Homework # 3       Physics 412 - Spring 2015       Due Friday, February 13, 2015

Read:  B&J Chapters 3, 5

14. A Hamiltonian of a system has only two eigenstates $|\psi_1\rangle$ and $|\psi_2\rangle$. These two states form a complete orthonormal set. The action of the operator $R$ is define to be:

$$R |\psi_1\rangle = 3 |\psi_1\rangle - i \sqrt{3} |\psi_2\rangle$$

and

$$R |\psi_2\rangle = \sqrt{3} i |\psi_1\rangle + 5 |\psi_2\rangle$$

(a) Write down the matrix representation of the operator $R$.
(b) Is the operator Hermitian?
(c) Is the operator unitary?
(d) Determine the eigenvalues and normalized eigenvectors of the operator.
(e) Show that a matrix consisting of the normalized eigenvectors as columns is unitary.

15. Consider a system described by a Hamiltonian with three eigenvectors and eigenvalues: $\mathcal{H} |\psi_n\rangle = E_n |\psi_n\rangle$ for $n = 1, 2$ and $3$ with $E_n = n^2 E_0$. Given a state $|\psi\rangle = 4 i |\psi_1\rangle + \sqrt{3} i |\psi_2\rangle + \sqrt{6} |\psi_3\rangle$

(a) Normalize $|\psi\rangle$
(b) If you make a measurement of the energy on the state $|\psi\rangle$, what values are possible and with what probability do they occur?
(c) What is the average value of the energy of the state $|\psi\rangle$?
(d) What is the average value of the square of the energy of the state $|\psi\rangle$?

16. Using the basis in Prob. 15, another operator $B$ has the matrix form $B = \begin{pmatrix} \sqrt{2} & 0 & \sqrt{2} i \\ 0 & \sqrt{2} & 0 \\ -\sqrt{2} i & 0 & \sqrt{2} \end{pmatrix}$

(a) What are the eigenvectors and eigenvalues of this new operator $B$?
(b) Find the unitary transformation that diagonalizes the matrix $B$.
(c) What is the average value of the energy of the state $B|\psi\rangle$ where $|\psi\rangle = \frac{1}{2} (\sqrt{2}, 1, -i)$?
(d) Do $\mathcal{H}$ and $B$ commute?

17. Use the form of the Hamiltonian in Prob. 15 and the operator $B$ in Prob. 16. Suppose that when you measure the energy, you obtain the value $4 E_0$. Immediately afterwards you measure $B$. What values will you obtain for $B$ and with what probabilities?

18. Show that $\frac{d \langle A \rangle}{dt} = 0$ for $|\psi\rangle$ a stationary state and $A$ does not depend on time explicitly $\frac{d A}{dt} = 0$. Note: a stationary state is one for which $\mathcal{H} |\psi\rangle = E |\psi\rangle$ or $\Psi(x, t) = \psi(x) e^{-i E t/\hbar}$.

(b) Prove the equivalent relationship of the Virial Theorem in classical mechanics by considering $\frac{d \langle x^2 \rangle}{dt}$ for a stationary state $|\psi\rangle$.

19. Evaluate $\frac{d \langle x \rangle}{dt}$, $\frac{d \langle p_x \rangle}{dt}$ and $\frac{d \langle \mathcal{H} \rangle}{dt}$ assuming that $\mathcal{H} = \frac{p_x^2}{2 m} + \frac{1}{2} m \omega^2 x^2 + V_0 \left( \frac{x}{x_0} \right)^3$. How does these compared to their classical analogs?
2x2 Unitary and Hermition Operator

A Hamiltonian of a system has only two eigenstates $|\psi_1\rangle$ and $|\psi_1\rangle$. These two states form a complete ortho-normal set. The action of the operator $R$ is define to be: $R |\psi_1\rangle = 3 |\psi_1\rangle - i \sqrt{3} |\psi_2\rangle$ and $R |\psi_2\rangle = i \sqrt{3} |\psi_1\rangle + 5 |\psi_2\rangle$

(a) Write down the matrix representation of the operator $R$
(b) Is the operator Hermitian?
(c) Is the operator unitary?
(d) Determine the eigenvalues and eigenvectors of the operator.

(a) Write down the matrix representation of the operator $R$.

The elements of $R$ are specified by

$$ R_{ij} = \langle \psi_i | R | \psi_j \rangle \quad \text{where} \quad R = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \quad (1) $$

By definition, operating $R$ on the state $|\psi_1\rangle$ gives

$$ R |\psi_1\rangle = 3 |\psi_1\rangle - i \sqrt{3} |\psi_2\rangle \quad (2) $$

Therefore the matrix element $\langle \psi_1 | R | \psi_1 \rangle$ becomes

$$ \langle \psi_1 | R | \psi_1 \rangle = \langle \psi_1 | (3 |\psi_1\rangle - i \sqrt{3} |\psi_2\rangle \rangle = 3 \quad (3) $$

where we have used the fact that the states are orthonormal $\langle \psi_i | \psi_j \rangle = \delta_{ij}$. Similarly

$$ \langle \psi_1 | R | \psi_2 \rangle = \langle \psi_1 | (i \sqrt{3} |\psi_1\rangle + 5 |\psi_2\rangle \rangle = i \sqrt{3} \quad (4) $$

$$ \langle \psi_2 | R | \psi_1 \rangle = \langle \psi_2 | (3 |\psi_1\rangle - i \sqrt{3} |\psi_2\rangle \rangle = -i \sqrt{3} \quad (5) $$

$$ \langle \psi_2 | R | \psi_2 \rangle = \langle \psi_2 | (i \sqrt{3} |\psi_1\rangle + 5 |\psi_2\rangle \rangle = 5 \quad (6) $$

The matrix form of $R$ is therefore

$$ R = \begin{pmatrix} 3 & i \sqrt{3} \\ -i \sqrt{3} & 5 \end{pmatrix} \quad (7) $$

As a check one can write the basis in vector notation, $|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ so that

$$ R |\psi_1\rangle = \begin{pmatrix} 3 & i \sqrt{3} \\ -i \sqrt{3} & 5 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 3 \\ -i \sqrt{3} \end{pmatrix} \quad (8) $$

which agrees with the above definition. Similarly
\[ R|\psi_2\rangle = \begin{pmatrix} 3 & i\sqrt{3} \\ -i\sqrt{3} & 5 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} i\sqrt{3} \\ 5 \end{pmatrix} \] (9)

(b) Is the operator Hermitian?

The Hermitian adjoint of the matrix form of the operator is the complex conjugate of the transposed matrix.

\[ R^\dagger = \begin{pmatrix} 3 & i\sqrt{3} \\ -i\sqrt{3} & 5 \end{pmatrix}^\dagger = \begin{pmatrix} 3 & -i\sqrt{3} \\ i\sqrt{3} & 5 \end{pmatrix}^* = \begin{pmatrix} 3 & i\sqrt{3} \\ -i\sqrt{3} & 5 \end{pmatrix} \] (10)

The operator is therefore Hermitian because \( R = R^\dagger \)

(b) Is the operator unitary?

By definition a unitary operator does not change the norm. As we can see from the form of the transformations, the resulting vectors \( R|\psi_1\rangle \) and \( R|\psi_2\rangle \) are not normalized and therefore \( R \) is not unitary. Alternatively, one can check that \( R^\dagger R = 1 \) i.e.

\[ R^\dagger R = \begin{pmatrix} 3 & i\sqrt{3} \\ -i\sqrt{3} & 5 \end{pmatrix}^\dagger \begin{pmatrix} 3 & i\sqrt{3} \\ -i\sqrt{3} & 5 \end{pmatrix} = \begin{pmatrix} 3 & i\sqrt{3} \\ -i\sqrt{3} & 5 \end{pmatrix} \begin{pmatrix} 3 & i\sqrt{3} \\ -i\sqrt{3} & 5 \end{pmatrix} = \begin{pmatrix} 12 & 8i\sqrt{3} \\ -8i\sqrt{3} & 28 \end{pmatrix} \neq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \] (11)

(d) Determine the eigenvalues and eigenvectors of the operator.

To determine the eigenvalues, one set the determinant of \( R - \lambda I \) equal to zero and solve for \( \lambda \)

\[ \text{det}(R - \lambda I) = \text{det}\left[ \begin{pmatrix} 3 - \lambda & i\sqrt{3} \\ -i\sqrt{3} & 5 - \lambda \end{pmatrix} \right] \]

\[ = (3 - \lambda)(5 - \lambda) - (i\sqrt{3})(-i\sqrt{3}) \]

\[ = (15 - 8\lambda + \lambda^2) - (3) = 12 - 8\lambda + \lambda^2 = (-6 + \lambda)(-2 + \lambda) = 0 \] (12)

Therefore the eigenvalues are

\[ \lambda \to 2 \]
\[ \lambda \to 6 \] (13)

Note that \( |\lambda|^2 \neq 1 \) for each eigenvalue as expected for the eigenvalues of a non-unitary operator. The corresponding eigenfunctions are obtained by substituting the eigenvalues into the

\[ (R - \lambda I) \begin{pmatrix} a \\ b \end{pmatrix} = 0 \] and solve for \( a \) and \( b \). For the first eigenvalue

\[ \lambda_1 = 2 \] (14)
\[
R - I \lambda = \begin{pmatrix} 3 - \lambda & i \sqrt{3} \\ -i \sqrt{3} & 5 - \lambda \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a + i \sqrt{3} b \\ -i \sqrt{3} a + 3b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\]  
(15)

Solving the two equations
\[
\begin{align*}
a + i \sqrt{3} b &= 0 & a &= -i \sqrt{3} b \\
-i \sqrt{3} a + 3b &= 0 & a &= -i \sqrt{3} b
\end{align*}
\]  
(16)

which are equivalent. Taking \( b = 1 \), the state becomes
\[
|\psi_{\lambda=2}\rangle \propto \begin{pmatrix} -i \sqrt{3} \\ 1 \end{pmatrix}
\]  
(17)

To obtain the normalized state, one must divide the state by the square root of the norm. The norm of the state is given by the inner product of the state with itself
\[
(i \sqrt{3}, 1) \begin{pmatrix} -i \sqrt{3} \\ 1 \end{pmatrix} = 4
\]  
(18)

The normalized state is therefore
\[
|\psi_{\lambda=2}\rangle = \frac{1}{2} \begin{pmatrix} -i \sqrt{3} \\ 1 \end{pmatrix} = \begin{pmatrix} -i \sqrt{3} \\ 2 \\ 1 \\ 2 \end{pmatrix}
\]  
(19)

The second eigenfunction
\[
\lambda_2 = 6
\]  
(20)

\[
R - I \lambda = \begin{pmatrix} 3 - \lambda & i \sqrt{3} \\ -i \sqrt{3} & 5 - \lambda \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -3a + i \sqrt{3} b \\ -i \sqrt{3} a - b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\]  
(21)

Solving the two equations
\[
\begin{align*}
-3a + i \sqrt{3} b &= 0 & a &= \frac{ib}{\sqrt{3}} \\
-i \sqrt{3} a - b &= 0 & a &= \frac{ib}{\sqrt{3}}
\end{align*}
\]  
(22)

which are equivalent. Taking \( b = 1 \), the state becomes
\[
|\psi_{\lambda=6}\rangle \propto \begin{pmatrix} i \\ \sqrt{3} \\ 1 \end{pmatrix}
\]  
(23)
The normal is given by the inner product of the state with itself

\[
\left( -\frac{i}{\sqrt{3}}, 1 \right) \left( \frac{i}{\sqrt{3}}, 1 \right) = \frac{4}{3}
\]  

(24)

Dividing the state by the square root of the norm to obtain the normalize eigenstate

\[
|\psi_{\lambda=6}\rangle = \frac{\sqrt{3}}{2} \left( \frac{i}{\sqrt{3}}, 1 \right) = \left( \frac{i}{2}, \frac{\sqrt{3}}{2} \right)
\]

(25)

Because the two eigenvectors have different eigenvalues, they are orthogonal.

\[
\langle \psi_{\lambda=6} | \psi_{\lambda=2} \rangle = \left( -\frac{i}{2}, \frac{\sqrt{3}}{2} \right) \left( -\frac{i\sqrt{3}}{2}, 1 \right) = 0
\]

(26)
Discrete Hamiltonian

Consider a system described by a Hamiltonian with three eigenvectors and eigenvalues: \( \mathcal{H} |\psi_n\rangle = \epsilon_n |\psi_n\rangle \) for \( n = 1, 2, 3 \) with \( \epsilon_n = n^2 \epsilon_0 \). Given the state \( |\psi\rangle = 4i |\psi_1\rangle + i \sqrt{3} |\psi_2\rangle + \sqrt{6} |\psi_3\rangle \)

(a) Normalize \( |\psi\rangle \)

(b) If you make a measurement of the energy, what values are possible and with what probability do they occur?

(c) What is the average value of the energy of the state \( |\psi\rangle \)?

(a) Normalize \( |\psi\rangle \)

Because \( |\psi_i\rangle \) are eigenstates of a Hermitian operator with different eigenvalues, they must be orthogonal to each other, \( \langle \psi_j | \psi_i \rangle = \delta_{ij} \). Remembering to take the complex conjugate when we form the bra \( \langle \psi \) |

\[
\langle \psi | \psi \rangle = \left( -4i \langle \psi_1 | -i \sqrt{3} \langle \psi_2 | + \sqrt{6} \langle \psi_3 | \right) \left( 4i |\psi_1\rangle + i \sqrt{3} |\psi_2\rangle + \sqrt{6} |\psi_3\rangle \right)
= 16 \langle \psi_1 | \psi_1 \rangle + 4 \sqrt{3} \langle \psi_2 | \psi_1 \rangle + 4i \sqrt{6} \langle \psi_3 | \psi_1 \rangle + 4 \sqrt{3} \langle \psi_1 | \psi_2 \rangle + 3 \langle \psi_2 | \psi_2 \rangle + \langle \psi_1 | \psi_3 \rangle - 3i \sqrt{2} \langle \psi_3 | \psi_2 \rangle + 6 \langle \psi_3 | \psi_3 \rangle
= 16 + 3 + 6 = 25
\]

Therefore to normalize the state, one multiplies the state by \( \frac{1}{\sqrt{\langle \psi | \psi \rangle}} = \frac{1}{5} \)

\[
|\psi\rangle = \frac{4}{5} i |\psi_1\rangle + \frac{1}{5} i \sqrt{3} |\psi_2\rangle + \frac{1}{5} \sqrt{6} |\psi_3\rangle
\]

Alternatively denoting \( |\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \) and \( |\psi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \) then the matrix form for \( |\psi\rangle \) becomes

\[
|\psi\rangle = \begin{pmatrix} 4i \\ \frac{1}{5} i \sqrt{3} \\ \frac{1}{5} \sqrt{6} \\ \frac{1}{5} \end{pmatrix}
\]

Checking the normalization
\[
\langle \psi | \psi \rangle = \begin{pmatrix}
\frac{4i}{5}, \frac{i \sqrt{3}}{5}, \frac{\sqrt{6}}{5}
\end{pmatrix}^* \begin{pmatrix}
\frac{4i}{5} \\
\frac{i \sqrt{3}}{5} \\
\frac{\sqrt{6}}{5}
\end{pmatrix}
\]
\[
= \begin{pmatrix}
\frac{4i}{5}, \frac{-i \sqrt{3}}{5}, \frac{-\sqrt{6}}{5}
\end{pmatrix}^* \begin{pmatrix}
\frac{4i}{5} \\
\frac{i \sqrt{3}}{5} \\
\frac{\sqrt{6}}{5}
\end{pmatrix}
\]
\[
= \frac{16}{25} + \frac{3}{25} + \frac{6}{25} = 1
\]

(b) If you make a measurement of the energy, what values are possible and with what probability do they occur?

Whenever you make a single measurement, one always measures an eigenvalue and the probability of measuring a particular eigenvalue is equal to the absolute square of the coefficient of the corresponding eigenfunction in the expansion of the original state.

For this problem, the result of a single measurement can be \( \varepsilon_1 = \varepsilon_0 \), \( \varepsilon_2 = 4 \varepsilon_0 \), \( \varepsilon_3 = 9 \varepsilon_0 \) with probabilities \( \frac{16}{25} \), \( \frac{3}{25} \), \( \frac{6}{25} \) respectively.

(c) What is the average value of the energy of the state?

Formally, the average value of the energy is the expectation value evaluated with the normalized wavefunction.

\[
\langle \psi | \mathcal{H} | \psi \rangle = -\frac{4}{5} \langle \psi | \psi \rangle - \frac{1}{5} i \sqrt{3} \langle \psi | \psi \rangle + \frac{1}{5} \sqrt{6} \langle \psi | \psi \rangle \mathcal{H} \left( -\frac{i}{5} \langle \psi | \psi \rangle + \frac{1}{5} i \sqrt{3} \langle \psi | \psi \rangle + \frac{1}{5} \sqrt{6} \langle \psi | \psi \rangle \right)
\]
\[
= \left( -\frac{4}{5} \langle \psi | \psi \rangle - \frac{1}{5} i \sqrt{3} \langle \psi | \psi \rangle + \frac{1}{5} \sqrt{6} \langle \psi | \psi \rangle \right) \mathcal{H} \left( -\frac{i}{5} \langle \psi | \psi \rangle + \frac{4}{5} i \sqrt{3} \langle \psi | \psi \rangle + \frac{4}{5} \sqrt{6} \langle \psi | \psi \rangle \right)
\]
\[
= \frac{16}{25} \varepsilon_0 \langle \psi | \psi \rangle + \frac{4}{25} \sqrt{3} \varepsilon_0 \langle \psi | \psi \rangle + \frac{4}{25} \sqrt{6} \varepsilon_0 \langle \psi | \psi \rangle + \frac{16}{25} \sqrt{3} \varepsilon_0 \langle \psi | \psi \rangle + \frac{12}{25} \varepsilon_0 \langle \psi | \psi \rangle
\]
\[
= 16 \varepsilon_0 + 12 \varepsilon_0 + 54 \varepsilon_0 + 82 \varepsilon_0
\]

Alternatively in matrix language,
\[ \langle \psi | \mathcal{H} | \psi \rangle = \left( -\frac{4i}{5}, -i \frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \begin{pmatrix} \varepsilon_0 & 0 & 0 \\ 0 & 4 \varepsilon_0 & 0 \\ 0 & 0 & 9 \varepsilon_0 \end{pmatrix} \begin{pmatrix} \frac{4i}{5} \\ i \frac{\sqrt{3}}{5} \\ \frac{\sqrt{6}}{5} \end{pmatrix} \]

\[ = \left( -\frac{4i}{5}, -i \frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \begin{pmatrix} 4 \varepsilon_0 \\ \frac{5}{5} \\ \frac{\sqrt{3} \varepsilon_0}{5} \end{pmatrix} \]

\[ = \frac{16}{25} \varepsilon_0 + \frac{4}{25} \varepsilon_0 + \frac{6}{25} \varepsilon_0 = \frac{82 \varepsilon_0}{25} \]

Finally one can use the probabilistic interpretation. The average energy is the energy eigenvalue times the appropriate probability i.e.,

\[ \langle \psi | \mathcal{H} | \psi \rangle = E_1 |c_1|^2 + E_2 |c_2|^2 + E_3 |c_3|^2 \]

\[ = \frac{16}{25} \varepsilon_1 + \frac{3}{25} \varepsilon_2 + \frac{6}{25} \varepsilon_3 = \frac{16}{25} \varepsilon_0 + \frac{4}{25} \varepsilon_0 + \frac{9}{25} \varepsilon_0 = \frac{82 \varepsilon_0}{25} \]  

(7)

(d) What is the average value of \( E^2 \) of the state \(|\psi\rangle\)?

Formally, the average value of \( E^2 \) is the expectation value of \( \mathcal{H}^2 \) evaluated with the normalized wavefunction.

\[ \langle \psi | \mathcal{H}^2 | \psi \rangle = \left( -\frac{4i}{5}, -i \frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \mathcal{H} \mathcal{H} \left( -\frac{4i}{5}, -i \frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \]

\[ = \left( -\frac{4i}{5}, -i \frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \mathcal{H} \left( -\frac{4i \varepsilon_0}{5}, -i \frac{\sqrt{3} \varepsilon_0}{5}, \frac{\sqrt{6} \varepsilon_0}{5} \right) \]

\[ = \left( \frac{48}{25} \varepsilon_0^2 + \frac{4}{25} \sqrt{3} \varepsilon_0^2 + \frac{4}{25} \frac{1}{\sqrt{6}} \varepsilon_0^2 + \frac{64}{25} \sqrt{3} \varepsilon_0^2 + \frac{48}{25} \varepsilon_0^2 \right) \]

\[ = \frac{16}{25} \varepsilon_0^2 + \frac{48 \varepsilon_0^2}{25} + \frac{486 \varepsilon_0^2}{25} \]

(8)

Alternatively in matrix language,
\[
\langle \psi | H H | \psi \rangle = \left( -\frac{4i}{5}, -i\frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \left( \begin{array}{ccc}
\varepsilon_0 & 0 & 0 \\
0 & 4\varepsilon_0 & 0 \\
0 & 0 & 9\varepsilon_0
\end{array} \right) \left( \begin{array}{c}
\varepsilon_0 \\
0 \\
0
\end{array} \right) = \frac{4i\varepsilon_0}{5} \begin{array}{c}
i\frac{\sqrt{3}}{5} \\
\frac{\sqrt{6}}{5}
\end{array}
\]

\[
= \left( -\frac{4i}{5}, -i\frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \left( \begin{array}{ccc}
\varepsilon_0 & 0 & 0 \\
0 & 4\varepsilon_0 & 0 \\
0 & 0 & 9\varepsilon_0
\end{array} \right) \left( \begin{array}{c}
\frac{4i\varepsilon_0}{5} \\
i\frac{\sqrt{3}\varepsilon_0}{5} \\
\frac{9\sqrt{6}\varepsilon_0}{5}
\end{array} \right)
\]

\[
= \left( -\frac{4i}{5}, -i\frac{\sqrt{3}}{5}, \frac{\sqrt{6}}{5} \right) \left( \begin{array}{c}
\frac{4i\varepsilon_0^2}{5} \\
i\frac{\sqrt{3}\varepsilon_0^2}{5} \\
\frac{81\sqrt{6}\varepsilon_0^2}{5}
\end{array} \right)
\]

\[
= \frac{16\varepsilon_0^2}{25} + \frac{48\varepsilon_0^2}{25} + \frac{486\varepsilon_0^2}{25} = 22\varepsilon_0^2
\]

Finally using the probabilities
\[
\langle \psi | H H | \psi \rangle = E_1^2 |c_1|^2 + E_2^2 |c_2|^2 + E_3^2 |c_3|^2
\]

\[
= \frac{16}{25} \varepsilon_1^2 + \frac{3}{25} \varepsilon_2^2 + \frac{6}{25} \varepsilon_3^2 = \frac{16}{25} \varepsilon_0^2 + \frac{16}{25} \varepsilon_0^2 + \frac{81}{25} \varepsilon_0^2 = 22\varepsilon_0^2
\]
B operator in basis of Hamiltonian

Using the basis described by a Hamiltonian with three eigenvectors and eigenvalues: \( \mathcal{H} |\psi_n\rangle = \varepsilon_n |\psi_n\rangle \) for \( n = 1, 2, 3 \) with \( \varepsilon_n = n^2 E_0 \). Another operator has the matrix form

\[
B = b \begin{pmatrix}
\sqrt{2} & 0 & i \sqrt{2} \\
0 & 2 & 0 \\
-2 & 0 & 2
\end{pmatrix}
\]

(a) What are the eigenfunctions and eigenvalues of this new operator?
(b) Find the unitary transformation that diagonalizes the matrix \( B \).
(c) What is the average value of the energy of the state \( B|\psi\rangle \) where \( |\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 2 \\ -i \end{pmatrix} \)?

(a) (a) What are the eigenfunctions and eigenvalues of this new operator?

To determine the eigenvalues, we substitute \( \lambda \) from the diagonal and set the determinant to zero

\[
det(B - I \lambda) = det\left[ \begin{array}{ccc}
\sqrt{2} & 0 & i \sqrt{2} \\
0 & \sqrt{2} & 0 \\
-2 & 0 & 2
\end{array} \right] = 0
\]

or

\[
(\sqrt{2} - \lambda)(\sqrt{2} - \lambda)(\sqrt{2} - \lambda) + \langle 0 | 0 \rangle (i \sqrt{2} - \lambda) + (i \sqrt{2} - \lambda) (0) = 0
\]

or

\[
(\sqrt{2} - \lambda)(2 \sqrt{2} - \lambda) \lambda = 0
\]

which has roots \( \lambda = 2 \sqrt{2} b, \sqrt{2} b, 0 \)

To find the eigenfunctions, we substitute the eigenvalue into the eigenfunction equation \( (B - \lambda I) |\psi\rangle = 0 \) and determine the the unknown coefficient.

For \( \lambda = 2 \sqrt{2} b \), we obtain 3 equations

\[
\begin{pmatrix}
\sqrt{2} & 0 & i \sqrt{2} \\
0 & \sqrt{2} & 0 \\
-2 & 0 & 2
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
a_3
\end{pmatrix}
= \begin{pmatrix}
\sqrt{2} b a_1 + i \sqrt{2} b a_3 \\
-\sqrt{2} b a_2 \\
-i \sqrt{2} b a_1 - \sqrt{2} b a_3
\end{pmatrix}
= 0
\]

or
\[ a_1 \rightarrow i a_3 \]
\[ a_2 \rightarrow 0 \quad \tag{5} \]

Setting \( a_1 = 1 \) and normalizing we obtained for \( \lambda = 2 \sqrt{2} \ b \)

\[
|\psi_1\rangle = \begin{pmatrix}
i \\
\sqrt{2} \\
0 \\
1 \\
\sqrt{2}
\end{pmatrix} \quad \tag{6}
\]

For \( \lambda = \sqrt{2} \ b \), the 3 equations become

\[
\begin{pmatrix}
0 & 0 & i \sqrt{2} \ b \\
0 & 0 & 0 \\
-i \sqrt{2} \ b & 0 & 0
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
a_3
\end{pmatrix} = \begin{pmatrix}
i \sqrt{2} \ b a_3 \\
0 \\
-i \sqrt{2} \ b a_1
\end{pmatrix} = 0 \quad \tag{7}
\]

or

\[ a_1 \rightarrow 0 \]
\[ a_3 \rightarrow 0 \quad \tag{8} \]

Now \( a_1 = 0 \) and \( a_3 = 0 \). Taking \( a_2 = 1 \) we have that

\[
|\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \tag{9}
\]

For \( \lambda = 0 \), the 3 equations become

\[
\begin{pmatrix}
\sqrt{2} \ b & 0 & i \sqrt{2} \ b \\
0 & \sqrt{2} \ b & 0 \\
-i \sqrt{2} \ b & 0 & \sqrt{2} \ b
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
a_3
\end{pmatrix} = \begin{pmatrix}
\sqrt{2} \ b a_1 + i \sqrt{2} \ b a_3 \\
\sqrt{2} \ b a_2 \\
-i \sqrt{2} \ b a_1 + \sqrt{2} \ b a_3
\end{pmatrix} = 0 \quad \tag{10}
\]

or

\[ a_1 \rightarrow -i a_3 \]
\[ a_2 \rightarrow 0 \quad \tag{11} \]
\[ |\psi_3\rangle = \begin{pmatrix} -\frac{i}{\sqrt{2}} \\ 0 \\ 1 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \]

The eigenvalues and eigenvectors are therefore

\[ \lambda_1 = 2\sqrt{2} \ b \ |b_1\rangle = \begin{pmatrix} \frac{i}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \]

\[ \lambda_2 = \sqrt{2} \ b \ |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \]

\[ \lambda_3 = 0 \ |b_3\rangle = \begin{pmatrix} -\frac{i}{\sqrt{2}} \\ 0 \\ 1 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \] (13)

(b) Find the unitary transformation that diagonalizes the matrix \( B \).

The unitary transformation that diagonalizes \( B \) is obtained by using the previously found eigenfunctions as the columns of the unitary matrix

\[ U = \begin{pmatrix} \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \\ 1 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \] (14)

To verify this result, we check to see whether \( U^\dagger B U \) is diagonal with the eigenvalues on the diagonal

\[ U^\dagger B U = \begin{pmatrix} \frac{i}{\sqrt{2}} & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{i}{\sqrt{2}} & 0 & i\sqrt{2} b \\ 0 & \frac{i}{\sqrt{2}} & 0 \\ -i\sqrt{2} b & 0 & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \\ 1 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \]
which is the diagonal matrix, with the eigenvalues along the diagonal.

(c) What is the average value of the energy of the state $B|\psi\rangle$?

As before, the energy is obtained by evaluating $\langle \phi | H | \phi \rangle$ where $| \phi \rangle$ is the normalized version of $B|\psi\rangle$. Evaluating $B|\psi\rangle$

$$
|B\psi\rangle = \begin{pmatrix}
\sqrt{2} b & 0 & i \sqrt{2} b \\
0 & \sqrt{2} b & 0 \\
-i \sqrt{2} b & 0 & \sqrt{2} b
\end{pmatrix}
\begin{pmatrix}
1 \\
\sqrt{2} \\
1/2 \\
i
\end{pmatrix}
$$

$$
= \begin{pmatrix}
\frac{1}{\sqrt{2}} b \\
\frac{1}{2} b \\
\frac{1}{2} i \left( 2 + \sqrt{2} \right) b
\end{pmatrix}
$$

(16)

As one can see, the resulting state is not normalized. Remembering that $B$ is a Hermitian operator and therefore $b$ is a real number, the norm of the state is

$$
\langle B\psi | B\psi \rangle = \begin{pmatrix}
\frac{1}{\sqrt{2}} b \\
\frac{1}{2} b \\
\frac{1}{2} i \left( 2 + \sqrt{2} \right) b
\end{pmatrix}
\begin{pmatrix}
\frac{1}{\sqrt{2}} b \\
\frac{1}{2} b \\
\frac{1}{2} i \left( 2 + \sqrt{2} \right) b
\end{pmatrix}
$$

$$
= \frac{1}{2} \left( 7 + 4 \sqrt{2} \right) b^2
$$

(17)

Therefore the normalized form of $|B\psi\rangle$ (call it $|\phi\rangle$)
\[ |\phi\rangle = \begin{pmatrix} \frac{2 + \sqrt{2}}{\sqrt{14 + 8 \sqrt{2}}} \\ 1 \\ \frac{1}{\sqrt{7 + 4 \sqrt{2}}} \\ -\frac{i (2 + \sqrt{2})}{\sqrt{14 + 8 \sqrt{2}}} \end{pmatrix} \]

and therefore

\[
\langle \phi | H | \phi \rangle = \begin{pmatrix} \frac{2 + \sqrt{2}}{\sqrt{14 + 8 \sqrt{2}}} \\ 1 \\ \frac{1}{\sqrt{7 + 4 \sqrt{2}}} \\ -\frac{i (2 + \sqrt{2})}{\sqrt{14 + 8 \sqrt{2}}} \end{pmatrix} \begin{pmatrix} E_0 & 0 & 0 \\ 0 & 4E_0 & 0 \\ 0 & 0 & 9E_0 \end{pmatrix} \begin{pmatrix} \frac{2 + \sqrt{2}}{\sqrt{14 + 8 \sqrt{2}}} \\ 1 \\ \frac{1}{\sqrt{7 + 4 \sqrt{2}}} \\ -\frac{i (2 + \sqrt{2})}{\sqrt{14 + 8 \sqrt{2}}} \end{pmatrix} \]

\[
= \frac{10 \left(2 + \sqrt{2}\right)^2 E_0}{14 + 8 \sqrt{2}} + \frac{4 E_0}{7 + 4 \sqrt{2}}
\]

\[
= \frac{2}{17} \left(39 + 2 \sqrt{2}\right) E_0
\]

(d) Do \(H\) and \(B\) commute?

To test whether \(H\) and \(B\) commute, we can just multiply their matrix representations and test whether \(HB = BH\)

\[
H B = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & 4E_0 & 0 \\ 0 & 0 & 9E_0 \end{pmatrix} \begin{pmatrix} \sqrt{2} b & 0 & i \sqrt{2} b \\ 0 & \sqrt{2} b & 0 \\ -i \sqrt{2} b & 0 & \sqrt{2} b \end{pmatrix}
\]
\[ bE_0 \begin{pmatrix} \sqrt{2} & 0 & i \sqrt{2} \\ 0 & 4\sqrt{2} & 0 \\ -9i \sqrt{2} & 0 & 9\sqrt{2} \end{pmatrix} \]

and

\[
B \mathcal{H} = \begin{pmatrix} \sqrt{2} b & 0 & i \sqrt{2} b \\ 0 & \sqrt{2} b & 0 \\ -i \sqrt{2} b & 0 & \sqrt{2} b \end{pmatrix} \begin{pmatrix} E_0 & 0 & 0 \\ 0 & 4E_0 & 0 \\ 0 & 0 & 9E_0 \end{pmatrix} \]

\[= bE_0 \begin{pmatrix} \sqrt{2} & 0 & 9i \sqrt{2} \\ 0 & 4\sqrt{2} & 0 \\ -i \sqrt{2} & 0 & 9\sqrt{2} \end{pmatrix} \] (21)

and so \( \mathcal{H} \) and \( B \) do not commute.
Measurement of B operator after measurement of the Energy

Using the basis described by a Hamiltonian with three eigenvectors and eigenvalues: \( \mathcal{H} |\psi_n\rangle = \varepsilon_n |\psi_n\rangle \) for \( n = 1, \ 2, \ 3 \) with \( \varepsilon_n = n^2 E_0 \). another operator has the matrix form

\[
B = \begin{pmatrix}
\sqrt{2} & 0 & i \sqrt{2} \\
0 & \sqrt{2} & 0 \\
-i \sqrt{2} & 0 & \sqrt{2}
\end{pmatrix}
\]

Suppose that when you measure the energy, you obtain the value 4\( E_0 \). Immediately afterwards you measure \( B \). What values will you obtain for \( B \) and with what probabilities?

If you measure the energy 4\( E_0 \) then the original wavefunction will have collapsed into \( |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \) If you then measure \( B \) you can only measure an eigenvalue of \( B \), \( \lambda = 2 \sqrt{2} \ b \), \( \sqrt{2} \ b \), \( 0 \). To determine the probability, we need to expand \( |\psi_2\rangle \) in terms of the eigenstates of \( B \)

\[
\lambda_1 = 2 \sqrt{2} \ b \quad |b_1\rangle = \begin{pmatrix} i \\ \sqrt{2} \\ 0 \\ 1 \\ \sqrt{2} \end{pmatrix}
\]

\[
\lambda_2 = \sqrt{2} \ b \quad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}
\]

\[
\lambda_3 = 0 \quad |b_3\rangle = \begin{pmatrix} -i \\ \sqrt{2} \\ 0 \\ 1 \\ \sqrt{2} \end{pmatrix}
\]

Remember that in the expansion

\[
|\psi_2\rangle = \sum_{n=1}^{3} c_n |b_n\rangle
\]

the coefficients \( c_n \) are obtained by taking the inner product with one of the eigenstates of \( B \).
\[ c_1 = \langle b_1 | \psi_2 \rangle = \begin{pmatrix} -\frac{i}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0 \]

\[ c_2 = \langle b_2 | \psi_2 \rangle = (0, 1, 0) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 1 \]

\[ c_3 = \langle b_3 | \psi_2 \rangle = \begin{pmatrix} \frac{i}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0 \]

and therefore the probabilities of measuring the eigenvalues of \( B \) are

\[ \lambda_1 = 2 \sqrt{2} \quad p_1 = 0 \]

\[ \lambda_2 = \sqrt{2} \quad p_2 = 1 \]  \hspace{1cm} (5)

\[ \lambda_3 = 0 \quad p_3 = 0 \]
Virial Theorem

Show that \( \frac{d\langle A \rangle}{dt} = 0 \) for \(|\psi\rangle\) a stationary state and \( A \) does not depend on time explicitly \( \frac{dA}{dt} = 0 \).

Note: a stationary state is one for which \( \mathcal{H} |\psi\rangle = E |\psi\rangle \) or \( \Psi[x, t] = \psi[x] e^{-iE\psi \hbar} \).

(b) Prove the equivalent relationship of the Virial Theorem in classical mechanics by considering \( \frac{d\langle xp\rangle}{dt} \) for a stationary state \(|\psi\rangle\).

(a) For a general operator and state, the Ehrenfest relationship is

\[
\frac{\partial \langle A \rangle}{\partial t} = \frac{\partial \langle A | \psi \rangle}{\partial t} = \frac{i}{\hbar} \langle \psi | [\mathcal{H}, A] | \psi \rangle + \left( \psi \left| \frac{\partial A}{\partial t} \right| \psi \right) \quad (1)
\]

If \( A \) does not depend on time explicitly, \( \frac{dA}{dt} = 0 \) and we have that

\[
\frac{\partial \langle A \rangle}{\partial t} = \frac{i}{\hbar} \langle \psi | [\mathcal{H}, A] | \psi \rangle \quad (2)
\]

Expanding the commutator

\[
\frac{\partial \langle A \rangle}{\partial t} = \frac{i}{\hbar} \langle \psi | (\mathcal{H} A - A \mathcal{H}) | \psi \rangle = \frac{i}{\hbar} \left( \langle \psi | \mathcal{H} A | \psi \rangle - \langle \psi | A \mathcal{H} | \psi \rangle \right) \quad (3)
\]

Because the Hamiltonian is a Hermitian operator we can move the operator to act on the first state

\[
\frac{\partial \langle A \rangle}{\partial t} = \frac{i}{\hbar} \left( \langle \mathcal{H} \psi | A | \psi \rangle - \langle \psi | A \mathcal{H} | \psi \rangle \right) \quad (4)
\]

But \( \mathcal{H} |\psi\rangle = E |\psi\rangle \)

\[
\frac{\partial \langle A \rangle}{\partial t} = \frac{i}{\hbar} \left( \langle E \psi | A | \psi \rangle - \langle \psi | AE | \psi \rangle \right) \quad (5)
\]

Given that \( E \) is a real constant, the above becomes

\[
\frac{\partial \langle A \rangle}{\partial t} = \frac{i}{\hbar} \left( E \langle \psi | A | \psi \rangle - E \langle \psi | A \psi \rangle \right) = 0 \quad (6)
\]

(b) Prove the equivalent relationship of the Virial Theorem in classical mechanics by considering \( \frac{d\langle xp\rangle}{dt} \) for a stationary state \(|\psi\rangle\).

Because neither \( x \) or \( p \) depend explicitly on time, the time rate of change of the expectation value of \( xp \) for a stationary state becomes

\[
\frac{\partial \langle xp\rangle}{\partial t} = \langle \psi | [\mathcal{H}, A] | \psi \rangle = 0 \quad (7)
\]
Writing the Hamiltonian as $\mathcal{H} = \frac{p^2}{2m} + V(x)$ and expanding using the commutator relationship, $[\mathcal{H}, x p] = x[\mathcal{H}, p] + [\mathcal{H}, x]p$, we have that

$$[\mathcal{H}, x p] = x[\mathcal{H}, p] + [\mathcal{H}, x]p$$

$$= x[V(x), p] + \left[\frac{p^2}{2m}, x\right]p$$

(8)

where we have used the fact that $\left[\frac{p^2}{2m}, p\right] = 0$ and $[V(x), x] = 0$. Reducing the commutators further

$$[V(x), p] \psi(x) = \left(V(x)\left(-i\hbar \frac{\partial}{\partial x}\right) - \left(-i\hbar \frac{\partial}{\partial x}\right)V(x)\right)\psi(x)$$

$$= -i\hbar V(x) \frac{\partial \psi(x)}{\partial x} + i\hbar \frac{\partial V(x)}{\partial x} \psi(x) + i\hbar V(x) \frac{\partial \psi(x)}{\partial x}$$

$$= i\hbar \frac{\partial V(x)}{\partial x} \psi(x)$$

(9)

and so

$$[V(x), p] = i\hbar \frac{\partial V(x)}{\partial x}$$

(10)

Similarly

$$\left[\frac{p^2}{2m}, x\right] = \frac{p}{2m} [p, x] + [p, x] \frac{p}{2m}$$

$$= \frac{p}{2m} \left(-i\hbar\right) + \left(-i\hbar\right) \frac{p}{2m}$$

$$= -i\frac{p\hbar}{m}$$

(11)

Combining these together

$$\langle \psi | [\mathcal{H}, x p] | \psi \rangle = \langle \psi | x[V(x), p] | \psi \rangle + \langle \psi | \left[\frac{p^2}{2m}, x\right]p | \psi \rangle$$

$$= \langle \psi | x i\hbar \frac{\partial V(x)}{\partial x} | \psi \rangle + \langle \psi | -i\frac{p\hbar}{m} p | \psi \rangle = 0$$

(12)

or

$$\langle \psi | x \frac{\partial V(x)}{\partial x} | \psi \rangle = \langle \psi | \frac{p^2}{m} | \psi \rangle = 2 \langle \psi | \frac{p^2}{2m} | \psi \rangle = 2 \langle \psi | KE | \psi \rangle$$

(13)

The average kinetic energy, $\langle KE \rangle$ is equal to one-half the average of $x \frac{\partial V(x)}{\partial x}$. 
Time Dependence of Operators

Evaluate \( \frac{d\langle x \rangle}{dt} \), \( \frac{d\langle p_x \rangle}{dt} \) and \( \frac{d\langle H \rangle}{dt} \) assuming that \( H = \frac{p_x^2}{2m} + \frac{1}{2} m \omega^2 x^2 + V_0 \left( \frac{x}{x_0} \right)^3 \). How does these compared to their classical analogs?

For a general operator

\[
\frac{\partial \langle A \rangle}{\partial t} = \frac{i}{\hbar} \langle [H, A] \rangle + \frac{\partial A}{\partial t}
\]

(1)

None of the above operators have an explicit time dependence, therefore \( \frac{\partial A}{\partial t} = 0 \) for each of them.

(a) \( \frac{d\langle x \rangle}{dt} \)

\[
\frac{\partial \langle x \rangle}{\partial t} = \frac{i}{\hbar} \langle [H, x] \rangle
\]

(2)

The only terms in the Hamiltonian which do not commute with \( x \) are the momenta terms \( x \) commutes with \( x^2 \) and \( x^3 \). In particular,

\[
[H, x] = \left[ \frac{p^2}{2m}, x \right]
\]

(3)

Using the rule

\[
\]

(4)

we have that

\[
\left[ \frac{p^2}{2m}, x \right] = \frac{1}{2m} \left( p[p, x] + [p, x] p \right)
\]

(5)

but the commutator of \( p \) and \( x \) is just \(-i\hbar\) and so

\[
\left[ \frac{p^2}{2m}, x \right] = -\frac{i\hbar}{m}
\]

(6)

and so

\[
\frac{\partial \langle x \rangle}{\partial t} = \frac{i}{\hbar} \left( \langle [H, x] \rangle \right) = \frac{i}{\hbar} \left( \frac{p^2}{2m}, x \right) = \langle \frac{p}{m} \rangle
\]

(7)

which states that the time rate of change of the average position is the average momentum divided by the mass or the average velocity.

(b) \( \frac{d\langle p \rangle}{dt} \)
\[ \frac{\partial \langle p \rangle}{\partial t} = \frac{i \langle [\mathcal{H}, p]\rangle}{\hbar} \quad (8) \]

The only terms in the Hamiltonian which do not commute with \( p \) are the position terms in the potential (\( p \) commutes with \( p^2 \). In particular, \[ [\mathcal{H}, p] = \left[ \frac{1}{2} m x^2 \omega^2 + \frac{x^3 V_0}{x_0^3}, p \right] = \frac{1}{2} m \omega^2 [x^2, p] + \frac{V_0 [x^3, p]}{x_0^3} \quad (9) \]

we have that \[ [x^2, p] = x [x, p] + x [x, p] \quad (11) \]
but the commutator of \( x \) and \( p \) is just \( i \hbar \) and so \[ [x^2, p] = 2i x \hbar \quad (12) \]
Similarly \[ [x^3, p] = x [x^2, p] + x^2 [x, p] \quad (13) \]
Using the result from Eq. 12 \[ [x^3, p] = 2i x^2 \hbar + i x^2 \hbar = 3i x^2 \hbar \quad (14) \]
and so \[ \frac{\partial \langle p \rangle}{\partial t} = \frac{i \langle [\mathcal{H}, p]\rangle}{\hbar} = \frac{1}{2} m \omega^2 \langle [x^2, p]\rangle + \frac{V_0 \langle [x^3, p]\rangle}{x_0^3} \]
\[ = -m \omega^2 \langle x \rangle - \frac{3V_0 \langle x^2 \rangle}{x_0^3} \quad (15) \]
which states that the time rate of change of the average momentum is the average force determined by \[ \left( -\frac{\partial V[x]}{\partial x} \right) = -m \omega^2 \langle x \rangle - \frac{3V_0 \langle x^2 \rangle}{x_0^3} \quad (16) \]

(c) For \( \frac{d}{dt} \langle \mathcal{H} \rangle \)
\[ \frac{\partial \langle \mathcal{H} \rangle}{\partial t} = \frac{i \langle [\mathcal{H}, \mathcal{H}]\rangle}{\hbar} \quad (17) \]
but since the Hamiltonian commutes with itself, the time rate of change of the average energy is zero
\[ \frac{\partial \langle \mathcal{H} \rangle}{\partial t} = 0 \]