Chapter 1: Review of Quantum Mechanics

1.1 Postulates of Quantum Mechanics

1.1.1 Postulates One, Two, and Three

There are several postulates of quantum mechanics. These are postulates since they cannot be derived from some other deeper theory. They are known only from experiments. The first few are:

1) The state of physical system at time 't' is described by a vector (or a ket), denoted by $|\psi(t)\rangle$, that belongs to a Hilbert space. The state vector captures all information that is knowable about the physical system.
2) Every measurable quantity A (like position or momentum of a particle) is described by an operator $\hat{A}$ that acts in the Hilbert space.
3) The only possible out come of a measurement of the quantity A is one of the eigenvalues of the operator $\hat{A}$.

Hilbert Spaces

A Hilbert space is just a fancy name for a linear vector space with certain properties. Vectors $|v\rangle$, $|u\rangle$, $|w\rangle$,… belong to a Hilbert space H if and only if:

(1) For some operation, denoted by '+', the vector $|v\rangle + |u\rangle$ belongs to H if $|v\rangle$ and $|u\rangle$ belong to H.

(2) $|v\rangle + |u\rangle = |u\rangle + |v\rangle$.

(3) $|v\rangle + (|u\rangle + |w\rangle) = (|v\rangle + |u\rangle) + |w\rangle$.

(4) There is a 'zero vector' 0 such that $|v\rangle + 0 = |v\rangle$.

(5) For any $|v\rangle$ there exists a vector $|-v\rangle$ such that $|v\rangle + |-v\rangle = 0$.

(6) For a complex number α, $\alpha|v\rangle \in$ H if $|v\rangle \in$ H.

(7) For a complex number α, $\alpha(|v\rangle + |u\rangle) = \alpha|v\rangle + \alpha|u\rangle$.

(8) For complex numbers α, β, $(\alpha + \beta)|v\rangle = \alpha|v\rangle + \beta|v\rangle$.

(9) The inner product of two vectors $|v\rangle$ and $|u\rangle$, denoted by $\langle u|v\rangle$, has the following properties:

(a) $\langle u|v\rangle = \langle v|u\rangle^*$.

(b) $\langle v|v\rangle \geq 0$, with equality if and only if $|v\rangle = 0$.

$\sqrt{\langle v|v\rangle}$ is called the magnitude of the vector.

(10) An operator $\hat{O}$ acting in the Hilbert space H has the property that for any vector $|v\rangle$ belonging to H, $\hat{O}|v\rangle$ is also some vector belonging to H.

Examples: There are many examples of Hilbert spaces besides the Hilbert space of quantum states. For example, the space spanned by 2-dimensional column vectors form a Hilbert space in which the vectors

are column vectors, $|v\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$, $|u\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$,… where $\{a,b,c,d,...\}$ are complex numbers. The inner product $\langle u|v\rangle$ is $\begin{bmatrix} c^* & d^* \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$. The operators are 2×2 matrices $\begin{bmatrix} e & f \\ g & h \end{bmatrix}$.

Properties of Operators in Hilbert Space

Eigenvectors and Eigenvalues: A vector $|v\rangle$ is an eigenvector of an operator $\hat{O}$ if and only if $\hat{O}|v\rangle = \lambda |v\rangle$ and the complex number λ is called the eigenvalue corresponding to the eigenvector $|v\rangle$. In general, an operator $\hat{O}$ can have many eigenvalues $\lambda_1, \lambda_2, \lambda_3 ....$ and the corresponding eigenvectors are $|v_1\rangle, |v_2\rangle, |v_3\rangle, ...$ i.e. $\hat{O}|v_k\rangle = \lambda_k |v_k\rangle$.

Adjoint Operators: The adjoint operator $\hat{O}^+$ corresponding to $\hat{O}$ is defined by the following relation,

$$\langle u|\hat{O}|v\rangle = \langle v|\hat{O}^+|u\rangle^* \qquad (1)$$

Let $|w\rangle = \hat{O}|v\rangle$. The left hand side in (1) is then $\langle u|w\rangle$. But (by property 9(a) of Hilbert spaces) $\langle u|w\rangle = \langle w|u\rangle^*$. Comparing with right hand side of (1) we get $\langle w| = \langle v|\hat{O}^+$. We can state the properties of bra $\langle w|$ corresponding to ket $|w\rangle$,

(a) if $|w\rangle = \alpha|v\rangle + \beta|u\rangle$ then $\langle w| = \alpha^* \langle v| + \beta^* \langle u|$.

(b) if $|w\rangle = \hat{O}|v\rangle$ then $\langle w| = \langle v|\hat{O}^+$.

Hermitian Operators: An operator $\hat{O}$ is Hermitian (or self-adjoint) if and only if $\hat{O} = \hat{O}^+$. In quantum mechanics, operators corresponding to observables are always Hermitian since Hermitian operators have real eigenvalues.

Basis Vectors

Any set of vectors that belong to H and 'span' H (i.e. where any vector in H can be written as a sum of vectors belonging to this set) is called a basis set. The minimum number of vectors in a basis set is called the dimentionality of H. For example, if $|v_1\rangle, |v_2\rangle, |v_3\rangle ... |v_n\rangle$ span an n-dimensional Hilbert space then any other vector $|w\rangle$ in H can be written as $|w\rangle = \sum_{k=1}^{n} a_k |v_k\rangle$. Usually basis sets are chosen such that all vectors in it are mutually orthogonal. For example, for the Hilbert space of 2-dimensional column vectors a basis set is $\begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

Orthonormal Basis: In the expansion $|w\rangle = \sum_{k=1}^{n} a_k |v_k\rangle$ the expansion coefficients a_j can be determined by multiplying both sides with the bra $\langle v_j|$,

$$\langle v_j | w \rangle = \langle v_j | \left(\sum_{k=1}^{n} a_k | v_k \rangle \right)$$

$$\Rightarrow \langle v_j | w \rangle = \sum_{k=1}^{n} a_k \langle v_j | v_k \rangle$$

Since for orthogonal basis set $\langle v_j | v_k \rangle = 0$ unless $j = k$,

$$\Rightarrow \quad \langle v_j | w \rangle = a_j \langle v_j | v_j \rangle$$

$$\Rightarrow \quad a_j = \frac{\langle v_j | w \rangle}{\langle v_j | v_j \rangle}$$

If the basis set is orthonormal then $\langle v_j | v_k \rangle = \delta_{jk}$ and in this case, $a_j = \langle v_j | w \rangle$.

Complete Basis: The completeness of an orthonormal basis set (i.e. the fact that the vectors in the set span the entire Hilbert space) is usually expressed as,

$$\sum_{k=1}^{n} | v_k \rangle \langle v_k | = \hat{1} \qquad (2)$$

Note that a combination of the form $|u\rangle\langle w|$ is actually an operator. To see this note that if $|u\rangle\langle w|$ acts on any vector $|v\rangle$ one obtains $(|u\rangle\langle w|)|v\rangle = \langle w | v \rangle$ which is another vector, and this is a property of an operator (property 10 of a Hilbert space). The operator $\hat{1}$ is the identity operator with the property that for any vector $|v\rangle$, $\hat{1}|v\rangle = |v\rangle$ (i.e. $\hat{1}$ does 'nothing'). To see why for a complete basis $\sum_{k=1}^{n} |v_k\rangle\langle v_k|$ equals $\hat{1}$ apply it to any vector $|w\rangle$ and see the result,

$$\left(\sum_{k=1}^{n} | v_k \rangle \langle v_k | \right) | w \rangle$$

$$= \sum_{k=1}^{n} | v_k \rangle \ \langle v_k | w \rangle$$

$$= \sum_{k=1}^{n} \langle v_k | w \rangle \ | v_k \rangle$$

but, as found earlier, $\langle v_k | w \rangle = a_k$ is the expansion coefficient when $|w\rangle$ is expressed in terms of the orthonormal basis set,

$$\Rightarrow \quad \sum_{k=1}^{n} \langle v_k | w \rangle | v_k \rangle = \sum_{k=1}^{n} a_k | v_k \rangle = | w \rangle$$

Thus, $\left(\sum_{k=1}^{n} | v_k \rangle \langle v_k | \right) | w \rangle = | w \rangle$. Therefore, $\sum_{k=1}^{n} | v_k \rangle \langle v_k | = \hat{1}$.

The eigenvectors of a Hermitian operator can be chosen to be all orthogonal and they also form a complete set.

1.1.2 Postulate Four and Measurement of Physical Quantities in Quantum Mechanics

Suppose $\hat{A}$ is an operator corresponding to a physical quantity A of a physical system. And suppose the quantum state vector of the physical system $|\psi\rangle$ is (somehow) known. The question then is if A is measured experimentally what would be the result? Postulate 3 tells us that the result can only be *one* of the eigenvalues of the operator $\hat{A}$. Suppose all the eigenvalues of $\hat{A}$ are known and the corresponding eigenvectors are also known, and they satisfy $\hat{A}|v_k\rangle = \lambda_k|v_k\rangle$ where $k = 1,2,3,...n$. The question then is which eigenvalue of A is going to be obtained upon measurement. The answer given by quantum mechanics is that one cannot know the result of a measurement before making the measurement but when a measurement is made the probability for obtaining the result λ_k is given by $|\langle v_k|\psi\rangle|^2$. This is also a postulate of quantum mechanics.

Since the eigenvectors $|v_k\rangle$ form a complete set one may expand $|\psi\rangle$ as,

$$|\psi\rangle = \sum_{k=1}^{n} a_k|v_k\rangle \qquad \text{where} \qquad a_k = \langle v_k|\psi\rangle$$

Just before the measurement, $|\psi\rangle$ is in a 'linear superposition' of the eigenvectors of $\hat{A}$. When a measurement is made of the quantity A, the result λ_k is obtained with probability $|a_k|^2 \left(= |\langle v_k|\psi\rangle|^2\right)$.

The probabilities of all possible measurement outcomes must add up to unity, and this is easy to show. Start from $\langle\psi|\psi\rangle = 1$,

$$\begin{aligned} 1 &= \langle\psi|\psi\rangle \\ &= \langle\psi|\hat{1}|\psi\rangle \\ &= \langle\psi|\sum_{k=1}^{n}|v_k\rangle\langle v_k||\psi\rangle \\ &= \sum_{k=1}^{n}\langle\psi|v_k\rangle\langle v_k|\psi\rangle = \sum_{k=1}^{n}|a_k|^2 \end{aligned}$$

1.1.3 Postulate 5 and Collapse of the Quantum State upon Measurement

Consider a physical observable A and the corresponding operator $\hat{A}$, which has eigenvectors and eigenvalues given by $\hat{A}|v_k\rangle = \lambda_k|v_k\rangle$. The quantum state $|\psi\rangle$ in terms of the eigenvectors of $\hat{A}$ is assumed to be $|\psi\rangle = \sum_k a_k|v_k\rangle$. Suppose a measurement of A is made and the result λ_j is obtained. The question is what is the quantum state just after the measurement? The answer is not trivial. The quantum state of an object contains all the information that can be obtained about the object by making any kind of measurement. When some information has been obtained by making a measurement, the quantum state after the measurement must reflect this extraction of information. If the eigenvalue λ_j was measured then the quantum state just after the measurement must be $|v_j\rangle$ (i.e. the eigenvector corresponding to λ_j). If a second measurement of A is made just after the first measurement then the result λ_j will be obtained with probability one, and this is certainly aesthetically pleasing. This sudden collapse of the quantum state

from $\sum_k a_k|v_k\rangle$ to $|v_j\rangle$ upon measurement is called collapse of the quantum state and is a postulate of quantum mechanics.

Case of Degenerate Eigenvalues: Suppose the first two eigenvalues of $\hat{A}$ are identical (i.e. $\lambda_1 = \lambda_2 = \lambda$). The quantum state before the measurement of A is $|\psi\rangle = \sum_k a_k|v_k\rangle$. What is the quantum state after the measurement if the result λ is obtained? In this case, since the measurement result cannot distinguish between $|v_1\rangle$ and $|v_2\rangle$, the quantum state after the measurement must lie in the eigen-subspace corresponding to the eigenvalue λ, and is given as,

$$\frac{\left(a_1|v_1\rangle + a_2|v_2\rangle\right)}{\sqrt{|a_1|^2 + |a_2|^2}}$$

In more technical language, the measurement projects the quantum state into the eigen-subspace corresponding to the measurement result.

Mean Values of Operators

The mean value of an operator $\hat{A}$, with respect to a quantum state $|\psi\rangle$, is defined as the mean value of the observable A obtained by making measurements of A on many identical copies of the quantum state $|\psi\rangle$. If $\hat{A}$ has eigenvectors and eigenvalues given by, $\hat{A}|v_k\rangle = \lambda_k|v_k\rangle$, and $|\psi\rangle$ expressed in terms of $|v_k\rangle$ is $|\psi\rangle = \sum_k a_k|v_k\rangle$, then the probability of obtaining λ_k is $|a_k|^2$. Therefore, the mean value of A with respect to the state $|\psi\rangle$ is $\sum_k |a_k|^2 \lambda_k$. This can be written more generally as $\langle\psi|\hat{A}|\psi\rangle$ or just $\langle\hat{A}\rangle$.

Some Common Observables

(1) **Position of a Particle:** The operator $\hat{x}$ corresponds to the position of a particle in 1 dimension. Eigenvectors of $\hat{x}$ are $|x\rangle$ with corresponding eigenvalues x (i.e. $\hat{x}|x\rangle = x|x\rangle$).

Orthogonality relation: $\langle x'|x\rangle = \delta(x - x')$

Completeness relation: $\int_{-\infty}^{\infty} dx\,|x\rangle\langle x| = \hat{1}$

(2) **Momentum of a Particle:** The operator $\hat{p}$ corresponds to the momentum of a particle in 1 dimension. Eigenvectors of $\hat{p}$ are $|p\rangle$ with corresponding eigenvalues p (i.e. $\hat{p}|p\rangle = p|p\rangle$)

Orthogonality relation: $\langle p'|p\rangle = \delta(p' - p)$

Completeness relation: $\int_{-\infty}^{\infty} dp\,|p\rangle\langle p| = \hat{1}$

Wavefunction: Note that one can write that quantum state of a particle as,

$$|\psi\rangle = \hat{1}|\psi\rangle = \left(\int_{-\infty}^{\infty} dx\,|x\rangle\langle x|\right)|\psi\rangle = \int_{-\infty}^{\infty} dx\,\langle x|\psi\rangle|x\rangle$$

The amplitude $\langle x|\psi\rangle$ is usually denoted by $\psi(x)$ and is called the wavefunction of the particle.

$$\Rightarrow |\psi\rangle = \int_{-\infty}^{\infty} dx\,\psi(x)|x\rangle$$

Similarly,

$$|\psi\rangle = \int_{-\infty}^{\infty} dp\, \psi(p) |p\rangle$$

Question: What is $\langle p|x\rangle$? We cannot answer this unless we know something more about the properties of the operators $\hat{x}$ and $\hat{p}$. The classical description of a particle is "quantized" by imposing (as a postulate) a commutation relation. For a non-relativistic, spin-less, particle this commutation relation is $[\hat{x}, \hat{p}] = i\hbar$ i.e. $\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$. One can obtain the value of the inner product $\langle p|x\rangle$ from this commutation relation, as shown below.

$$\begin{aligned}
&[\hat{x}, \hat{p}] = i\hbar \\
&\Rightarrow \langle p| \, [\hat{x}, \hat{p}] \, |x\rangle = i\hbar \langle p|x\rangle \\
&\Rightarrow \langle p|\hat{x}\hat{p}|x\rangle - xp\langle p|x\rangle = i\hbar\langle p|x\rangle \\
&\Rightarrow (i\hbar + xp)\langle p|x\rangle = \langle p|\hat{x}\hat{p}|x\rangle \\
&\Rightarrow (i\hbar + xp)\langle p|x\rangle = \langle p|\hat{x}\hat{1}\hat{p}|x\rangle = \langle p|\hat{x}\left[\int dp'|p'\rangle\langle p'|\right]\hat{p}|x\rangle \\
&\Rightarrow (i\hbar + xp)\langle p|x\rangle = \int dp' \langle p|\hat{x}|p'\rangle p' \langle p'|x\rangle \\
&\Rightarrow (i\hbar + xp)\langle p|x\rangle = \int dp' p' \langle p|\hat{X}\left[\int dx'|x'\rangle\langle x'|\right]|p'\rangle\langle p'|x\rangle \\
&\Rightarrow (i\hbar + xp)\langle p|x\rangle = \int dp' \int dx' p' x' \langle p|x'\rangle\langle x'|p'\rangle\langle p'|x\rangle
\end{aligned}$$

The solution of the above integral equation can be found and it is,

$$\langle p|x\rangle = \frac{e^{-i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}$$

This is quite interesting; if $|\psi\rangle = \int dx\, \psi(x)|x\rangle$ and $|\psi\rangle = \int dx\, \psi(p)|p\rangle$, then it follows that,

$$\psi(x) = \langle x|\psi\rangle = \int dp\, \langle x|p\rangle\langle p|\psi\rangle = \int dp\, \frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}} \psi(p)$$

Similarly,

$$\psi(p) = \int_{-\infty}^{\infty} dx\, \psi(x) \frac{e^{-i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}$$

It follows from the commutation relation that the coefficients of momentum and position basis expansion have a Fourier transform relationship!!

It is also useful to know the action of the operators $\hat{x}$ and $\hat{p}$ on a state vector $|\psi\rangle$ (i.e. what are the states $\hat{p}|\psi\rangle$ and $\hat{x}|\psi\rangle$). We already know that $\langle x|\psi\rangle = \psi(x)$. We need to find $\langle x|\hat{x}|\psi\rangle$ and $\langle x|\hat{p}|\psi\rangle$.

1) $\langle x|\hat{x}|\psi\rangle$:

$$\begin{aligned}
\langle x|\hat{x}|\psi\rangle &= \left(\langle\psi|\hat{x}^+|x\rangle\right)^* = \left(\langle\psi|\hat{x}|x\rangle\right)^* = \left(x\langle\psi|x\rangle\right)^* \\
&= x\langle x|\psi\rangle = x\psi(x)
\end{aligned}$$

2) $\langle x|\hat{p}|\psi\rangle$:

A little more complicated,

$$\langle x|\hat{p}|\psi\rangle = \langle x|\hat{p}\hat{1}|\psi\rangle = \langle x|\hat{p}\int_{-\infty}^{\infty} dp\,|p\rangle\langle p|\,|\psi\rangle$$

$$= \int dp\, p\langle x|p\rangle\langle p|\psi\rangle = \int dp\, p\frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}\psi(p)$$

$$= \frac{\hbar}{i}\frac{\partial}{\partial x}\left[\int dp\frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}\psi(p)\right]$$

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

Therefore, $\hat{p}$ acts like a differential operator in the position representation!

3) $\langle p|\hat{x}|\psi\rangle$:

Proceed as before,

$$\langle p|\hat{x}|\psi\rangle = \langle p|\hat{x}\hat{1}|\psi\rangle = \langle p|\hat{x}\int dx\,|x\rangle\langle x|\,|\psi\rangle = \int dx\langle p|x\rangle\; x\psi(x)$$

$$= \int dx\frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}x\psi(x) = -\frac{\hbar}{i}\frac{\partial}{\partial p}\psi(p)$$

$\hat{x}$ acts like a differential operator in the momentum representation.

4) $\langle p|\hat{p}|\psi\rangle$:

$$\langle p|\hat{p}|\psi\rangle = \left(\langle\psi|\hat{p}|p\rangle\right)^* = \left(\langle\psi|\hat{p}|p\rangle\right)^* = \left(p\langle\psi|p\rangle\right)^*$$

$$= p\langle p|\psi\rangle = p\psi(p)$$

Standard Deviation of Observables

We saw earlier the expectation value, or the mean value, of an operator $\hat{A}$ is $\langle\psi|\hat{A}|\psi\rangle$. We will write this mean value as $\langle\hat{A}\rangle$. What about the standard deviation? Define a new operator $\Delta\hat{A}$ as,

$$\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$$

$$\Rightarrow \Delta\hat{A}^2 = \hat{A}^2 + \langle\hat{A}\rangle^2 - 2\hat{A}\langle\hat{A}\rangle$$

and,

$$\left\langle \Delta \hat{A}^2 \right\rangle = \langle \psi | \hat{A}^2 + \left\langle \hat{A} \right\rangle^2 - 2\hat{A}\left\langle \hat{A} \right\rangle | \psi \rangle$$

$$= \langle \psi | \hat{A}^2 | \psi \rangle - \left(\langle \psi | \hat{A} | \psi \rangle \right)^2$$

$$\left\langle \Delta \hat{A}^2 \right\rangle = \left\langle \hat{A}^2 \right\rangle - \left\langle \hat{A} \right\rangle^2$$

Heisenberg Uncertainty Relations

Suppose we have two operators $\hat{A}$ and $\hat{B}$. The Heisenberg Uncertainty Principle states that if $\left[\hat{A}, \hat{B}\right] = iC$ (where C is some real number) then for all possible states $|\psi\rangle$ the following relation holds,

$$\left\langle \Delta \hat{A}^2 \right\rangle \left\langle \Delta \hat{B}^2 \right\rangle \geq \frac{C^2}{4}$$

Proof: For some real number λ, consider the state $|\phi\rangle$ where $|\phi\rangle = \left(\Delta \hat{A} + i\lambda \Delta \hat{B}\right)|\psi\rangle$. Now we know that $\langle \phi | \phi \rangle \geq 0$, therefore,

$$\Rightarrow \qquad \langle \psi | \left(\Delta \hat{A}^+ - i\lambda \Delta \hat{B}^+\right)\left(\Delta \hat{A} + i\lambda \Delta \hat{B}\right) | \psi \rangle \geq 0$$

Suppose $\hat{A}$ and $\hat{B}$ are Hermitian, then,

$$\Rightarrow \qquad \langle \psi | \Delta \hat{A}^2 + \lambda^2 \Delta \hat{B}^2 + i\lambda \left[\Delta \hat{A}, \Delta \hat{B}\right] | \psi \rangle = 0$$

But since $\left[\Delta \hat{A}, \Delta \hat{B}\right] = \left[\hat{A}, \hat{B}\right] = iC$,

$$\Rightarrow \qquad \langle \psi | \Delta \hat{A}^2 + \lambda^2 \Delta \hat{B}^2 - \lambda C | \psi \rangle \geq 0$$

$$\Rightarrow \qquad \left\langle \Delta \hat{A}^2 \right\rangle + \lambda^2 \left\langle \Delta \hat{B}^2 \right\rangle - \lambda C \geq 0$$

The above must hold for all values of λ and this can only happen if,

$$C^2 - 4\left\langle \Delta \hat{A}^2 \right\rangle \left\langle \Delta \hat{B}^2 \right\rangle \leq 0$$

$$\Rightarrow \left\langle \Delta \hat{A}^2 \right\rangle \left\langle \Delta \hat{B}^2 \right\rangle \geq \frac{C^2}{4}$$

Example: We know that $\left[\hat{x}, \hat{p}\right] = i\hbar$, therefore,

$$\Rightarrow \qquad \left\langle \Delta \hat{x}^2 \right\rangle \left\langle \Delta \hat{p}^2 \right\rangle \geq \frac{\hbar^2}{4}$$

This should not be a surprise since we already know that the position and momentum representations of a quantum state are related by,

$$\psi(x) = \int_{-\infty}^{\infty} dp \frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}} \psi(p)$$

and this Fourier transform relationship implies that $\left\langle \Delta \hat{x}^2 \right\rangle \left\langle \Delta \hat{p}^2 \right\rangle \geq \frac{\hbar^2}{4}$

The Hamiltonian Operator

The energy of a particle of mass m and momentum p in a potential $V(x)$ is given classically as,

$$H = \frac{p^2}{2m} + V(x)$$

In quantum mechanics, the energy is given by the Hamiltonian operator $\hat{H}$. For a free particle,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

1.1.4 Postulate 6 and Time Development in Quantum Mechanics

The time evolution of a quantum state $|\psi(t)\rangle$ is given by the Schrodinger equation (sixth postulate):

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

This is a first order linear differential equation. Therefore, if $|\psi(t=0)\rangle$ is known, then using this as the boundary condition $|\psi(t)\rangle$ can be determined for all $t \geq 0$. The formal solution of the above equation, for a time independent Hamiltonian, is,

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(t=0)\rangle$$

Stationary States

The eigenvectors of the energy operator $\hat{H}$ are called stationary states since they don't evolve in time other than acquiring a time dependent phase factor.

Example: Suppose $\hat{H}$ has eigenvectors $|e_k\rangle$ with eigenvalues ε_k (i.e. $\hat{H}=|e_k\rangle=\varepsilon_k|e_k\rangle$). Since $\hat{H}$ is Hermitian, its eigenvectors form a complete set (i.e $\sum_k |e_k\rangle\langle e_k| = \hat{1}$) and any arbitrary quantum state can be expanded in terms of $|e_k\rangle$. Suppose $|\psi(t=0)\rangle = \sum_k c_k|e_k\rangle$. Assume, $|\psi(t)\rangle = \sum_k c_k(t)|e_k\rangle$, and plug in the Schrodinger equation,

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

$$\sum_k i\hbar\frac{\partial c_k(t)}{\partial t}|e_k\rangle = \sum_k c_k(t)\hat{H}|e_k\rangle = \sum_k c_k(t)\,\varepsilon_k|e_k\rangle$$

Multiply by bra $\langle e_j|$ on both sides to get,

$$i\hbar\frac{\partial c_i(t)}{\partial t} = \varepsilon_j c_j(t)$$

Solution is,

$$c_j(t) = c_j(t=0)e^{-i\frac{\varepsilon_j t}{\hbar}} = c_j e^{-i\frac{\varepsilon_j t}{\hbar}}$$

$$\Rightarrow \quad |\psi(t)\rangle = \sum_k c_k(t)|e_k\rangle = \sum_k c_k\, e^{\frac{-i\varepsilon_k t}{\hbar}}|e_k\rangle$$

This implies $\left|\langle e_j|\psi(t)\rangle\right|^2 = \left|\langle e_j|\psi(t=0)\rangle\right|^2$ for all times. The probability of being in particular energy eigenstate does not change with time. That is why energy eigenstates are called stationary states.

Matrix Representation of Operators

Suppose vectors $|\omega_k\rangle$ form a complete set (i.e. $\sum_k |\omega_k\rangle\langle\omega_k| = \hat{1}$). Any operator can be written as.

$$\begin{aligned}\hat{A} &= \hat{1}\,\hat{A}\,\hat{1} \\ &= \sum_k |\omega_k\rangle\langle\omega_k|\,\hat{A}\,\sum_j |\omega_j\rangle\langle\omega_j| \\ &= \sum_{kj}\langle\omega_k|\hat{A}|\omega_j\rangle\,|\omega_k\rangle\langle\omega_j|\end{aligned}$$

Let, $A_{kj} = \langle\omega_k|\hat{A}|\omega_j\rangle$. Then,

$$\hat{A} = \sum_{kj} A_{kj}\,|\omega_k\rangle\langle\omega_j|$$

We can represent $\hat{A}$ in matrix form by choosing a mapping between basis vectors $|\omega_k\rangle$ and column vectors. For example, let,

$$|\omega_1\rangle = \begin{bmatrix}1\\0\\0\\\vdots\end{bmatrix} \quad |\omega_2\rangle = \begin{bmatrix}0\\1\\0\\\vdots\end{bmatrix} \quad |\omega_3\rangle = \begin{bmatrix}0\\0\\1\\\vdots\end{bmatrix} \quad \ldots\ldots$$

The operator $\hat{A}$ is then a matrix,

$$\hat{A} = \begin{bmatrix}A_{11} & A_{12} & \ldots. \\ A_{21} & A_{22} & \\ \vdots & & \ddots\end{bmatrix}$$

If the basis set chosen consists of eigenvectors of $\hat{A}$ then $A_{kj} = \langle\omega_k|\hat{A}|\omega_j\rangle = \delta_{kj}\,A_{jj}$ and in this basis set the operator $\hat{A}$ is represented by a diagonal matrix,

$$\hat{A} = \begin{bmatrix}A_{11} & 0 & 0 & \ldots \\ 0 & A_{22} & & \\ 0 & & & \\ \vdots & & & \ddots\end{bmatrix}$$

Hamiltonian Operator in a Different Form

We know that for a particle in a potential,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

Suppose $\hat{H}$ has eigenvectors $|e_k\rangle$ with eigenvalues ε_k (i.e. $\hat{H}|e_k\rangle = \varepsilon_k|e_k\rangle$). Using these energy eigenvectors, we can write $\hat{H}$ in a different form,

$$\hat{H} = \hat{1}\,\hat{H}\,\hat{1}$$
$$= \left(\sum_k |e_k\rangle\langle e_k|\right)\hat{H}\left(\sum_j |e_j\rangle\langle e_j|\right)$$
$$= \sum_j \sum_k |e_k\rangle \langle e_k|e_j\rangle\, \varepsilon_j\, \langle e_j|$$
$$= \sum_j \sum_k |e_k\rangle\, \delta_{kj}\, \varepsilon_j\, \langle e_j|$$
$$\hat{H} = \sum_k \varepsilon_k\, |e_k\rangle\langle e_k|$$

Now suppose we have a Hamiltonian $\hat{H}_o$,

$$\hat{H}_o = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

and we found the eigenvectors $|e_k\rangle$ and eigenvalues ε_k (i e. $\hat{H}_o|e_k\rangle = \varepsilon_k|e_k\rangle$). Now suppose an additional potential $U(\hat{x})$ is added to $\hat{H}_o$ so that the full Hamiltonian is now $\hat{H}$, where,

$$\hat{H} = \hat{H}_o + U(\hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x}) + U(\hat{x})$$
$$\hat{H} = \hat{1}\,\hat{H}\,\hat{1} = \hat{1}\,(\hat{H}_o + U(\hat{x}))\,\hat{1}$$
$$= \left(\sum_k |e_k\rangle\langle e_k|\right)\left(\hat{H}_o + U(\hat{x})\right)\sum_j |e_j\rangle\langle e_j|$$
$$\hat{H} = \sum_k \varepsilon_k\, |e_k\rangle\langle e_k| + \sum_k \sum_j U_{kj}\, |e_k\rangle\langle e_j| \qquad \left\{U_{kj} = \langle e_k|U(\hat{x})|e_j\rangle\right.$$

The first part is `diagonal' in the basis used. The second part is not diagonal.

1.2 Dynamics of a Two-Level System

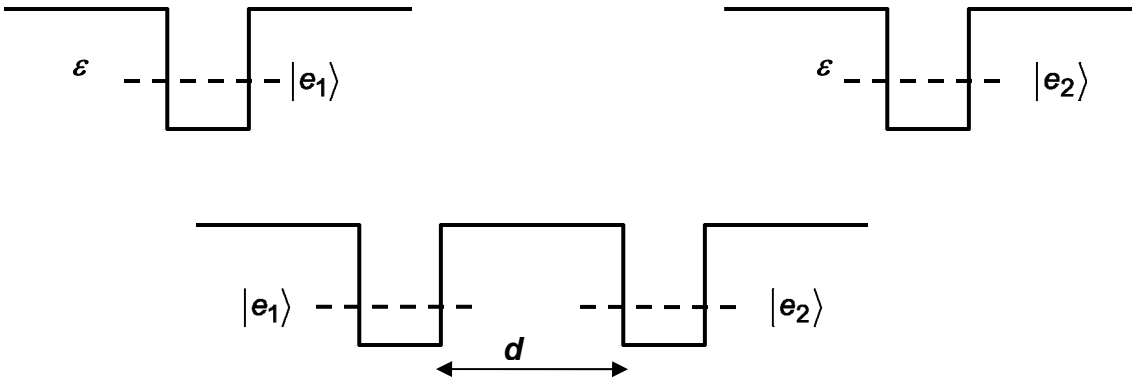
Suppose $\hat{H}_o$ has only two important eigenvectors; $|e_1\rangle$ and $|e_2$ which are degenerate, i.e.,

$$\hat{H}_o = \varepsilon|e_1\rangle\langle e_1| + \varepsilon|e_2\rangle\langle e_2|$$

Suppose a small potential is added to the Hamiltonian,

$$\hat{H} = \hat{H}_o + U(\hat{x})$$
$$= \varepsilon|e_1\rangle\langle e_1| + \varepsilon|e_2\rangle\langle e_2| - U|e_1\rangle\langle e_2| - U|e_2\rangle\langle e_1| \qquad \begin{cases} U_{12} = U_{21} = -U \\ U_{11} = U_{22} = 0 \end{cases}$$

Physical Realization: A coupled quantum well system, shown below, is a two-level system. $\hat{H}_o$ corresponds to the Hamiltonian when the two potential wells were very far apart, and $\hat{H}$ corresponds to the potential when the two wells are close. If d is small, the quantum states $|e_1\rangle$ and $|e_2\rangle$ get `coupled' via tunneling through the barrier. This tunneling is described by the additional potential $U(\hat{x})$.



Suppose at time $t=0$ the particle is placed in well #1 so that $|\psi(t=0)\rangle=|e_1\rangle$. We need to find the particle wavefunction for $t\geq 0$.

Solution by Expansion in the Original Eigenstates: Assume the following solution for $t\geq 0$,

$$|\psi(t)\rangle = c_1(t)|e_1\rangle + c_2(t)|e_2\rangle$$

with the boundary condition $c_1(t=0)=1$ and $c_2(t=0)=0$) and plug into the Schrodinger equation to get,

$$i\hbar\frac{\partial}{\partial t}\left[c_1(t)|e_1\rangle + c_2(t)|e_2\rangle\right] = \hat{H}\left[c_1(t)|e_1\rangle + c_2(t)|e_2\rangle\right]$$

Multiply by the bras $\langle e_1|$ and then $\langle e_2|$ to get two equations,

$$i\hbar\frac{\partial}{\partial t}c_1(t) = \varepsilon\, c_1(t) - U\, c_2(t)$$

$$i\hbar\frac{\partial}{\partial t}c_2(t) = \varepsilon\, c_2(t) - U\, c_1(t)$$

The matrix form of the above two equations is,

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix} = \begin{bmatrix} \varepsilon & -U \\ -U & \varepsilon \end{bmatrix}\begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix}$$

Solution, subject to the initial conditions, is,

$$c_1(t) = e^{-i\frac{\varepsilon\, t}{\hbar}}\cos\left(\frac{Ut}{\hbar}\right)$$

$$c_2(t) = i\, e^{-i\frac{\varepsilon\, t}{\hbar}}\sin\left(\frac{Ut}{\hbar}\right)$$

and,

$$\left|\langle e_1|\psi(t)\rangle\right|^2 = |c_1(t)|^2 = \cos^2\left(\frac{Ut}{\hbar}\right).$$

$$\left|\langle e_2|\psi(t)\rangle\right|^2 = |c_2(t)|^2 = \sin^2\left(\frac{Ut}{\hbar}\right).$$

The quantum state oscillates in time between $|e_1\rangle$ and $|e_2\rangle$.

Solution by Expansion in the Exact Eigenstates: Start from,

$$\hat{H} = \hat{H}_o + U(\hat{x})$$
$$= \varepsilon|e_1\rangle\langle e_1| + \varepsilon|e_2\rangle\langle e_2| - U|e_1\rangle\langle e_2| - U|e_2\rangle\langle e_1|$$

We can diagonalize the new Hamiltonian. In matrix representation, where $|e_1\rangle = \begin{bmatrix}1\\0\end{bmatrix}$ and $|e_2\rangle = \begin{bmatrix}0\\1\end{bmatrix}$, $\hat{H}$ is,

$$\hat{H} = \begin{bmatrix}\varepsilon & -U\\ -U & \varepsilon\end{bmatrix}$$

Eigenvalues of $\hat{H}$ are $\varepsilon - U$ and $\varepsilon + U$ and the corresponding eigenvectors are $\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$ and $\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$, respectively, which correspond to states, $\frac{1}{\sqrt{2}}\left(|e_1\rangle + |e_2\rangle\right)$ and $\frac{1}{\sqrt{2}}\left(|e_1\rangle - |e_2\rangle\right)$, respectively. Let these states be $|v_1\rangle$ and $|v_2\rangle$, respectively. We can work out temporal dynamics using $|v_1\rangle$, $|v_2\rangle$ which are the eigenvectors of the full Hamiltonian. The initial state is,

$$|\psi(t=0)\rangle = |e_1\rangle = \frac{1}{\sqrt{2}}\left(|v_1\rangle + |v_2\rangle\right)$$

Since $|v_1\rangle$ and $|v_2\rangle$ are the energy eigenstates, they are stationary states. So using the earlier result, the state at a later time is,

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(t=0)\rangle$$
$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{\frac{-i}{\hbar}(\varepsilon-U)t}|v_1\rangle + e^{\frac{-i}{\hbar}(\varepsilon+U)t}|v_2\rangle\right]$$

It follows that,

$$\left|\langle v_1|\psi(t)\rangle\right|^2 = \left|\langle v_1|\psi(t=0)\rangle\right|^2 = \frac{1}{2}$$
$$\left|\langle v_2|\psi(t)\rangle\right|^2 = \left|\langle v_2|\psi(t=0)\rangle\right|^2 = \frac{1}{2}$$

But now if we evaluate $\left|\langle e_1|\psi(t)\rangle\right|^2$ we get,

$$\left|\langle e_1|\psi(t)\rangle\right|^2 = \left|\frac{1}{\sqrt{2}}\left(\langle v_1| + \langle v_2|\right)|\psi(t)\rangle\right|^2 = \cos^2\left(\frac{Ut}{\hbar}\right).$$

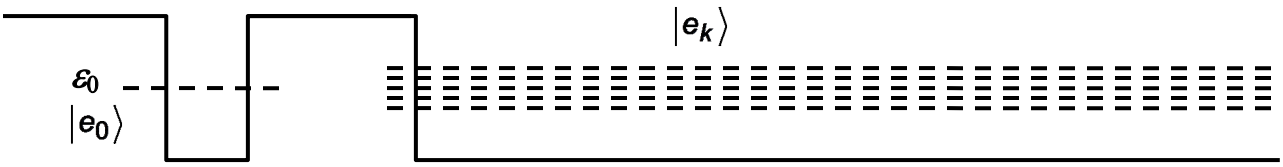
and similarly,

$$\left|\langle e_2|\psi(t)\rangle\right|^2 = \sin^2\left(\frac{Ut}{\hbar}\right)$$

which are the same results obtained earlier via a different method.

1.3 Fermi's Golden Rule

Now consider the problem of one level coupled with infinitely many levels, as shown below.



The Hamiltonian can be written as,

$$\hat{H} = \varepsilon_0 |e_0\rangle\langle e_0| + \sum_{k=1}^{\infty} \varepsilon_k |e_k\rangle\langle e_k| - \sum_{k=1}^{\infty} \left[U_k |e_0\rangle\langle e_k| + U_k^* |e_k\rangle\langle e_0| \right]$$

The levels ε_1 to ε_∞ are described by a density of levels (or density of states) $D(E)$ that has units equal to the number of levels per unit energy interval, and can be written as,

$$D(E) = \sum_{k=1}^{\infty} \delta(E - \varepsilon_k)$$

One cannot diagonalize this giant Hamiltonian. Suppose $|\psi(t=0)\rangle = |e_0\rangle$, then one may ask the question: what is the escape time of the particle from the well? As before, let the solution be of the form,

$$|\psi(t)\rangle = c_0(t)|e_0\rangle + \sum_{k=1}^{\infty} c_k(t)|e_k\rangle$$

And plug this solution in the Schrodinger equation to get the following equations,

$$i\hbar \frac{\partial}{\partial t} c_0(t) = \varepsilon_0 \, c_0(t) - \sum_{k=1}^{\infty} U_k \, c_k(t)$$

$$i\hbar \frac{\partial}{\partial t} c_k(t) = \varepsilon_k \, c_k(t) - U_k^* \, c_0(t)$$

The initial conditions are,

$$c_0(t=0) = 1$$

$$c_k(t=0) = 0 \qquad \{k = 1,2,3,\ldots\ldots$$

Suppose,

$$b_0(t) = c_0(t) e^{+\frac{i\varepsilon_0 t}{\hbar}}$$

$$b_k(t) = c_k(t) e^{+\frac{i\varepsilon_k t}{\hbar}}$$

This gives us,

$$\hbar \frac{\partial b_0(t)}{\partial t} = - \sum_{k=1}^{\infty} U_k \, e^{-i\frac{(\varepsilon_k - \varepsilon_0)t}{\hbar}} \, b_k(t)$$

$$i\hbar \frac{\partial b_k(t)}{\partial t} = - U_k^* \, b_0(t) e^{i\frac{(\varepsilon_k - \varepsilon_0)t}{\hbar}}$$

$$\Rightarrow b_k(t) = \frac{i}{\hbar} U_k^* \int_0^t b_0(t') e^{i\frac{(\varepsilon_k - \varepsilon_0)t'}{\hbar}} dt'$$

Use this expression in the equation for $b_0(t)$ to get,

$$\Rightarrow \frac{\partial b_0(t)}{\partial t} = -\frac{1}{\hbar^2} \sum_{k=1}^{\infty} |U_k|^2 \int_0^t dt' e^{-i\frac{(\varepsilon_k - \varepsilon_0)}{\hbar}(t-t')} \, b_0(t')$$

Since $b_0(t)$ is expected to change in time slowly compared to the exponential term, we can pull it out of the integral to get,

$$\Rightarrow \frac{\partial b_0(t)}{\partial t} = -\left\{ \frac{1}{\hbar^2} \sum_{k=1}^{\infty} |U_k|^2 \int_0^t dt' e^{-i\frac{(\varepsilon_k - \varepsilon_0)}{\hbar}(t-t')} \right\} b_0(t)$$

This gives,

$$\frac{\partial |b_0(t)|^2}{\partial t} = -2\ \text{Real}\left\{ \sum_{k=1}^{\infty} \frac{|U_k|^2}{\hbar^2} \int_0^t dt' e^{-i\frac{(\varepsilon_k - \varepsilon_0)}{\hbar}(t-t')} \right\} |b_0(t)|^2$$

$$= -2\ \text{Real}\left\{ \sum_{k=1}^{\infty} \frac{|U_k|^2}{\hbar^2} \pi\hbar\,\delta(\varepsilon_k - \varepsilon_0) \right\} |b_0(t)|^2$$

$$= -\left\{ \frac{2\pi}{\hbar} \sum_{k=1}^{\infty} |U_k|^2 \delta(\varepsilon_k - \varepsilon_0) \right\} |b_0(t)|^2$$

The above equations shows that the probability of finding the particle at any later time to be in the initial state decays as,

$$\frac{\partial |b_0(t)|^2}{\partial t} = -\Gamma\ |b_0(t)|^2$$

where the decay rate Γ is,

$$\Gamma = \frac{2\pi}{\hbar} \sum_{k=1}^{\infty} |U_k|^2 \delta(\varepsilon_k - \varepsilon_0)$$

If we replace the summation $\sum_{k=1}^{\infty}$ by the integral $\int_{-\infty}^{\infty} dE\ \mathrm{D}(E)$, and $|U_k|^2$ by $|U(E)|^2$, then we get,

$$\Gamma = \frac{2\pi}{\hbar} \int_{-\infty}^{+\infty} dE\ D(E) |U(E)|^2 \delta(E - \varepsilon_0)$$

$$= \frac{2\pi}{\hbar} |U(\varepsilon_0)|^2 D(\varepsilon_0)$$

The above relation is called Fermi's Golden Rule.

Conclusion: When the number of possible final states is infinite, there are no oscillations. There is just a decay of the initial state into the final states and the decay rate is given by the Fermi's Golden Rule.

1.4 Heisenberg and Schrodinger Pictures in Quantum Mechanics

1.4.1 The Schrodinger Picture

In quantum mechanics, one is usually interested in calculating expectation values of operators, e.g. quantities like $\langle \psi(t) | \hat{A} | \psi(t) \rangle$. The calculation proceeds as follows:

i) Given the initial state $|\psi(t=0)\rangle$, calculate $|\psi(t)\rangle$ for $t \geq 0$ using the Schrodinger equation,

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

The formal solution is $|\psi(t)\rangle = e^{-i\frac{\hat{H}t}{\hbar}}|\psi(t=0)\rangle$. The operator exponential is to be interpreted as its Taylor series expansion, i.e.,

$$e^{-i\frac{\hat{H}}{\hbar}t} = 1 - \frac{i}{\hbar}\hat{H}t - \frac{\hat{H}^2}{2\hbar^2}t^2 + \ldots\ldots$$

ii) Once $|\psi(t)\rangle$ is known, calculate $\langle\psi(t)|\hat{A}|\psi(t)\rangle$.

This method, which we have been using so far, is called the Schrodinger's picture. In the Schrodinger picture, the state vectors are time dependent and the operators are time independent.

1.4.2 The Heisenberg Picture

There is another equivalent way to calculate expectation values of operators. First note that,

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(t=0)|e^{i\frac{\hat{H}}{\hbar}t}\ \hat{A}\ e^{\frac{-i\hat{H}}{\hbar}t}|\psi(t=0)\rangle$$

If one defines a time-dependent operator $\hat{A}(t)$ as,

$$\hat{A}(t) = e^{i\frac{\hat{H}}{\hbar}t}\ \hat{A}\ e^{-i\frac{\hat{H}}{\hbar}t}$$

then $\langle\psi(t)|\hat{A}|\psi(t)\rangle$ becomes $\langle\psi(t=0)|\hat{A}(t)|\psi(t=0)\rangle$. In this new form, the quantum state does not change with time but the operator evolves in time. This is called the Heisenberg picture. In the Heisenberg picture the operators are time dependent,

$$\hat{A}(t) = e^{i\frac{\hat{H}}{\hbar}t}\ \hat{A}\ e^{-i\frac{\hat{H}}{\hbar}t}$$

One can differentiate both sides with respect to time to get,

$$i\hbar\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}\right]$$

The above equation is called the Heisenberg equation. The calculation procedure in the Heisenberg picture is as follows:

i) Given an initial state $|\psi(t=0)\rangle$ and an operator $\hat{A}$, calculate $\hat{A}(t)$ using the Heisenberg equation,

$$i\hbar\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}\right]$$

with $\hat{A}(t=0) = \hat{A}$ as the boundary condition.

ii) Once $\hat{A}(t)$ is known, the mean value of $\hat{A}$ at time t is obtained as follows,

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(t=0)|\hat{A}(t)|\psi(t=0)\rangle = \left\langle\hat{A}(t)\right\rangle$$

In the Heisenberg picture, the operators are time dependent and the state vectors are time independent (one just uses the initial state for calculations). Note that:

(a) $\hat{H}(t) = e^{i\frac{\hat{H}}{\hbar}t}\ \hat{H}\ e^{-i\frac{\hat{H}}{\hbar}t} = \hat{H}$, the Hamiltonian operator is time-independent.

(b) If $\left[\hat{A}, \hat{B}\right] = \hat{C}$ then the equal time commutation relation at a later time is,

$$\left[\hat{A}(t),\hat{B}(t)\right]=e^{i\frac{\hat{H}}{\hbar}t}\left(\hat{A}\,\hat{B}-\hat{B}\,\hat{A}\right)e^{-i\frac{\hat{H}}{\hbar}t}=e^{i\frac{\hat{H}}{\hbar}t}\,\hat{C}\,e^{-i\frac{\hat{H}}{\hbar}t}=\hat{C}(t)$$

The form of the equal-time commutation relations do not change with time. The equal-time commutation relations represent fundamental properties of physical systems and their form are time independent.

A Two-Level System in the Heisenberg Picture

The two-level system discussed earlier is described by the Hamiltonian,

$$\hat{H}=\varepsilon|e_1\rangle\langle e_1|+\varepsilon|e_2\rangle\langle e_2|-U|e_1\rangle\langle e_2|-U|e_2\rangle\langle e_1|$$

Suppose, $|\psi(t=0)\rangle=|e_1\rangle$. We need to find $\left|\langle e_1|\psi(t)\rangle\right|^2$ and $\left|\langle e_2|\psi(t)\rangle\right|^2$ using the Heisenberg picture.

We define the following number operators,

$$\hat{N}_1=|e_1\rangle\langle e_1| \quad \hat{N}_2=|e_2\rangle\langle e_2|$$

Then the desired quantities can be written as,

$$\left|\langle e_1|\psi(t)\rangle\right|^2=\langle\psi(t)|\hat{N}_1|\psi(t)\rangle=\langle\psi(t=0)|\hat{N}_1(t)|\psi(t=0)\rangle$$

$$\left|\langle e_2|\psi(t)\rangle\right|^2=\langle\psi(t=0)|\hat{N}_2(t)|\psi(t=0)\rangle.$$

So we need to find $\hat{N}_1(t)$ and $\hat{N}_2(t)$. We also define operators $\hat{\sigma}_-$ and $\hat{\sigma}_+$ as,

$$\hat{\sigma}_-=|e_1\rangle\langle e_2| \quad \hat{\sigma}_+=|e_2\rangle\langle e_1| \qquad \left\{\hat{\sigma}_-^+=\hat{\sigma}_+\right\}$$

$\hat{H}$ is then,

$$\hat{H}=\varepsilon\left(\hat{N}_1+\hat{N}_2\right)-U\left(\hat{\sigma}_-+\hat{\sigma}_+\right)$$

You can verify that the following commutation relations hold,

$$\left[\hat{N}_1,\hat{\sigma}_-\right]=\hat{\sigma}_- \qquad \left[\hat{N}_2,\hat{\sigma}_-\right]=-\hat{\sigma}_-$$

$$\left[\hat{N}_1,\hat{\sigma}_+\right]=-\hat{\sigma}_+ \qquad \left[\hat{N}_2,\hat{\sigma}_+\right]=\hat{\sigma}_+$$

$$\left[\hat{\sigma}_+,\hat{\sigma}_-\right]=\hat{N}_2-\hat{N}_1$$

Using the Heisenberg equation we get,

$$i\hbar\frac{d\hat{N}_1(t)}{dt}=\left[\hat{N}_1(t),\hat{H}\right]=U\left[\hat{\sigma}_+(t)-\hat{\sigma}_-(t)\right]=-i\hbar\frac{d\hat{N}_2(t)}{dt}$$

$$i\hbar\frac{d\hat{\sigma}_-(t)}{dt}=\left[\hat{\sigma}_-(t),\hat{H}\right]=U\left[\hat{N}_2(t)-\hat{N}_1(t)\right]=-i\hbar\frac{d\hat{\sigma}_+(t)}{dt}$$

Note that,

$$\frac{d}{dt}\left[\hat{N}_1(t)+\hat{N}_2(t)\right]=0\Rightarrow\hat{N}_1(t)+\hat{N}_2(t)=\hat{N}_1+\hat{N}_2$$

Define, $\hat{N}_d(t)=\hat{N}_2(t)-\hat{N}_1(t)$. The equation for $\hat{N}_d(t)$ is,

$$\frac{d^2\hat{N}_d(t)}{dt}=-\frac{4U^2}{\hbar^2}\hat{N}_d(t)$$

The above equation can be solved with the two boundary conditions,

$$\hat{N}_d(t=0)=\hat{N}_d=\hat{N}_2-\hat{N}_1 \qquad \left.\frac{d\hat{N}_d(t)}{dt}\right|_{t=0}=\frac{2iU}{\hbar}\left(\hat{\sigma}_+-\hat{\sigma}_-\right)$$

Solution is,

$$\hat{N}_d(t)=\hat{N}_d\cos\left(\frac{2U}{\hbar}t\right)+i\left(\hat{\sigma}_+-\hat{\sigma}_-\right)\sin\left(\frac{2U}{\hbar}t\right)$$

It follows that,

$$\hat{N}_1(t) = \frac{\left[\hat{N}_1(t)+\hat{N}_2(t)\right]-\hat{N}_d(t)}{2} = \frac{\left(\hat{N}_1+\hat{N}_2\right)-\hat{N}_d(t)}{2}$$
$$= \hat{N}_1\cos^2\left(\frac{U}{\hbar}t\right) + \hat{N}_2\sin^2\left(\frac{U}{\hbar}t\right) - \frac{i}{2}\left(\hat{\sigma}_+ - \hat{\sigma}_-\right)\sin\left(\frac{2U}{\hbar}t\right)$$

and

$$\hat{N}_2(t) = \hat{N}_1\sin^2\left(\frac{Ut}{\hbar}\right) + \hat{N}_2\cos^2\left(\frac{Ut}{\hbar}\right) + \frac{i}{2}\left(\hat{\sigma}_+ - \hat{\sigma}_-\right)\sin\left(\frac{2Ut}{\hbar}\right)$$

The above two operator expressions for $\hat{N}_1(t)$ and $\hat{N}_2(t)$ might look strange. The answer for the Heisenberg operators $\hat{N}_1(t)$ and $\hat{N}_2(t)$ has been expressed in terms of the Schrodinger operators $\hat{N}_1$, $\hat{N}_2$, $\hat{\sigma}_+$, and $\hat{\sigma}_-$, and we already know the action of these Schrodinger operators on the quantum states. We can now obtain,

$$\left|\langle e_1|\psi(t)\rangle\right|^2 = \langle\psi(t=0)|\hat{N}_1(t)|\psi(t=0)\rangle$$
$$= \langle e_1|\hat{N}(t)|e_1\rangle$$
$$= \cos^2\left(\frac{Ut}{\hbar}\right).$$

and,

$$\left|\langle e_2|\psi(t)\rangle\right|^2 = \langle e_1|\hat{N}_2(t)|e_1\rangle = \sin^2\left(\frac{U}{\hbar}t\right).$$

These results are the same as found earlier using the Schrodinger equation.

1.5 Quantum Mechanical Measurements

1.5.1 Commutation Relations in Quantum Mechanics and Physical Measurements

In quantum mechanics, commutation relations have an intimate connection with physical measurements and this connection will be explored in the following Sections.

Commutation Relations and Common Eigenvectors

We know from linear algebra that if two matrices commute then they can both have the same set of eigenvectors. In quantum mechanics, if two operators $\hat{A}$ and $\hat{B}$ commute (i.e $\left[\hat{A},\hat{B}\right]=0$) then they also can have the same set of eigenvectors.

Outline of the Proof: Suppose $\hat{A}$ has eigenvector $|v_k\rangle$ with eigenvalues λ_k i.e $\hat{A}|v_k\rangle = \lambda_k|v_k\rangle$. Since $\left[\hat{A},\hat{B}\right]=0$,

$$\Rightarrow \hat{A}\,\hat{B} - \hat{B}\,\hat{A} = 0$$
$$\Rightarrow \left(\hat{A}\,\hat{B} - \hat{B}\,\hat{A}\right)|v_k\rangle = 0$$
$$\Rightarrow \hat{A}\,\hat{B}|v_k\rangle - \lambda_k\,\hat{B}|v_k\rangle = 0$$
$$\Rightarrow \hat{A}\left(\hat{B}|v_k\rangle\right) = \lambda_k\left(\hat{B}|v_k\rangle\right)$$

$\Rightarrow \hat{B}|v_k\rangle$ is also an eigenvector of $\hat{A}$ with eigenvalue λ_k. If $\hat{A}$ has all distinct eigenvalues then $\hat{B}|v_k\rangle$ must be proportional to $|v_k\rangle$ (i.e $\hat{B}|v_k\rangle \propto |v_k\rangle$) and this means that $|v_k\rangle$ is also an eigenvector of $\hat{B}$. If $\hat{A}$ has many eigenvectors with the same eigenvalue λ_k then $\hat{B}|v_k\rangle$ must at least lie in this eigensubspace of $\hat{A}$ even if $\hat{B}|v_k\rangle$ is not proportional to $|v_k\rangle$. In this case, the vectors in this eigensubspace of $\hat{A}$ can be chosen such that they are also eigenvectors of $\hat{B}$ (a proof of this can be found in any text on linear algebra).

Commutation Relations and Simultaneous Measurements

Consider two operators $\hat{A}$ and $\hat{B}$ that have eigenvectors and (all distinct) eigenvalues given by,

$$\hat{A}|v_k\rangle = \alpha_k |v_k\rangle \qquad \hat{B}|u_k\rangle = \beta_k |u_k\rangle$$

1) Supppose the observable A is measured for a state $|\psi\rangle$. The a-priori probability of obtaining the result α_k is $\left|\langle v_k|\psi\rangle\right|^2$. Suppose α_j was obtained. Immediately after the measurement the quantum state $|\psi\rangle$ collapses to $|v_j\rangle$. All subsequent measurements of A (done fast enough so that no evolution described by the Schrodinger equation takes place during this time) will yield the result α_j.

2) Now suppose the observable A is measured for a state $|\psi\rangle$. Suppose α_j was obtained and immediately after this measurement the quantum state $|\psi\rangle$ collapsed to $|v_j\rangle$. Now suppose the observable B is measured. The a-priori probability of obtaining β_k is $\left|\langle u_k|v_j\rangle\right|^2$. Suppose β_j was obtained. Immediately after the measurement the quantum state $|v_j\rangle$ collapses to $|u_j\rangle$. If now A is again measured, the probability of obtaining α_k is $\left|\langle v_k|u_j\rangle\right|^2$. The measurement of B `disturbed' the quantum state so that the second measurement of A gave a different result than the first. We say that A and B are not *simultaneously measurable*. Measurement of one quantity disturbs the value of the other quantity.

3) Suppose $\left[\hat{A},\hat{B}\right] = 0$. Then $\hat{A}$ and $\hat{B}$ have the same set of eigenvectors, say $|\omega_k\rangle$. In other words,

$$\hat{A}|\omega_k\rangle = \alpha_k |\omega_k\rangle$$
$$\hat{B}|\omega_k\rangle = \beta_k |\omega_k\rangle$$

Now suppose the following sequence of events: A is measured $\rightarrow$ result α_j is obtained $\rightarrow B$ is measured $\rightarrow$ result β_j obtained. But now all subsequent measurements of A and/or B will give the results α_j and β_j, respectively. We say that if $\hat{A}$ and $\hat{B}$ commute they are simultaneously measurable (i.e. measurement of one quantity does not disturb the value of the other quantity). Of course, it has been implicitly assumed that all measurements are done in a time period short enough that no time evolution of the quantum state occurs.

1.5.2 Quantum Mechanical Decoherence

Decoherence is one of the least understood as well as the most misunderstood concept in quantum mechanics. A simple picture of decoherence is presented here. Consider the superposition state $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$ of a particle. A measurement is made to determine whether the particle is in $|v_1\rangle$ or $|v_2\rangle$. If the result is $|v_1\rangle$ and the state immediately after the measurement is $|v_1\rangle$ (i.e. $|\psi\rangle = |v_1\rangle$). If the result is $|v_2\rangle$ then just after the measurement, $|\psi\rangle = |v_2\rangle$. In either case, the action of measurement destroys the linear superposition state given by $c_1|v_1\rangle + c_2|v_2\rangle$ and replaces it by either $|v_1\rangle$ or $|v_2\rangle$ depending upon the measurement outcome. In other words, the acquisition of information (by intelligent beings) can destroy quantum mechanical linear superpositions. An intelligent being does not need to make a direct measurement. He/she can perhaps use, say a photon or phonon, and scatter it off the particle to determine whether the particle is in $|v_1\rangle$ state or in $|v_2\rangle$ state. Any such procedure that gives the intelligent being information about whether the particle is in $|v_1\rangle$ or $|v_2\rangle$ destroys the linear superposition and collapses the quantum state of the particle into either $|v_1\rangle$ or $|v_2\rangle$.

Now suppose the test particle is interacting with its environment. If there is a way by which an intelligent being can determine whether the particle is in $|v_1\rangle$ or $|v_2\rangle$ by just observing the environment then the linear superposition state of the particle will still get destroyed. Linear superpositions can therefore be short lived and can easily get destroyed by interaction with the environment (even if no intelligent being is actively making a measurement).

A question to ask here is if there a way to quantify this destruction of quantum mechanical linear superpositions. For the state $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$, consider the products $c_1^* c_2$ and $c_2^* c_1$. These products are indicative of the linear superposition in the state $|\psi\rangle$. If these products are zero then a linear superposition does not exist. The operators $\hat{\sigma}_- == |v_1\rangle\langle v_2|$ and $\hat{\sigma}_+ == |v_2\rangle\langle v_1|$ generate these products given a state $|\psi\rangle$,

$$\langle\psi|\hat{\sigma}_-|\psi\rangle = c_1^* c_2 \qquad \langle\psi|\hat{\sigma}_+|\psi\rangle = c_2^* c_1$$

The interaction of a particle with its environment can make these products go to zero as time progresses, i.e.,

$$\langle\psi(t)|\hat{\sigma}_-|\psi(t)\rangle = \; c_1^*(t)c_2(t) \xrightarrow{t\to\infty} 0$$

and,

$$\langle\psi(t)|\hat{\sigma}_+|\psi(t)\rangle = \; c_2^*(t)c_1(t) \xrightarrow{t\to\infty} 0$$

This phenomenon which results in the destruction of quantum mechanical superpositions is called quantum mechanical decoherence.

A Paradox: We started from a state $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$ and reached the conclusion that as time progresses, $|\psi\rangle$ will either collapse into $|v_1\rangle$ or $|v_2\rangle$ by interaction with the environment (i.e. the linear superposition will get destroyed). Suppose a new basis set is introduced,

$$|v_+\rangle = \frac{1}{\sqrt{2}}\left(|v_1\rangle + |v_2\rangle\right) \quad |v_-\rangle = \frac{1}{\sqrt{2}}\left(|v_1\rangle - |v_2\rangle\right)$$

Then starting from $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$ one ends up in $|v_1\rangle$ or $|v_2\rangle$ which one can also write as, $\frac{1}{\sqrt{2}}\left(|v_+\rangle + |v_-\rangle\right)$ and $\frac{1}{\sqrt{2}}\left(|v_+\rangle - |v_-\rangle\right)$, respectively. We said linear superpositions get destroyed by interaction with the environment. Then now come we end up in linear superposition states after interaction with the environment? Of course, any state can be written as a linear superposition state by choosing an appropriate basis set. Whether or not linear superpositions in a particular basis representation get destroyed depends on the nature of the interaction between the particle and the environment and exactly what information is extracted by the environment during the interaction. Suppose the interaction of the particle, initially in state $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$, is such that an intelligent observer by looking later at the environment can figure out whether the particle was in $|v_+\rangle$ or $|v_-\rangle$. We can write $|\psi\rangle$ as,

$$|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle = \frac{(c_1+c_2)}{\sqrt{2}}|v_+\rangle + \frac{(c_1-c_2)}{\sqrt{2}}|v_-\rangle$$

As time progresses the linear superposition between $|v_+\rangle$ and $|v_-\rangle$ will get destroyed and the particle state will end up in $|v_+\rangle$ or $|v_-\rangle$, which are $\frac{1}{\sqrt{2}}\left(|v_1\rangle + |v_2\rangle\right)$ and $\frac{1}{\sqrt{2}}\left(|v_1\rangle - |v_2\rangle\right)$, respectively.

1.6 The Quantum Mechanical Density Operator

1.6.1 Pure States and Statistical Mixtures

Consider two sets of quantum states:

Set A: A large number of identical copies of the linear superposition state, $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$

Set B: A large number of states $|v_1\rangle$ and $|v_2\rangle$. The numbers of $|v_1\rangle$ states and $|v_2\rangle$ states are in the ratio $|c_1|^2 : |c_2|^2$.

Set A consists of pure states $|\psi\rangle$. Set B is a statistical mixture of states $|v_1\rangle$ and $|v_2\rangle$. Suppose the states $|v_1\rangle, |v_2\rangle$ are eigenstates of an operator $\hat{O}$ with corresponding eigenvalues λ_1 and λ_2, respectively. If the mean value of $\hat{O}$ is measured for sets A and B, the same result $\left(\lambda_1|c_1|^2 + \lambda_2|c_2|^2\right)$ will be obtained for both sets. Is there a way to handle the distinction between pure states (set A) and a statistical mixture (set B)? The answer is yes, and the density operator is the tool designed to handle pure states and statistical mixtures on equal footing.

1.6.2 The Density Operator and the Density Matrix in Quantum Mechanics

Density operators are a useful way to represent quantum states. Density operators can also describe dynamics of quantum states (including decoherence) in a simple way. Density operators can also represent statistical mixtures in addition to pure quantum states. Most generally, a quantum state is not represented by a state vector $|\psi\rangle$, but by a density operator $\hat{\rho}$.

For a pure state $|\psi\rangle$ the density operator $\hat{\rho}$ is $|\psi\rangle\langle\psi|$. If $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$, as in the case of set A above, $\hat{\rho}$ is,

$$\hat{\rho} = |c_1|^2|v_1\rangle\langle v_1| + |c_2|^2|v_2\rangle\langle v_2| + c_1^* c_2|v_2\rangle\langle v_1| + c_2^* c_1|v_1\rangle\langle v_2|$$

The density operator, like all quantum mechanical operators, can be put in a matrix form. In matrix representation, using the basis $|v_1\rangle$ and $|v_2\rangle$ (i.e. $|v_1\rangle \rightarrow \begin{bmatrix}1\\0\end{bmatrix}$ and $|v_2\rangle \rightarrow \begin{bmatrix}0\\1\end{bmatrix}$), the density operator is,

$$\hat{\rho} = \begin{bmatrix} |c_1|^2 & c_2^* c_1 \\ c_1^* c_2 & |c_2|^2 \end{bmatrix} \qquad (1)$$

The diagonal elements of $\hat{\rho}$ indicate the occupation probabilities, and the off-diagonal elements represent coherences. For a statistical mixture, as in the case of set B above, the density operator is,

$$\hat{\rho} = |c_1|^2 \, |v_1\rangle\langle v_1| + |c_2|^2 \, |v_2\rangle\langle v_2|$$

In matrix form,

$$\hat{\rho} = \begin{bmatrix} |c_1|^2 & 0 \\ 0 & |c_2|^2 \end{bmatrix} \qquad (2)$$

Comparing (2) to (1), we see that the off-diagonal elements of the density matrix are absent for a statistical mixture. We also know that decoherence can destroy linear superposition and reduce a large collection of states of the form $c_1|v_1\rangle + c_2|v_2\rangle$ to a statistical mixture that has states $|v_1\rangle$ and $|v_2\rangle$ with probabilities $|c_1|^2$ and $|c_2|^2$. Thus we expect,

$$\hat{\rho} = \begin{bmatrix} |c_1|^2 & c_2^* c_1 \\ c_1^* c_2 & |c_2|^2 \end{bmatrix} \xrightarrow{\text{Decoherence}} \hat{\rho} = \begin{bmatrix} p_1 & 0 \\ 0 & p_2 \end{bmatrix}$$

Decoherence can destroy off diagonal elements of the density operator (or the density matrix).

Mean Values of Operators Using the Density Operator/Matrix: The mean value of an observable A with respect to the state $|\psi\rangle$ was $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$. The mean value of A with respect to the density operator $\hat{\rho}$ is defined as,

$$\langle \hat{A} \rangle = \text{Trace}\{\hat{\rho}\,\hat{A}\}$$

Suppose, $\hat{\rho} = |\psi\rangle\langle\psi|$ where $|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle$, and $|v_1\rangle$ and $|v_2\rangle$ form a complete basis. Then,

$$\begin{aligned}
\text{Trace}\{|\psi\rangle\langle\psi|\hat{A}\} &= \sum_n \langle v_n| \, |\psi\rangle\langle\psi|\hat{A}\,|v_n\rangle \\
&= \langle v_1|\psi\rangle\langle\psi|\hat{A}|v_1\rangle + \langle v_2|\psi\rangle\langle\psi|\hat{A}|v_2\rangle \\
&= |c_1|^2 \langle v_1|\hat{A}|v_1\rangle + |c_2|^2 \langle v_2|\hat{A}|v_2\rangle \\
&\quad + c_2^* c_1 \langle v_2|\hat{A}|v_1\rangle + c_1^* c_2 \langle v_1|\hat{A}_1\,|v_2\rangle \\
&= \langle \psi | \hat{A} | \psi \rangle
\end{aligned}$$

On the other hand if $\hat{\rho}$ represents a statistical mixture of $|v_1\rangle$ and $|v_2\rangle$ with probabilities $|c_1|^2$ and $|c_2|^2$ then,

$$\begin{aligned}
\langle \hat{A} \rangle = \text{Trace}\{\hat{\rho}\,\hat{A}\} &= \text{Trace}\left\{\left(|c_1|^2 |v_1\rangle\langle v_1| + |c_2|^2 |v_2\rangle\langle v_2|\right)\hat{A}\right\} \\
&= |c_1|^2 \langle v_1| \, \hat{A}|v_1\rangle + |c_2|^2 \langle v_2|A|v_2\rangle
\end{aligned}$$

A More Complicated Example: Suppose we have a statistical mixture of states $|v_+\rangle = \frac{1}{\sqrt{2}}\left(|v_1\rangle + |v_2\rangle\right)$ and $|v_-\rangle = \frac{1}{\sqrt{2}}\left(|v_1\rangle - |v_2\rangle\right)$ with probabilities p_+ and p_-, respectively. In this case we have a *statistical mixture of linear superposition states*. Then,

$$\hat{\rho} = p_+ |v_+\rangle\langle v_+| + p_- |v_-\rangle\langle v_-| \quad \{ p_+ + p_- = 1$$

We can write the above expression as,

$$\hat{\rho} = \frac{p_+}{2}\left[|v_1\rangle\langle v_1| + |v_2\rangle\langle v_2| + |v_1\rangle\langle v_2| + |v_2\rangle\langle v_1|\right]$$
$$+ \frac{p_-}{2}\left[|v_1\rangle\langle v_1| + |v_2\rangle\langle v_2| - |v_1\rangle\langle v_2| - |v_2\rangle\langle v_1|\right]$$
$$= \frac{1}{2}|v_1\rangle\langle v_1| + \frac{1}{2}|v_2\rangle\langle v_2| + \frac{(p_+ - p_-)}{2}|v_1\rangle\langle v_2| + \frac{(p_+ - p_-)}{2}|v_2\rangle\langle v_1|$$

Note that the density matrix was diagonal in the $|v_+\rangle, |v_-\rangle$ basis but has off-diagonal elements in the $|v_1\rangle, |v_2\rangle$ basis. The average value of the observable A is then,

$$\langle \hat{A} \rangle = \text{Trace}\left\{\hat{\rho}\,\hat{A}\right\} = \frac{1}{2}\langle v_1 |\hat{A}| v_1\rangle + \frac{1}{2}\langle v_2 |\hat{A}| v_2\rangle$$
$$+ \frac{(p_+ - p_-)}{2}\langle v_2 |\hat{A}| v_1\rangle + \frac{(p_+ - p_-)}{2}\langle v_1 |\hat{A}| v_2\rangle.$$

The above examples show that density operators/matrices can handle the most general types of situations.

1.6.3 Time Development of Density Operators

In the case of pure states, the average value of a quantity A at time "t" was shown to be,

$$\langle \hat{A}(t) \rangle = \langle \psi(t) |\hat{A}| \psi(t)\rangle \quad \rightarrow \quad \text{Schrodinger Picture (the state is time dependent)}$$
$$= \langle \psi(t=0) |\hat{A}(t)| \psi(t=0)\rangle \quad \rightarrow \quad \text{Heisenberg Picture (the operator is time dependent)}$$

There are also two ways to calculate averages when quantum states are described by density operators,

$$\langle \hat{A}(t) \rangle = \text{Trace}\left\{\hat{\rho}(t)\hat{A}(t=0)\right\} = \text{Trace}\left\{\hat{\rho}(t)\hat{A}\right\} \quad \rightarrow \quad \text{Schrodinger Picture (the state is time dependent)}$$
$$= \text{Trace}\left\{\hat{\rho}(t=0)\hat{A}(t)\right\} \quad \rightarrow \quad \text{Heisenberg Picture (the operator is time dependent)}$$

To see their equivalence, recall that,

$$\hat{A}(t) = e^{i\frac{\hat{H}}{\hbar}t}\,\hat{A}\,e^{-i\frac{\hat{H}}{\hbar}t}$$

So,

$$\text{Trace}\left\{\hat{\rho}(t=0)\hat{A}(t)\right\} = \text{Trace}\left\{\hat{\rho}(t=0)e^{i\frac{\hat{H}}{\hbar}t}\,\hat{A}\,e^{-i\frac{\hat{H}}{\hbar}t}\right\}$$

Use the result, $\text{Trace}\left\{\hat{A}\hat{B}\right\} = \text{Trace}\left\{\hat{B}\hat{A}\right\}$, to get,

$$\text{Trace}\left\{\hat{\rho}(t=0)\hat{A}(t)\right\} = \text{Trace}\left\{e^{\frac{-i\hat{H}}{\hbar}t}\,\hat{\rho}(t=0)e^{\frac{i\hat{H}}{\hbar}t}\;\hat{A}\right\}$$
$$= \text{Trace}\left\{\hat{\rho}(t)\hat{A}\right\}$$

where,

$$\hat{\rho}(t) = e^{\frac{-i\hat{H}}{\hbar}t}\,\hat{\rho}(t=0)e^{\frac{i\hat{H}}{\hbar}t}$$

After differentiating the above equation with respect to time we obtain the Schrodinger equation (not the Heisenberg equation) for the density operator,

$$i\hbar\frac{\partial\hat{\rho}(t)}{\partial t} = \left[\hat{H},\hat{\rho}(t)\right]$$

Note that the above equation is a little different from the Heisenberg equation for any other operator,

$$i\hbar\frac{\partial\hat{A}(t)}{\partial t} = \left[\hat{A}(t),\hat{H}\right]$$

An advantage of the Heisenberg picture is that we can calculate correlation functions of observables, such as,

$$\text{Trace}\left\{\hat{\rho}(t=0)\hat{A}(t_1)\hat{B}(t_2)\right\}$$

It is difficult to compute these quantities in the Schrodinger picture. In the Schrodinger picture, we can only easily compute equal time averages, e.g.,

$$\text{Trace}\left\{\hat{\rho}(t=0)\hat{A}(t_1)\hat{B}(t_1)\right\} = \text{Trace}\left\{\rho(t_1)\hat{A}\hat{B}\right\}$$

Two-level System via the Density Operator Formalism in the Schrodinger Picture

Consider the two-level system described by the Hamiltonian,

$$\hat{H} = \varepsilon\left(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2|\right) - U\left(|e_2\rangle\langle e_1| + |e_1\rangle\langle e_2|\right).$$

Suppose, $|\psi(t=0)\rangle = |e_1\rangle$. The density operator is then,

$$\hat{\rho}(t=0) = |\psi(t=0)\rangle\langle\psi(t=0)| = |e_1\rangle\langle e_1|$$

In the matrix form, with $|e_1\rangle \rightarrow \begin{bmatrix}1\\0\end{bmatrix}$ and $|e_2\rangle \rightarrow \begin{bmatrix}0\\1\end{bmatrix}$ as the basis, we get,

$$\hat{\rho}(t=0) = \begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}$$

Our goal is to find,

$$\left|\langle e_1|\psi(t)\rangle\right|^2 = \langle\psi(t)|e_1\rangle\langle e_1|\psi(t)\rangle = \text{Trace}\left\{\hat{\rho}(t)|e_1\rangle\langle e_1|\right\} = \rho_{11}(t)$$

Start from,

$$i\hbar\frac{\partial\hat{\rho}(t)}{\partial t} = \hat{H}\hat{\rho}(t) - \hat{\rho}(t)\hat{H} \qquad \left\{\hat{\rho}(t) = \begin{bmatrix}\rho_{11}(t) & \rho_{12}(t)\\ \rho_{21}(t) & \rho_{22}(t)\end{bmatrix}\right.$$

Take the matrix element of the above equation with $\langle e_1|$ and $|e_1\rangle$ to get,

$$i\hbar\frac{d}{dt}\rho_{11}(t) = U\left[\rho_{12}(t) - \rho_{21}(t)\right]$$

Take the matrix element with $\langle e_2|$ and $|e_1\rangle$ to get,

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho_{21}(t) = U\left[\rho_{22}(t) - \rho_{11}(t)\right]$$

Similarly,

$$i\hbar \frac{d}{dt}\rho_{22}(t) = -U\left[\rho_{12}(t) - \rho_{21}(t)\right]$$

$$i\hbar \frac{d}{dt}\rho_{12}(t) = -U\left[\rho_{22}(t) - \rho_{11}(t)\right]$$

Note that,

$$\frac{d}{dt}\left[\rho_{11}(t) + \rho_{22}(t)\right] = 0$$

$$\Rightarrow \rho_{11}(t) + \rho_{22}(t) = \rho_{11}(t=0) + \rho_{22}(t=0) = \rho_{11}(t=0)$$

The above equation described the conservation of probability during time evolution. Let,

$$\rho_d(t) = \rho_{22}(t) - \rho_{11}(t)$$

$$\rho_s(t) = \rho_{12}(t) - \rho_{21}(t)$$

Then,

$$\frac{d}{dt}\rho_d(t) = \frac{2iU}{\hbar}\rho_s(t)$$

and,

$$\frac{d}{dt}\rho_s(t) = \frac{2iU}{\hbar}\rho_d(t)$$

Combining the above two equation gives,

$$\frac{d^2}{dt^2}\rho_d(t) = -\left(\frac{2U}{\hbar}\right)^2 \rho_d(t)$$

The boundary conditions are,

$$\begin{cases} \rho_d(t=0) = \rho_{22}(t=0) - \rho_{11}(t=0) = -1 \\ \left.\dfrac{d}{dt}\rho_d(t)\right|_{t=0} = \dfrac{2iU}{\hbar}\rho_s(t=0) = \dfrac{2iU}{\hbar}\left[\rho_{12}(t=0) - \rho_{21}(t=0)\right] \end{cases}$$

The solution is,

$$\rho_d(t) = -\cos\left(\frac{2U}{\hbar}t\right).$$

$$\Rightarrow \rho_{11}(t) = \frac{\left[\rho_{11}(t) + \rho_{22}(t)\right] - \left[\rho_d(t)\right]}{2} = \frac{1 + \cos\left(\dfrac{2U}{\hbar}t\right)}{2} = \cos^2\left(\frac{Ut}{\hbar}\right).$$

$$\Rightarrow \rho_{22}(t) = \sin^2\left(\frac{Ut}{\hbar}\right).$$

So,

$$\left|\langle e_1 | \psi(t)\rangle\right|^2 = \mathrm{T_r}\left\{\hat{\rho}(t)|e_1\rangle\langle e_1|\right\} = \rho_{11}(t) = \cos^2\left(\frac{U}{\hbar}t\right).$$

This is the same result as obtained earlier by different methods.

Decoherence in the Density Operator Formalism

We first discuss the effects of decoherence. Averages computed via the density operator should be interpreted is an average sense, i.e. the average $\left\langle \hat{A}(t) \right\rangle = \text{Trace}\left\{ \hat{\rho}(t)\hat{A} \right\}$ could mean either one of the following:

a) Several identical copies of a system are prepared at $t = 0$ and the state of each system is represented by the density operator $\hat{\rho}(t = 0)$. At time t measurement of a quantity A is made on all copies of the system. The average of the results obtained corresponds to the quantity $\text{Trace}\left\{ \hat{\rho}(t)\hat{A} \right\}$.

b) A single system is prepared at $t = 0$ and the state of the system is represented by the density operator $\hat{\rho}(t = 0)$. At time t measurement of a quantity A is made. The system is then put (by some means) in the same state $\hat{\rho}(t = 0)$, and the process is repeated many times. The average of all the measurements corresponds to the quantity $\text{Trace}\left\{ \hat{\rho}(t)\hat{A} \right\}$.

We are now in a position to understand how decoherence will effect our results. Suppose we have N different copies of a two-level system, and all copies are prepared in the state $|e_1\rangle$ at time $t = 0$. So, assuming interpretation (a), the density operator of each system is,

$$\hat{\rho}(t = 0) = |e_1\rangle\langle e_1|$$

At later time t (assuming no decoherence),

$$\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|$$

$$= \cos^2\left(\frac{Ut}{\hbar}\right)|e_1\rangle\langle e_1| + \sin^2\left(\frac{Ut}{\hbar}\right)|e_2\rangle\langle e_2|$$

$$+ i\cos\left(\frac{Ut}{\hbar}\right)\sin\left(\frac{Ut}{\hbar}\right)|e_2\rangle\langle e_1| - i\cos\left(\frac{Ut}{\hbar}\right)\sin\left(\frac{Ut}{\hbar}\right)|e_1\rangle\langle e_2|$$

At time t consider the state of the j-th system,

$$|\psi(t)\rangle_j = \left\{\cos\left(\frac{Ut}{\hbar}\right)|e_1\rangle_j + i\sin\left(\frac{Ut}{\hbar}\right)|e_2\rangle_j\right\} e^{-i\frac{\varepsilon}{\hbar}t}$$

Suppose the j-th system at $t = t_1$ collapsed into $|e_1\rangle$ as a result of decoherence. For $t > t_1$, $|\psi(t)\rangle_j$ becomes,

$$|\psi(t)\rangle_j = \left\{\cos\left(\frac{U}{\hbar}(t - t_1)\right)|e_1\rangle_j + i\sin\left(\frac{U}{\hbar}(t - t_1)\right)|e_2\rangle_j\right\} e^{-i\frac{\varepsilon}{\hbar}(t - t_1)}$$

$$= \left\{\cos\left[\frac{Ut}{\hbar} + \phi_j\right]|e_1\rangle_j + i\sin\left(\frac{Ut}{\hbar} + \phi_j\right)|e_2\rangle_j\right\} e^{-i\frac{\varepsilon}{\hbar}(t - t_1)}$$

where, $\phi_j = -\frac{Ut_1}{\hbar}$. Now suppose at $t = t_2$ the k-th system collapsed into $-i|e_2\rangle$. For $t > t_2$,

$$|\psi(t)\rangle_k = \left\{\cos\left[\frac{Ut}{\hbar} + \phi_k - \frac{\pi}{2}\right]|e_1\rangle_k + i\sin\left(\frac{Ut}{\hbar} + \phi_k - \frac{\pi}{2}\right)|e_2\rangle_k\right\} e^{-i\frac{\varepsilon}{\hbar}(t - t_2)}$$

where $\phi_k = -\frac{Ut_2}{\hbar}$. As time progresses more and more systems will decohere and collapse into either $-i|e_2\rangle$ or $|e_1\rangle$. Since the times when the states of different systems collapse are random, the phases ϕ

will also be random. Therefore, in what follows, one can absorb the $\frac{\pi}{2}$ phase terms in it. The process of decoherence usually has an associated time scale, which we will call $1/\gamma$. For $t << 1/\gamma$, most systems will not have experienced a state collapse. For $t >> 1/\gamma$, most systems would have experienced a state collapse. At time t, the ensemble average of any observable quantity A (averaged over the entire system) will be,

$$\left\langle \hat{A}(t) \right\rangle = \frac{\sum_{p=1}^{N} {}_p\langle \psi(t) | \hat{A} | \psi(t) \rangle_p}{N}$$

$$= \frac{1}{N} \sum_{p=1}^{N} \left\{ \cos^2\left(\frac{Ut}{\hbar} + \phi_p\right) {}_p\langle e_1 | \hat{A} | e_1 \rangle_p + \sin^2\left(\frac{Ut}{\hbar} + \phi_p\right) {}_p\langle e_2 | \hat{A} | e_2 \rangle_p \right.$$

$$+ i \cos\left(\frac{Ut}{\hbar} + \phi_p\right) \sin\left(\frac{Ut}{\hbar} + \phi_p\right) {}_p\langle e_1 | \hat{A} | e_2 \rangle_p$$

$$\left. - i \cos\left(\frac{Ut}{\hbar} + \phi_p\right) \sin\left(\frac{Ut}{\hbar} + \phi_p\right) {}_p\langle e_2 | \hat{A} | e_1 \rangle_p \right\}$$

If $t >> 1/\gamma$, ϕ_p for every system will be non-zero and will have a random value. For N large, one can replace the sum over p by averaging with respect to ϕ assuming that ϕ is a random variable uniformly distributed in the interval from $0 \le \phi < 2\pi$, and the above expression becomes,

$$\left\langle \hat{A}(t >> 1/\gamma) \right\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi} \left\{ \cos^2\left(\frac{Ut}{\hbar} + \phi\right) \langle e_1 | \hat{A} | e_1 \rangle + \sin^2\left(\frac{Ut}{\hbar} + \phi\right) \langle e_2 | \hat{A} | e_2 \rangle \right.$$

$$\left. + i \frac{1}{2} \sin\left(2\frac{Ut}{\hbar} + 2\phi\right) \langle e_1 | \hat{A} | e_2 \rangle - i \frac{1}{2} \sin\left(2\frac{Ut}{\hbar} + 2\phi\right) \langle e_2 | \hat{A} | e_1 \rangle \right\}$$

$$= \frac{1}{2} \langle e_1 | \hat{A} | e_1 \rangle + \frac{1}{2} \langle e_2 | \hat{A} | e_2 \rangle$$

The above result is equivalent to the density matrix $\hat{\rho}(t)$ for $t >> 1/\gamma$ given by,

$$\hat{\rho}(t >> 1/\gamma) = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

A description of decoherence must therefore give the same results as obtained above. This can be done by modifying the equations for the off-diagonal components of the density matrix and introducing a decay term,

$$\frac{d}{dt} \rho_{12}(t) = -\gamma \, \rho_{12}(t) + i \frac{U}{\hbar} [\rho_{22}(t) - \rho_{11}(t)]$$

$$\frac{d}{dt} \rho_{21}(t) = -\gamma \, \rho_{21}(t) - i \frac{U}{\hbar} [\rho_{22}(t) - \rho_{11}(t)]$$

Now we get for,

$$\rho_d(t) = \rho_{22}(t) - \rho_{11}(t)$$

the equation,

$$\frac{d^2}{dt^2} \rho_d(t) + \gamma \frac{d}{dt} \rho_d(t) + \left(\frac{2U}{\hbar}\right)^2 \rho_d(t) = 0$$

Using the same boundary conditions as before we get the result,

$$\rho_d(t) = -e^{-\frac{\gamma}{2}t}\left[\cos\Omega t + \frac{\gamma}{2\Omega}\sin\Omega t\right]$$

$$\Omega = \sqrt{\left(\frac{2U}{\hbar}\right)^2 - \left(\frac{\gamma}{2}\right)^2}$$

and,

$$\rho_{11}(t) = \frac{1}{2}\left\{1 + e^{-\frac{\gamma}{2}t}\left[\cos\Omega t + \frac{\gamma}{2\Omega}\sin\Omega t\right]\right\}$$

$$\rho_{22}(t) = \frac{1}{2}\left\{1 - e^{-\frac{\gamma}{2}t}\left[\cos\Omega t + \frac{\gamma}{2\Omega}\sin\Omega t\right]\right\}$$

As $t \to \infty$,

$$\rho_{11}(t) \to \frac{1}{2}$$

$$\rho_{22}(t) \to \frac{1}{2}$$

and,

$$\rho_{12}(t) \to 0$$

$$\rho_{21}(t) \to 0$$

Therefore,

$$\hat{\rho}(t) \xrightarrow[t\to\infty]{} \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

This is just what was desired. Thus, introduction of coherence decay terms (i.e. γ) works as expected. Note that we arbitrarily inserted these coherence decay terms in the equations for $\rho_{12}(t)$ and $\rho_{21}(t)$. Question arises if there is a better description, or a better equation, for the density operator of the form,

$$i\hbar\frac{d}{dt}\hat{\rho}(t) = ??$$

whose matrix elements contain the decoherence terms for the off-diagonal components. It terms out there is such an equation, but it is complicated. It is much easier to do this is the Heisenberg picture using Langevin equations. We shall do this later in the course.

Two-level System via the Density Operator Formalism in the Heisenberg Picture

In the Heisenberg picture,

$$\left\langle \hat{A}(t) \right\rangle = \mathrm{Tr}\left\{\hat{\rho}(t=0)\hat{A}(t)\right\}$$

where,

$$i\hbar\frac{d}{dt}\hat{A}(t) = \left[\hat{A}(t), \hat{H}(t)\right]$$

We have as before,

$$\hbar\frac{d}{dt}\hat{N}_1(t) = U\left[\hat{\sigma}_+(t) - \hat{\sigma}_-(t)\right] \qquad (1)$$

$$i\hbar\frac{d}{dt}\hat{N}_2(t) = -U\left[\hat{\sigma}_+(t)-\hat{\sigma}_-(t)\right] \qquad (2)$$

$$i\hbar\frac{d}{dt}\hat{\sigma}_+(t) = -U\left[\hat{N}_2(t)-\hat{N}_1(t)\right] \qquad (3)$$

$$i\hbar\frac{d}{dt}\hat{\sigma}_-(t) = +U\left[\hat{N}_2(t)-\hat{N}_1(t)\right] \qquad (4)$$

Since,

$$\left.\begin{aligned}\rho_{11}(t) &= \text{Trace}\left\{\hat{\rho}(t)|e_1\rangle\langle e_1|\right\}\\ &= \text{Trace}\left\{\hat{\rho}(t)\hat{N}_1\right\}\\ &= \text{Trace}\left\{\hat{\rho}(t=0)\hat{N}_1(t)\right\}\\ \rho_{22}(t) &= \text{Trace}\left\{\hat{\rho}(t=0)\hat{N}_2(t)\right\}\\ \rho_{12}(t) &= \text{Trace}\left\{\hat{\rho}(t)\hat{\sigma}_+\right\} = \text{Trace}\left\{\hat{\rho}(t=0)\hat{\sigma}_+(t)\right\}\\ \rho_{21}(t) &= \text{Trace}\left\{\hat{\rho}(t=0)\hat{\sigma}_-(t)\right\}\end{aligned}\right\}$$

the average of equations (1)-(4) with respect to $\text{Trace}\left\{\hat{\rho}(t=0)\bullet\right\}$ gives the equations we obtained earlier for $\rho_{11}(t),\rho_{22}(t),\rho_{12}(t),\text{and }\rho_{21}(t)$ working in the Schrodinger picture. The solution of (1)-(4) is,

$$\hat{N}_1(t) = \hat{N}_1\cos^2\left(\frac{Ut}{\hbar}\right)+\hat{N}_2\sin^2\left(\frac{Ut}{\hbar}\right)-i\frac{1}{2}(\hat{\sigma}_+-\hat{\sigma}_-)\sin\left(\frac{2Ut}{\hbar}\right)$$

$$\Rightarrow\left\langle\hat{N}_1(t)\right\rangle = \text{Trace}\left\{\hat{\rho}(t=0)\hat{N}_1(t)\right\} = \text{Trace}\left\{|e_1\rangle\langle e_1|\hat{N}_1(t)\right\}$$

$$= \langle e_1|\hat{N}_1(t)|e_1\rangle = \cos^2\left(\frac{Ut}{\hbar}\right)$$

$$\Rightarrow\left\langle\hat{N}_2\right\rangle(t) = \sin^2\left(\frac{Ut}{\hbar}\right).$$

Now we want to introduce decoherence. We can try changing the equations for $\hat{\sigma}_+(t)$ and $\hat{\sigma}_-(t)$ as follows,

$$\frac{d}{dt}\hat{\sigma}_+(t) = -\gamma\hat{\sigma}_+(t)+i\frac{U}{\hbar}\left[\hat{N}_2(t)-\hat{N}_1(t)\right] \qquad (5)$$

$$\frac{d}{dt}\hat{\sigma}_-(t) = -\gamma\hat{\sigma}_+(t)-i\frac{U}{\hbar}\left[\hat{N}_2(t)-\hat{N}_1(t)\right] \qquad (6)$$

The motivation for adding these decay terms is that we know that,

$$\text{Trace}\left\{\hat{\rho}(t=0)\hat{\sigma}_+(t)\right\} = \text{Trace}\left\{\hat{\rho}(t)(t)\hat{\sigma}_+\right\} = \rho_{12}(t)$$

and,

$$\text{Trace}\left\{\hat{\rho}(t=0)\hat{\sigma}_-(t)\right\} = \rho_{21}(t)$$

Since we have already seen that the equations for $\rho_{12}(t)$ and $\rho_{21}(t)$ and know they have the decay terms, the modified equations for $\hat{\sigma}_+(t)$ and $\hat{\sigma}_-(t)$ ensure that we get the right equations for $\rho_{12}(t)$ and $\rho_{21}(t)$. The solution of (1) (2) (5) (6) with initial conditions,

$$\hat{N}_1(t=0)=\hat{N}_1 \quad \hat{N}_2(t=0)=N_2$$

$$\hat{\sigma}_-(t=0)=\hat{\sigma}_- \quad \hat{\sigma}_+(t=0)=\hat{\sigma}_+$$

is

$$\hat{N}_1(t) = \frac{\hat{N}_1}{2}\left\{1+e^{-\frac{\gamma}{2}t}\left(\cos\Omega t+\frac{\gamma}{2\Omega}\sin\Omega t\right)\right\}+\frac{\hat{N}_2}{2}\left\{1-e^{-\frac{\gamma}{2}t}\left(\cos\Omega t+\frac{\gamma}{2\Omega}\sin\Omega t\right)\right\}$$

$$-i\frac{U}{\hbar\Omega}(\hat{\sigma}_+-\hat{\sigma}_-)e^{-\frac{\gamma}{2}t}\sin(\Omega t) \qquad \left\{\Omega=\sqrt{\left(\frac{2U}{\hbar}\right)-\left(\frac{\gamma}{2}\right)^2}\right.$$

and,

$$\hat{N}_2(t) = 1-\hat{N}_1(t)$$

Finally,

$$\left\langle\hat{N}_1(t)\right\rangle = \mathrm{Tr}\left\{\hat{\rho}(t=0)\hat{N}_1(t)\right\}=\mathrm{Tr}\left\{|e_1\rangle\langle e_1|\hat{N}_1(t)\right\}=\langle e_1|\hat{N}_1(t)|e_1\rangle$$

$$=\frac{1}{2}\left\{1+e^{-\frac{\gamma}{2}t}\left(\cos\Omega t+\frac{\gamma}{2\Omega}\sin\Omega t\right)\right\}$$

which is the same result as before.

A Big Problem: We had said earlier that time evolution in the Heisenberg picture preserves the commutation relations between operators.

Proof: If $\left[\hat{A},\hat{B}\right]=\hat{C}$ then,

$$\left[\hat{A}(t),\hat{B}(t)\right]=e^{\frac{i}{\hbar}\hat{H}t}\left[\hat{A},\hat{B}\right]e^{\frac{-i}{\hbar}\hat{H}t}=e^{\frac{i}{\hbar}\hat{H}t}\hat{C}\,e^{\frac{-i}{\hbar}\hat{H}t}=\hat{C}(t)$$

Commutation relations are fundamental ingredients of the quantum mechanical description of any system and can never be violated. But if one adds extra terms to the right hand side of the Heisenberg equation,

$$i\hbar\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t),\hat{H}\right]$$

then there is no guarantee that the commutation of $\hat{A}(t)$ with other operators will be preserved during time evolution. For example, to model decoherence we changed the equation for $\hat{\sigma}_+(t)$ given by,

$$\frac{d}{dt}\hat{\sigma}_+(t)=-\frac{i}{\hbar}\left[\hat{\sigma}_+(t),\hat{H}\right]=\frac{i}{\hbar}U\left[\hat{N}_2(t)-\hat{N}_1(t)\right]$$

to,

$$\frac{d}{dt}\hat{\sigma}_+(t)=-\gamma\,\hat{\sigma}_+(t)-\frac{i}{\hbar}\left[\hat{\sigma}_+(t),\hat{H}\right]=-\gamma\,\hat{\sigma}_+(t)+\frac{i}{\hbar}U\left[\hat{N}_2(t)-\hat{N}_1\right]$$

The original equation preserved the commutation relations, such as,

$$\left[\hat{N}_1(t),\hat{\sigma}_+(t)\right]=-\hat{\sigma}_+(t)$$

The modified equation *does not* preserve such commutations In modeling decoherence, we changed the equations in a way that spoiled the quantum mechanical consistency of the equations. We did not detect this problem in the Schrodinger picture since we took averages of the density operator equation,

$$\rho_{11}(t)=\langle e_1|\hat{\rho}(t)|e_1\rangle$$

$$\rho_{22}(t)=\langle e_2|\hat{\rho}(t)|e_2\rangle$$

$$\rho_{12}(t)=\langle e_1|\hat{\rho}(t)|e_2\rangle$$

$$\rho_{21}(t)=\langle e_2|\hat{\rho}(t)|e_1\rangle$$

and introduced decoherence into not the operator equations but the equations for complex numbers (e.g. $\rho_{21}(t)$ and $\rho_{12}(t)$). Later in the course, we will see that decoherence introduces noise into the system that is in some sense fundamental. This noise will be studied with Heisenberg-Langevin equations.

1.7 Product Hilbert Spaces

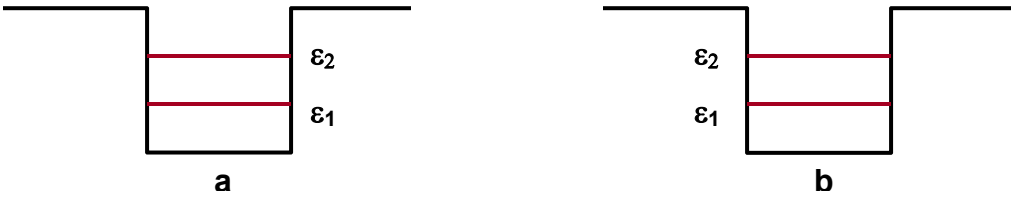
The Hilbert space of two independent quantum systems is obtained by "sticking" together the Hilbert spaces of the individual systems. For example, consider two systems, system "a" and system "b", with quantum states $|\phi\rangle_a$ and $|x\rangle_b$, respectively. The state $|\psi\rangle$ of the combined system is written as,

$$|\psi\rangle = |\phi\rangle_a \otimes |x\rangle_b$$

An operator in this enlarged Hilbert space is written as a tensor product, $\hat{A}\otimes\hat{B}$, where the operator $\hat{A}$ (or $\hat{B}$) acts only in the Hilbert space of system "a" (or system "b") as follows,

$$\hat{A}\otimes\hat{B}\,|\psi\rangle = \hat{A}\otimes\hat{B}\;\;|\phi\rangle_a \otimes |\chi\rangle_b = \hat{A}\;|\phi\rangle_a \otimes \hat{B}\,|\chi\rangle_b$$

Example: Two Different Two-Level Systems:



The Hamiltonian for two different two-level systems is,

$$\hat{H} = \hat{H}_a \otimes \hat{1}_b + \hat{1}_a \otimes \hat{H}_b$$

which, with a slight abuse of notation, is more commonly written as,

$$\hat{H} = \hat{H}_a + \hat{H}_b$$

Here,

$$\hat{H}_a = \varepsilon_1 |e_1\rangle_a \;{}_a\langle e_1| + \varepsilon_2 |e_2\rangle_a \;{}_a\langle e_1|$$

$$\hat{H}_b = \varepsilon_1 |e_1\rangle_b \;{}_b\langle e_1| + \varepsilon_2 |e_2\rangle_b \;{}_b\langle e_1|$$

An eigenstate of the combined system is, for example,

$$|e_1\rangle_a \otimes |e_2\rangle_b$$

And the action of the Hamiltonian on the eigenstate is,

$$\begin{aligned}\hat{H}|e_1\rangle_a \otimes |e_2\rangle_b &= \hat{H}_a \otimes \hat{1}_b \left\{|e_1\rangle_a \otimes |e_2\rangle_b\right\} + 1_a \otimes \hat{H}_b \left\{|e_1\rangle_a \otimes |e_2\rangle_b\right\} \\ &= \hat{H}_a\;|e_1\rangle_a \otimes 1_b |e_2\rangle_b + 1_a |e_1\rangle_a \otimes \hat{H}_b |e_2\rangle_b \\ &= \varepsilon_1 \left\{|e_1\rangle_a \otimes |e_2\rangle_b\right\} + \varepsilon_2 \left\{|e_1\rangle_a \otimes |e_2\rangle_b\right\} \\ &= (\varepsilon_1 + \varepsilon_2)|e_1\rangle_a \otimes |e_2\rangle_b\end{aligned}$$

Note that each operator in the tensor product acts on the state belonging to its own Hilbert space.

Example: Two Different Radiation Modes in a Cavity

The Hamiltonian for two different modes ("1" and "2") of radiation in a cavity is,

$$\hat{H} = \hat{H}_1 \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{H}_2 = \hat{H}_1 + \hat{H}_2 = \hbar\omega_1\,\hat{a}_1^+\,\hat{a}_1 + \hbar\omega_2\,\hat{a}_2^+\,\hat{a}_2$$

Eigenstates of the above Hamiltonian are of the form,

$$|n\rangle_1 \otimes |m\rangle_2$$

$$\Rightarrow \hat{H}|n\rangle_1 \otimes |m\rangle_2 = \left(\hat{H}_1 + \hat{H}_2\right)|n\rangle_1 \otimes |m\rangle_2$$

$$= \hat{H}_1|n\rangle_1 \otimes |m\rangle_2 + |n\rangle_1 \otimes \hat{H}_2|m\rangle_2$$

$$= \left(n\hbar\omega_1 + m\hbar\omega_1\right)|n\rangle_1 \otimes |m\rangle_2$$

1.8 Entangled States

1.8.1 Introduction

States belonging to a combined Hilbert space of two systems, "a" and "b", are of two types:

1) Unentangled states
2) Entangled states

States of the type $|\phi\rangle_a \otimes |x\rangle_b$ that can be written as,

$$|\text{a unique state of system "a"}\rangle_a \otimes |\text{a unique state of system "b"}\rangle_b$$

are unentangled states. Examples of unentangled states for two different two-level systems are,

i) $|\psi\rangle = |e_1\rangle_a \otimes |e_2\rangle_b$

ii) $|\psi\rangle = \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_a + |e_2\rangle_a\right)\right] \otimes \left[|e_1\rangle_b\right] = \frac{1}{\sqrt{2}}\left\{|e_1\rangle_a \otimes |e_1\rangle_b + |e_2\rangle_a \otimes |e_1\rangle_b\right\}$

iii) $|\psi\rangle = |e_1\rangle_a \otimes \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_b - |e_2\rangle_b\right)\right] = \frac{1}{\sqrt{2}}\left\{|e_1\rangle_a \otimes |e_1\rangle_b - |e_1\rangle_a \otimes |e_2\rangle_b\right\}$

iv) $|\psi\rangle = \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_a + |e_2\rangle_a\right)\right] \otimes \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_b + |e_2\rangle_b\right)\right]$

For entangled states, this "separation" is not possible. For example, consider the entangled state,

$$\frac{1}{\sqrt{2}}\left[|e_1\rangle_a \otimes |e_2\rangle_b - |e_2\rangle_a \otimes |e_1\rangle_b\right]$$

The state above cannot be written in the form, $|\phi\rangle_a \otimes |x\rangle_b$.

1.8.2 Entangled States and Quantum Measurements

Entangled states have some interesting consequences when it comes to measurements. First, consider the complicated un-entangled state of two different two-level systems,

$$\left[\left(\frac{\sqrt{3}}{2}|e_1\rangle_a + \frac{1}{2}|e_2\rangle_a\right)\right] \otimes \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_b + |e_2\rangle_b\right)\right]$$

Suppose we measure the energy of system "b". Possible outcomes and the corresponding probabilities are,

$$\begin{cases} \varepsilon_1 \leftrightarrow \text{probability} = \frac{1}{2} \\ \varepsilon_2 \leftrightarrow \text{probability} = \frac{1}{2} \end{cases}$$

Suppose we measure the energy of system "a". Possible outcomes and the corresponding probabilities are,

$$\begin{cases} \varepsilon_1 \leftrightarrow \text{probability} = \dfrac{3}{4} \\ \varepsilon_2 \leftrightarrow \text{probability} = \dfrac{1}{4} \end{cases}$$

Now suppose we made an energy measurement on system "a" and obtained the result ε_1. Right after this measurement the state of the full system is,

$$|e_1\rangle_a \otimes \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_b + |e_2\rangle_b\right)\right].$$

If after the measurement on system "a", we make a measurement on system "b", the possible outcomes and the corresponding associated probabilities are,

$$\begin{cases} \varepsilon_1 \leftrightarrow \text{probability} = \dfrac{1}{2} \\ \varepsilon_2 \leftrightarrow \text{probability} = \dfrac{1}{2} \end{cases}$$

Therefore, measurement on system "a" has not changed the measurement results (i.e possible outcomes and the corresponding probabilities) for system "b". Now consider the entangled state,

$$\frac{\sqrt{3}}{2}|e_1\rangle_a \otimes |e_2\rangle_b - \frac{1}{2}|e_2\rangle_a \otimes |e_1\rangle_b$$

For energy measurement on system "a", possible outcomes and the corresponding probabilities are,

$$\begin{cases} \varepsilon_1 \leftrightarrow \text{probability} = \dfrac{3}{4} \\ \varepsilon_2 \leftrightarrow \text{probability} = \dfrac{1}{4} \end{cases}$$

For energy measurement on system "b", we have,

$$\begin{cases} \varepsilon_1 \leftrightarrow \text{probability} = \dfrac{1}{4} \\ \varepsilon_2 \leftrightarrow \text{probability} = \dfrac{3}{4} \end{cases}$$

Suppose we made an energy measurement on system "a" and obtained the result ε_1. Right after this measurement the state of the combined system collapses into the state,

$$|e_1\rangle_a \otimes |e_2\rangle_b$$

If after the measurement on system "a", we make an energy measurement on system "b", the only possible outcome is ε_2 with probability one. Therefore, for entangled states measurement on one subsystem, changes the measurement results (i.e possible outcomes and the corresponding probabilities) for the other subsystem.

1.9 Density Operators for Joint Hilbert Spaces

1.9.1 Density Operators for Entangled and Unentangled States

If the quantum state of a system consisting of two subsystems "a" and "b" is an unentangled state like,

$$|\psi\rangle = |\phi\rangle_a \otimes |x\rangle_b$$

then the density operator $\hat{\rho}$ for the system is,

$$\hat{\rho} = |\psi\rangle\langle\psi|$$
$$= \left\{|\phi\rangle_a \otimes |x\rangle_b\right\}\left\{{}_a\langle\phi| \otimes {}_b\langle x|\right\}$$
$$\hat{\rho} = |\phi\rangle_a\ {}_a\langle\phi| \otimes |x\rangle_b\ {}_b\langle x|$$
$$\hat{\rho} = \hat{\rho}_a \otimes \hat{\rho}_b$$

Where, $\hat{\rho}_a = |\phi\rangle_a\ {}_a\langle\phi|$ and $\hat{\rho}_b = |x\rangle_b\ {}_b\langle x|$. Therefore, the density operator can be written as a tensor product of the density operators of the subsystems. Another example is,

$$|\psi\rangle = \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_a + |e_2\rangle_a\right)\right] \otimes \left[\frac{1}{\sqrt{2}}\left(|e_1\rangle_b - |e_2\rangle_b\right)\right]$$
$$\hat{\rho} = \hat{\rho}_a \otimes \hat{\rho}_b$$

where,

$$\hat{\rho}_a = \frac{1}{2}\left\{|e_1\rangle_a\ {}_a\langle e_1| + |e_1\rangle_a\ {}_a\langle e_2| + |e_2\rangle_a\ {}_a\langle e_1| + |e_2\rangle_a\ {}_a\langle e_2|\right\}$$
$$\hat{\rho}_b = \frac{1}{2}\left\{|e_1\rangle_b\ {}_b\langle e_1| - |e_1\rangle_b\ {}_b\langle e_2| - |e_2\rangle_b\ {}_b\langle e_1| + |e_2\rangle_b\ {}_b\langle e_2|\right\}$$

Now consider the entangled state,

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left\{|e_1\rangle_a \otimes |e_2\rangle_b - |e_2\rangle_a \otimes |e_1\rangle_b\right\}$$
$$\hat{\rho} = |\psi\rangle\langle\psi|$$
$$= \frac{1}{2}\left\{|e_1\rangle_a\ {}_a\langle e_1| \otimes |e_2\rangle_b\ {}_b\langle e_2| + |e_2\rangle_a\ {}_a\langle e_2| \otimes |e_1\rangle_b\ {}_b\langle e_1|\right.$$
$$\left. - |e_1\rangle_a\ {}_a\langle e_2| \otimes |e_2\rangle_b\ {}_b\langle e_1| - |e_2\rangle_a\ {}_a\langle e_1| \otimes |e_1\rangle_b\ {}_b\langle e_2|\right\}$$

The density operator $\hat{\rho}$ for entangled states cannot be written as a tensor product, $\hat{\rho}_a \otimes \hat{\rho}_b$.

Recall that $\text{Trace}\{\ \}$ operation means trace with respect to all the states of the full Hilbert space that form a complete set. As an example, consider two different two-level systems "a" and "b". The full Hilbert space consists of the following four states which form a complete set,

$$|1\rangle = |e_1\rangle_a \otimes |e_1\rangle_b$$
$$|2\rangle = |e_2\rangle_a \otimes |e_1\rangle_b$$
$$|3\rangle = |e_1\rangle_a \otimes |e_2\rangle_b$$
$$|4\rangle = |e_2\rangle_a \otimes |e_2\rangle_b$$

The average energy is calculated as,

$$\text{Trace}\left\{\hat{\rho}\hat{H}\right\} = \sum_{k=1}^{4}\langle k|\hat{\rho}\hat{H}|k\rangle$$

Suppose, $|\psi\rangle = |e_1\rangle_a \otimes |e_2\rangle_b$. Then,

$$\hat{\rho} = |\psi\rangle\langle\psi| = |e_1\rangle_a\ {}_a\langle e_1| \otimes |e_2\rangle_b\ {}_b\langle e_2|$$

and,

$$\text{Trace}\left\{\hat{\rho}\left(\hat{H}_a+\hat{H}_b\right)\right\}=\text{Trace}\left\{|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|\left(\hat{H}_a+\hat{H}_b\right)\right\}$$

$$=\sum_{k=1}^{4}\langle k|\left(|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|\right)\left(\hat{H}_a+\hat{H}_b\right)|k\rangle$$

$$={}_a\langle e_1|\otimes{}_b\langle e_1|\left(|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|\right)\left(\hat{H}_a+\hat{H}_b\right)|e_1\rangle_a\otimes|e_1\rangle_b$$

$$+{}_a\langle e_2|\otimes{}_b\langle e_1|\left(|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|\right)\left(\hat{H}_a+\hat{H}_b\right)|e_2\rangle_a\otimes|e_1\rangle_b$$

$$+{}_a\langle e_1|\otimes{}_b\langle e_2|\left(|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|\right)\left(\hat{H}_a+\hat{H}_b\right)|e_1\rangle_a\otimes|e_2\rangle_b$$

$$+{}_a\langle e_2|\otimes{}_b\langle e_2|\left(|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|\right)\left(\hat{H}_a+\hat{H}_b\right)|e_2\rangle_a\otimes|e_2\rangle_b$$

$$=\text{ only the third line above gives a nonzero answer equal to }\left(\varepsilon_1+\varepsilon_2\right)$$

Note that an expression of the form,

$${}_a\langle x|\otimes{}_b\langle\phi|\quad\left\{|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|\right\}|x\rangle_a\otimes|\phi\rangle_b$$

equals,

$${}_a\langle x|e_1\rangle_a\,{}_a\langle e_1|x\rangle_a\,\,{}_b\langle\phi|e_2\rangle_b\,{}_b\langle e_2|\phi\rangle_b$$

1.9.2 Partial Traces and Density Operators of Subsystems

Sometimes a density operator for two (or more) systems contains too much information. The purpose of the density operator is to allow one to calculate averages. If one is interested in only system "a" but has the joint density operator $\hat{\rho}$ for system "a" and system "b", then one needs to "extract" a density operator $\hat{\rho}_a$ for system "a". This is done as follows. The density operator for system "a" is extracted from $\hat{\rho}$ by doing a partial trace with respect to the states belonging to system "b", i.e.,

$$\hat{\rho}_a=\text{Tracep}\{\hat{\rho}\}$$

$$={}_b\langle e_1|\hat{\rho}|e_1\rangle_b+{}_b\langle e_2|\hat{\rho}|e_2\rangle_b$$

For unentangled states, we know that,

$$\hat{\rho}=\hat{\rho}_a\otimes\hat{\rho}_b$$

Therefore,

$$\text{Tracep}\{\hat{\rho}\}={}_b\langle e_1|\hat{\rho}_a\otimes\hat{\rho}_b|e_1\rangle_b+{}_b\langle e_2|\hat{\rho}_a\otimes\hat{\rho}_b|e_2\rangle_b$$

$$=\hat{\rho}_a\,{}_b\langle e_1|\hat{\rho}_b|e_1\rangle_b+\hat{\rho}_a\,{}_b\langle e_2|\hat{\rho}_b|e_2\rangle_b$$

$$=\hat{\rho}_a\left[{}_b\langle e_1|\hat{\rho}_b|e_1\rangle_b+{}_b\langle e_2|\hat{\rho}_b|e_2\rangle_b\right]$$

$$=\hat{\rho}_a\,\text{Tracep}\{\hat{\rho}_b\}=\hat{\rho}_a$$

Now consider the entangled state,

$$|\psi\rangle=\left\{\frac{\sqrt{3}}{2}|e_1\rangle_a\otimes|e_2\rangle_b+\frac{1}{2}|e_2\rangle_a\otimes|e_1\rangle_b\right\}$$

$$\hat{\rho}=\frac{1}{4}\{3|e_1\rangle_a\,{}_a\langle e_1|\otimes|e_2\rangle_b\,{}_b\langle e_2|+\sqrt{3}|e_1\rangle_a\,{}_a\langle e_2|\otimes|e_2\rangle_b\,{}_b\langle e_1|$$

$$+\sqrt{3}|e_2\rangle_a\,{}_a\langle e_1|\otimes|e_1\rangle_b\,{}_b\langle e_2|+|e_2\rangle_a\,{}_a\langle e_2|\otimes|e_1\rangle_b\,{}_b\langle e_1|\}$$

$$\begin{aligned}\hat{\rho}_a &= \text{Tracep}\,\{\hat{\rho}\} \\ &= {}_b\langle e_1|\hat{\rho}|e_1\rangle_b + {}_b\langle e_2|\hat{\rho}|e_2\rangle_b \\ &= \left\{\frac{3}{4}|e_1\rangle_a\ {}_a\langle e_1| + \frac{1}{4}|e_2\rangle_a\ {}_a\langle e_2|\right\} \\ \hat{\rho}_a &= \begin{bmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{bmatrix}\end{aligned}$$

Therefore, $\hat{\rho}_a$ is a statistical mixture of states $|e_1\rangle_a$ and $|e_2\rangle_a$ with probabilities $\frac{3}{4}$ and $\frac{1}{4}$, respectively. But note that just by looking at the full state,

$$|\psi\rangle = \left\{\frac{\sqrt{3}}{2}|e_1\rangle_a \otimes |e_2\rangle_b + \frac{1}{2}|e_2\rangle_a \otimes |e_1\rangle_b\right\}$$

one can tell that a measurement of the energy of system "a" will yield outcomes ε_1 and ε_2 with probabilities $\frac{3}{4}$ and $\frac{1}{4}$, respectively. The extracted density operator $\hat{\rho}_a$ tells exactly this but in a formal way. Usually, entangled states of two systems yield statistical mixture like density operators for any subsystem after the partial trace operation.