1) An operator $A$, corresponding to a physical observable, has two normalized eigenstates $|\phi_1\rangle$ and $|\phi_2\rangle$ with non-degenerate eigenvalues $a_1$ and $a_2$, respectively. A second operator $B$, corresponding to a different physical observable, has normalized eigenstates $|\chi_1\rangle$ and $|\chi_2\rangle$, with eigenvalues $b_1$ and $b_2$, respectively. The two sets of eigenstates are related by

$$|\phi_1\rangle \propto 2|\chi_1\rangle + 3|\chi_2\rangle \quad (1)$$
$$|\phi_2\rangle \propto 3|\chi_1\rangle - 2|\chi_2\rangle \quad (2)$$

The physical observable corresponding to $A$ is measured and the value $a_1$ is obtained. Immediately afterwards, the physical observable corresponding to $B$ is measured, and again immediately after that the one corresponding to $A$ is remeasured. What is the probability of obtaining $a_1$ a second time?

**Ans**: First let’s normalized the wave functions:

$$|\phi_1\rangle = \frac{1}{\sqrt{13}} (2|\chi_1\rangle + 3|\chi_2\rangle) \quad (3)$$
$$|\phi_2\rangle = \frac{1}{\sqrt{13}} (3|\chi_1\rangle - 2|\chi_2\rangle) \quad (4)$$

After the first measurement of $A$, we know that the state must have “collapsed” into the eigenstate $|\phi_1\rangle$. If we now measure $B$, the result can be either $b_1$ or $b_2$ with the following probability

$$P(b_1) = |\langle \chi_1 | \phi_1 \rangle|^2 \quad (5)$$
$$P(b_2) = |\langle \chi_2 | \phi_1 \rangle|^2 \quad (6)$$

The wave function will now be either $|\chi_1\rangle$ or $|\chi_2\rangle$, depending on whether we got $b_1$ or $b_2$. If we now measure $A$ again, the probability to measure $a_1$ is given by

$$P(a_1) = |\langle \phi_1 | \chi_1 \rangle|^2 P(b_1) + |\langle \phi_1 | \chi_2 \rangle|^2 P(b_2) = |\langle \phi_1 | \chi_1 \rangle|^4 + |\langle \phi_1 | \chi_2 \rangle|^4 = \frac{97}{169}. \quad (7)$$

2) The ammonia molecule NH$_3$ has two different possible configurations: One (which we will call $|1\rangle$), where the nitrogen atom is located above the plane spanned by the three
H atoms, and the other one (which we will call $|2\rangle$) where it is below. These two states span the Hilbert space in our simple example. In both states, the expectation value of the energy $\langle n | H | n \rangle$ is the same, $E(n = 1, 2)$. On the other hand, the two states are not eigenstates of the Hamiltonian; in fact, we have $\langle 2 | H | 1 \rangle = \langle 1 | H | 2 \rangle = -V$ (where $V$ is some positive number).

1) Write down the Hamiltonian in Dirac form and in matrix form.

**Answ:** The Dirac form is

$$H = E(|1\rangle \langle 1| + |2\rangle \langle 2|) - V(|2\rangle \langle 1| + |1\rangle \langle 2|).$$

and the matrix form is

$$H = \begin{pmatrix} E & -V \\ -V & E \end{pmatrix}$$

(9)

2) Find both eigenvalues and normalized eigenvectors. Which state is the ground state?

**Answ:** The eigenvalues are $\varepsilon_{1,2} = E \pm V$.

The ground state has energy $\varepsilon_1 = E - V$ and eigenstate $|\phi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$. The excited state energy is $\varepsilon_2 = E + V$ with eigenstate $|\phi_2\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$.

3) Where is nitrogen in the two eigenstates, i.e., what is the probability to find nitrogen atom above or below in the two states?

**Answ:** These two states are linear superpositions of the two eigenstates to the operator measuring the position of the N atom. In fact, it is clear that for both of them, the probability to find the N either above or below the $H_3$ plane is 50%. Nitrogen is in both positions at once.

4) Consider the parity operator in which all coordinates change sign ($x \rightarrow -x$). Is parity well defined in the two eigenstates? If yes, what is the value of the parity operator in the two cases?

**Answ:** Under the parity operation, all coordinates change sign, interchanging the meaning of up and down. This means that $|1\rangle \rightarrow |2\rangle$ and $|2\rangle \rightarrow |1\rangle$ under this operation.

Applying this to the two energy eigenstates, we find that the ground state is invariant (it is an eigenstate of the parity operator with eigenvalue +1 even parity) and the excited state acquires a minus sign (it is also an eigenstate under parity, but with eigenvalue -1, i.e., odd parity).

3) Consider the following three operators (representing physical observable) on the two dimensional Hilbert space:

$$S_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(10)

$$S_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

(11)

$$S_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(12)
(1) Assume $S_z$ is measured and one finds the value -1. Immediately afterwards, what are $\langle S_x \rangle$, $\langle S_x^2 \rangle$ and $\Delta S_x \equiv \sqrt{\langle S_x^2 \rangle - \langle S_x \rangle^2}$.

**Ans.:** After measurement, the system is in the eigenstate $|\psi\rangle = (0, 1)$ of $S_z$. Hence, we can calculate

\begin{align*}
\langle S_x \rangle &= \langle \psi | S_x | \psi \rangle = 0 \quad \text{(13)} \\
\langle S_x^2 \rangle &= \langle \psi | S_x^2 | \psi \rangle = 1 \quad \text{(14)} \\
\Delta S_x &= 1 \quad \text{(15)}
\end{align*}

(2) What are the possible values one could measure for $S_x$, and what are their possibilities if it is measured immediately after measurement in (1).

**Ans.:** Eigenstates of $S_x$ are

\begin{align*}
|\phi_1\rangle &= \frac{1}{\sqrt{2}} (1, 1) \\
|\phi_2\rangle &= \frac{1}{\sqrt{2}} (1, -1)
\end{align*} \quad \text{(16)} \quad \text{(17)}

The first with eigenvalue $s_x = 1$ and the second with $s_x = -1$. Hence, one could measure either +1 or -1.

We measure $s_x = 1$ with probability $P(1) = |\langle \phi_1 | \psi \rangle|^2 = 1/2$ and $P(-1) = |\langle \phi_2 | \psi \rangle|^2 = 1/2$.

(3) Explicitly calculate the commutators between any two of the three operators above (all 3). Is it possible to prepare a state of the system with well-defined values for all three?

**Ans.:** After some algebra, we get

\begin{align*}
[S_x, S_y] &= S_x S_y - S_y S_x = 2i S_z \quad \text{(18)} \\
[S_y, S_z] &= 2i S_x \quad \text{(19)} \\
[S_z, S_x] &= 2i S_y \quad \text{(20)}
\end{align*}

Since these operators do not commute, it is not possible to find simultaneous eigenvectors to any two of them.

4) The normalized wave function $\psi(x, t)$ satisfies the time-dependent Schroedinger equation for a free particle of mass $m$ moving in 1D. Consider a second wave function of the form $\phi(x, t) = \exp(i(ax - bt)) \psi(x - vt, t)$.

- Show that $\phi(x, t)$ obeys the same time-dependent Schroedinger equation as $\psi(x, t)$ when constants $a$ and $b$ are chosen appropriately. What should the values of $a$ and $b$ be (express them in terms of $v$)?

**Ans.:** We need to show that

$$
\frac{ih}{dt} \frac{d\phi}{dt} = -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2}
$$
and we know that
\[ i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \]

We first compute derivatives of \( \phi \) using its given form:
\[ \frac{d\phi}{dt} = -ib\phi - ve^{i(ax-bt)} \frac{\partial}{\partial x} \psi(x-vt,t) + e^{i(ax-bt)} \frac{\partial}{\partial t} \psi(x-vt,t) \]  
\[ \frac{\partial^2 \phi}{\partial x^2} = -a^2 \phi + 2iae^{i(ax-bt)} \frac{\partial}{\partial x} \psi(x-vt,t) + e^{i(ax-bt)} \frac{\partial^2}{\partial x^2} \psi(x-vt,t) \]

When we plug these derivatives into the Schrödinger equation for \( \phi \) and take into account that \( \psi \) satisfies the same equation, we get
\[ i\hbar \left[ -ib\phi - ve^{i(ax-bt)} \frac{\partial}{\partial x} \psi(x-vt,t) \right] = -\frac{\hbar^2}{2m} \left[ -a^2 \phi + 2iae^{i(ax-bt)} \frac{\partial}{\partial x} \psi(x-vt,t) \right] \]

This is satisfies when the first (second) term on the rhs is equal to the first (second) term on the lhs, which gives
\[ \hbar b = \frac{\hbar^2 a^2}{2m} \]  
\[ i\hbar v = \frac{ia\hbar^2}{m} \]

and hence we need to require
\[ a = \frac{mv}{\hbar} \]  
\[ b = \frac{mv^2}{2\hbar} \]

- Calculate the expectation value of position \( \langle X \rangle \), momentum \( \langle P \rangle \), and energy \( \langle H \rangle \) for particle in the state \( \phi(x,t) \) in terms of those for particle in the state \( \psi(x,t) \). Show that uncertainty in the momentum is the same in both states.

**Answ.:**
\[ \langle X \rangle_\phi = \int \phi^*(x)x\phi(x)dx = \int \psi^*(x-vt,t)x\psi(x-vt,t)dx = \int \psi^*(x',t)(x'+vt)\psi(x',t)dx' = vt + \langle X \rangle_\psi \]
\[ \langle P \rangle_\phi = -i\hbar \int \phi^*(x) \frac{\partial}{\partial x} \phi(x)dx = -i\hbar \int \phi^*[ia\phi + e^{i(ax-bt)} \frac{\partial}{\partial x} \psi]dx = \hbar a + \langle P \rangle_\psi = mv + \langle P \rangle_\psi \]
\[ \langle H \rangle_\phi = -\frac{\hbar^2}{2m} \int \phi^*[a^2 - 2iae^{i(ax-bt)} \frac{\partial}{\partial x} \psi + e^{i(ax-bt)} \frac{\partial^2}{\partial x^2} \psi]dx = \frac{\hbar^2 a^2}{2m} + \frac{a\hbar}{m} \langle P \rangle_\psi + \langle H \rangle_\psi = \frac{1}{2}mv^2 + v \langle P \rangle_\psi + \langle H \rangle_\psi \]
\[(\Delta P)^2_\phi = 2m \langle H \rangle_\phi - \langle P \rangle^2_\phi = m^2v^2 + 2mv \langle P \rangle_\psi + 2m \langle H \rangle_\psi - (mv + \langle P \rangle_\psi)^2 \]
\[= \langle P^2 \rangle_\psi - \langle P \rangle^2_\psi = (\Delta P)^2_\psi \quad (30)\]

What physical interpretation can be given to the transformation from the state \(\psi(x, t)\) to the state \(\phi(x, t)\)?

**Answ.:**
\(\phi\) describes the same state as \(\psi\), except from a coordinate system that is moving towards the left with velocity \(v\). In that coordinate system, the system seems to be moving to the right with additional velocity \(v\) and therefore additional momentum \(mv\). The total kinetic energy increases accordingly.