = (1/\sqrt{2}, 0, -1/\sqrt{2}), \\
\lambda = -1 \quad \Rightarrow & \sqrt{2}x_1 + x_2 = 0,\ x_2 + \sqrt{2}x_3 = 0 & \Rightarrow \vec{u}_- = (-1/2, 1/\sqrt{2}, -1/2), \\
\lambda = 1 \quad \Rightarrow & -\sqrt{2}x_1 + x_2 = 0,\ -x_2 + \sqrt{2}x_3 = 0 & \Rightarrow \vec{u}_+ = (1/2, 1/\sqrt{2}, 1/2).
\end{array}$$

b) The eigenvalues are $0, \pm 1$ so we have a spin 1 system, and the matrix is probably related to operators for spin 1. Later on, when we shall study angular momentum, this matrix will re-appear and that is why we called it J_z as above. Spin 1 appears in many different systems; for example in the hyperfine structure of the Hydrogen atom, in many elementary particles (ρ, ϕ, W, Z), and in the isospin symmetry of pions.

6. Consider the following Hamiltonian for a 2-state system:

$$H = a(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|)\,.$$

The matrix representation of H in the basis $|1\rangle$ and $|2\rangle$ is given by:

$$H \to \begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle \end{pmatrix}$$

Let us compute $\langle 1|H|1\rangle$:

$$\begin{aligned} \langle 1|H|1\rangle &= \langle 1|\left[a\left(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\right)\right]|1\rangle \\ &= a(\langle 1|1\rangle\langle 1|1\rangle - \langle 1|2\rangle\langle 2|1\rangle + \langle 1|1\rangle\langle 2|1\rangle + \langle 1|2\rangle\langle 1|1\rangle) \\ &= a(1-0+0+0) \\ &= a \end{aligned}$$

Likewise,

$$\begin{aligned} \langle 1|H|2\rangle &= a \\ \langle 2|H|1\rangle &= a \\ \langle 2|H|2\rangle &= -a \end{aligned}$$

Therefore, we have

$$H \to a\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

The eigenvalues E of H are the solutions of $\det(H - EI) = 0$, that is

$$\begin{aligned} \det\begin{pmatrix} a-E & a \\ a & -a-E \end{pmatrix} &= 0 \\ -(a-E)(a+E) - a^2 &= 0 \\ -(a^2 - E^2) - a^2 &= 0 \\ E^2 = 2a^2 &= 0 \\ \Rightarrow E = \pm\sqrt{2}a & \end{aligned}$$

Note that a general ket $|\alpha\rangle$ can be decomposed on the basis $|1\rangle$ and $|2\rangle$ as

$$|\alpha\rangle = \alpha_1|1\rangle + \alpha_2|2\rangle\ ,$$

so that the vector representation of $|\alpha\rangle$ on this basis is given by

$$|\alpha\rangle \to \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

In particular, the vector representations of the eigenkets of H on this basis are the eigenvector of the matrix representation of H on the same basis:

$$a\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = E\begin{pmatrix} x \\ y \end{pmatrix}$$

$$\Rightarrow \begin{cases} x + y = \frac{E}{a}x \\ x - y = \frac{E}{a}y \end{cases}$$

$$\Rightarrow y = \left(\frac{E}{a} - 1\right)x$$

Therefore, the eigenvectors have the form

$$\mathcal{N}\begin{pmatrix} 1 \\ \frac{E}{a} - 1 \end{pmatrix}$$

where $\mathcal{N}$ is a normalization factor: $\mathcal{N} = 1/\sqrt{1 + \left(\frac{E}{a} - 1\right)^2}$.

The eigenvalues and eigenkets of H are given by:

$$E = \sqrt{2}a \qquad \frac{1}{\sqrt{1 + (\sqrt{2} - 1)^2}}\left[|1\rangle + \left(\sqrt{2} - 1\right)|2\rangle\right]$$

$$E = -\sqrt{2}a \qquad \frac{1}{\sqrt{1 + (-\sqrt{2} - 1)^2}}\left[|1\rangle + \left(-\sqrt{2} - 1\right)|2\rangle\right]$$