Lecture 1: Hilbert Space and Phase Space
Friday, December 06, 2019

0.1 Hilbert Space and Phase Space

For a 1-D system, phase space has two variables, position x and "conjugate" momentum p. For a particle at (x_0, p_0) at t_0 the position in phase space evolves to a different position (x_1, p_1) at t_1. Position and momentum here are real numbers, and the evolution is continuous and deterministic.

For a quantum system, we use a Hilbert space. We will use the Hilbert space of a spin-1/2 particle, generally thought of as a two level system. The spin is thought of as a vector, and we will let this vector be aligned along the z axis. The Hilbert space is two dimensional, and the x-axis refers to $|z+\rangle$ while the y-axis refers to $|z-\rangle$, which are vectors pointing in the + and - z-directions. Regardless of the position along the +z axis, the particle has its spin in the +z position. All the states along that line, except for the origin, refer to particles with +z polarization. We can use a coefficient α to refer to the position along this axis, and all the +z polarized particles belong to the set $\alpha_+|z+\rangle$. Likewise, $\alpha_-|z-\rangle$ can take us along the z-axis.

In QM, we can have states which are off-axis, they have attributes of both properties. Let's call one such state $|\psi_0\rangle$. The set of equivalent vectors is a line in Hilbert space!It will evolve continuously in time to a state $|\psi_1\rangle$. Suppose $|\psi_1\rangle$ is perpendicular to $|\psi_0\rangle$. This state is completely different from the original, it shares no attributes with the original like the two z-states. Such states are orthogonal.

The Hilbert space is a complex vector space:

- $c|\psi\rangle \in \mathcal{H}$
- $|\psi\rangle + |\phi\rangle \in \mathcal{H}$
- Inner product: ket notation
  - ket vectors are elements of the Hilbert space: $|\psi\rangle \in \mathcal{H}$
  - bra vectors are elements of the adjoint/dual space: $\langle\psi| \in \mathcal{H}^\dagger$
  - $\langle\psi| \equiv (|\psi\rangle)^\dagger$
  - $\langle\psi| : |\phi\rangle \to c \in \mathbb{C}$
  - $\langle\psi| : |\psi\rangle \to \langle\psi|\psi\rangle = ||\psi||^2$, the squared norm of the vector

$$|\psi\rangle = a_+|z+\rangle + a_-|z-\rangle$$

$$|\phi\rangle = b_+|z+\rangle + b_-|z-\rangle$$

$$\langle\psi| = \langle z+|a_+^* + \langle z-|a_-^*$$

$\langle\psi|\psi\rangle = |a_+|^2 + |a_-|^2$ because

$$\langle z+|z-\rangle = 0$$

$$\langle\psi|\phi\rangle = a_+^* b_+ + a_-^* b_- = \langle\phi|\psi\rangle^*$$

Operators

$$A\colon \mathcal{H} \to \mathcal{H}$$

$$A\colon |\psi\rangle \to |\phi\rangle \equiv |A\psi\rangle$$

It is sufficient to make a list of what operators do to orthogonal elements, which will be equivalent to the complete set of all possible inner products.

Matrix Element

$$\langle\chi|A|\psi\rangle = \langle\chi|A\psi\rangle = \langle\chi|\phi\rangle$$

(A does not operate on χ)

The adjoint operator $A^\dagger$:

$$^\dagger\colon \langle\chi| \to \langle\chi|A^\dagger \equiv (A|\chi\rangle)^\dagger$$

$$\langle\chi|A^\dagger\psi\rangle = (\langle\chi|A^\dagger)|\psi\rangle = (|A\chi\rangle)^\dagger|\psi\rangle = (\langle\psi|A|\chi\rangle)^* = \langle\psi|A\chi\rangle^*$$

We will (almost always) talk about "Normal" Operators. Say N is a normal operator:

$$N^\dagger N = NN^\dagger$$

Hermitian operators are normal: $H = H^\dagger$ —associated with physical properties, eigenvalues are real

Unitary operators are normal: $U^\dagger U = UU^\dagger = I$, the identity—these are associated with time evolution of quantum systems. Their eigenvalues have unit magnitude, time evolution will keep states on the unit circle.

Note: the unit complex "circle" is a 4-D sphere called the Bloch sphere

1. $N|\psi\rangle = \lambda|\psi\rangle \Rightarrow \langle\psi|N^\dagger = \lambda^*|\psi\rangle$
    1. $||(N-\lambda I)|u\rangle||^2 = 0 = \langle u|(N^\dagger - \lambda^* I)(N-\lambda I)|u\rangle = ||\langle u|(N^\dagger - \lambda^* I)||^2$
2. $N|u_i\rangle = \lambda_i|u_i\rangle$ and $N|u_j\rangle = \lambda_j|u_j\rangle$. Then $\lambda_i \neq \lambda_j \Rightarrow \langle u_i|u_j\rangle = 0$
    1.
3. H (a Hermitian operator) has real eigenvalues
4. Eigenvalues of U (a Unitary operator) have unit magnitude
    1. $(\langle u|U^\dagger)(U|u\rangle) = \lambda^*\lambda\langle u|u\rangle = \langle u|u\rangle$ since $U^\dagger U = I$

Projectors Projectors are operators which project any state to the specified projection subspace. In general, a projector $P = P^2$ can be defined using the inner product of two states:

$$\langle\psi|\phi\rangle|\psi\rangle = |\psi\rangle\langle\psi|\phi\rangle = P_\psi|\phi\rangle$$

if $|\psi\rangle$ is normalized (in general, $P_\psi = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$).

The dimension of the subspace onto which the state is being projected is the dimension of the projector, and $\dim P = \text{Tr } P$, the trace of the projector matrix (called a dyad).

Note: In the textbook, the projector of a given state is often denoted by $[\psi]$.

Say we are defining the usual spin-1/2 system on the basis $z+$ and $z-$. The projectors onto those states are:

$$[z+] = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

and

$$[z-] = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Note that trace of both of these projectors is equal to 1, meaning the projected subspaces are one-dimensional.

Suppose we had a Normal operator A with eigenvectors denoted by α_i and eigenvalues a_i.

$A|\alpha_i\rangle = a_i|\alpha_i\rangle$.

We can define a projector for each eigenvector (assuming they are not degenerate/have different eigenvalues):

$$P_i = |\alpha_i\rangle\langle\alpha_i|$$

If $\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$, $P_i P_j = \delta_{ij} P_i$.

Spectral Decomposition For any operator, we can find a decomposition based on the sum of projectors multiplied by the corresponding eigenvalues:

$$A = \sum_i a_i P_i$$

Physical Variables and Properties In *Classical* phase space, we can have properties like the energy $H(\gamma)$ at some point γ in phase space. We can also make claims like $H(\phi) < E_0$ (ϕ has this "property"). Physical properties in phase space are subsets of the phase space.

In the *Quantum* Hilbert space, we say that physical properties are ***linear*** subspaces of $\mathcal{H}$. S_z has value $+\frac{\hbar}{2}$ for $\{|\psi\rangle \mid |\psi\rangle = c|z+\rangle\}, \quad c \neq 0$.

Review of Properties *Classical*: "The energy is less than x" is a subset of the phase space. In particular, it's the set of points in phase space such that the property is true. Alternatively, we could define a function P for a property $\mathcal{P}$. This "indicator" function is defined as:

$$P(\gamma) = \begin{cases} 1 & \mathcal{P} \text{ is true} \\ 0 & \mathcal{P} \text{ is false} \end{cases}$$

Quantum: A property $\mathcal{P}$ is a linear subspace of the Hilbert space. Algebraically, we can also define:

$$\mathcal{P} = \{|\psi\rangle \in \mathcal{H} \mid P_{\mathcal{P}}|\psi\rangle = |\psi\rangle\}$$

Here, the projector acts like an indicator function, since if the system does not have the property, the projector will return zero.

$$I = P_{z+} + P_{z-}$$

Logical Reasoning

Classical:

Q	(x¡0)
$\mathcal{P} \cap \mathcal{Q}$	Disjunction $\mathcal{PQ}$
$P(\gamma)Q(\gamma)$	$\mathcal{P} \cup \mathcal{Q}$
$((H\gamma) < E_0)$	$P(\gamma) + Q(\gamma) - P(\gamma)Q(\gamma)$
	$((H\gamma) < E_0)(x < 0)$

Identities:

- $\neg(\mathcal{P} \cap \mathcal{Q}) = (\neg\mathcal{P} \cup \neg\mathcal{Q})$
- $\neg(\mathcal{P} \cup \mathcal{Q}) = (\neg\mathcal{P} \cap \neg\mathcal{Q})$
- $\mathcal{P} \cup (\mathcal{Q} \cap \mathcal{R}) = (\mathcal{P} \cup \mathcal{Q}) \cap (\mathcal{P} \cup \mathcal{R})$
- $\mathcal{P} \cap (\mathcal{Q} \cup \mathcal{R}) = (\mathcal{P} \cap \mathcal{Q}) \cup (\mathcal{P} \cap \mathcal{R})$

This set of rules constitutes a "boolean algebra."

Quantum

Q	(S$_z = +\frac{\hbar}{2}$) is undefined
???	Disjunction $\mathcal{PQ}$
PQ or QP (should be the same if they commute)	???
$(S_x = +\frac{\hbar}{2})$	$P + Q - PQ$ or $P + Q - QP$
	$(S_x = +\frac{\hbar}{2})$
	(S$_x = -\frac{\hbar}{2}$)

Conditional Probabilities and the Born Rule Conditional probability: $0 \leq Pr(\mathcal{P} \mid \psi) \leq 1$ is the probability that the state is in the subspace P. If $|\psi\rangle \in \mathcal{P} \to Pr = 1$ and $|\psi\rangle \in \neg\mathcal{P} = \mathcal{P}^{\perp} \to Pr = 0$. Intermediate states (linear combinations of property states) could have a value between 0 and 1. For example, the probability for a particle in the state $|x+\rangle$ to have the property $|z+\rangle$ is $\frac{1}{2}$.

Suppose $\langle\psi|\psi\rangle = 1$. The Born rule states that $Pr(\mathcal{P} \mid \psi) = ||P|\psi\rangle||^2 = \langle\psi|P^\dagger P|\psi\rangle = \langle\psi|P|\psi\rangle$.

Density Operator (Matrix)

Pure State: $|\psi\rangle \to [\psi] = |\psi\rangle\langle\psi| = \rho$.

$$Pr(\mathcal{P} \mid \rho) = \langle\psi|P|\psi\rangle$$

Insert identities on either side of P:

$$Pr(\mathcal{P}|\rho) = \langle\psi|(\sum_m |m\rangle\langle m|)P(\sum_n |n\rangle\langle n|)|\psi\rangle = \sum_{mn}\langle\psi|m\rangle\langle m|P|n\rangle\langle n|\psi\rangle$$

The outermost brakets are just complex numbers, so we can move them around. Also, $\langle n|\psi\rangle\langle\psi|m\rangle = \langle n|\rho|m\rangle$:

$$Pr(\mathcal{P}|\rho) = \sum_n\sum_m \rho_{nm}P_{mn} = \sum_n (\rho P)_{nn} = Tr(\rho P)$$

Example:

$$|\psi\rangle = |x+\rangle = \frac{1}{\sqrt{2}}(|z+\rangle + |z-\rangle)$$

$$\rho = \frac{1}{2}(|z+\rangle\langle z+| + \dots)$$

In $z\pm$ basis,

$$\rho = \frac{1}{2}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}$$

In $x\pm$ basis, $\rho = \begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}$

Mixed State For example, take a state which is 75% $|x+\rangle$ and 25% $|x-\rangle$:

$$\frac{3}{4}\rho_{x+} + \frac{1}{4}\rho_{x-} = \rho = \begin{bmatrix}\frac{1}{2} & \frac{1}{4}\\ \frac{1}{4} & \frac{1}{2}\end{bmatrix}$$

in the z basis ($\rho = \begin{bmatrix}\frac{3}{4} & 0\\ 0 & \frac{1}{4}\end{bmatrix}$ in the x basis)

$$Pr([z+] \mid \rho) = Tr(\rho[z+]) = Tr(\begin{bmatrix}\frac{1}{2} & \frac{1}{4}\\ \frac{1}{4} & \frac{1}{2}\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}) = \frac{1}{2}$$

$$Pr([x+] \mid \rho) = Tr(\rho[x+]) = Tr(\begin{bmatrix}\frac{3}{4} & 0\\ 0 & \frac{1}{4}\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}) = \frac{3}{4}$$

In a pure state, $Tr(\rho) = 1$ and $Tr(\rho^2) = Tr(\rho) = 1$ since the density matrix for a pure state is a projector onto that state.

In a general density matrix, $Tr(\rho) = 1$, but $\rho^2 \neq \rho$, so $Tr(\rho^2) = Tr(\sum_j p_j P_j \sum_k p_k P_k) = \sum_j p_j^2$, so $\sum_j p_j^2 < 1$ unless $p_j = \delta_{jk}$. The trace of the density matrix squared is always non-zero in finite-dimension Hilbert spaces (could be zero in a maximally-mixed infinite-dimensional space).

Average Value of an Observable

$$A = \sum_a a P_a$$

For a state $|\psi\rangle$, the expectation value of the operator A is $\langle A\rangle_\psi = \sum_a aPr(A = a \mid \psi) = \sum_a a||P_a|\psi\rangle||^2 = \sum_a a\langle\psi|P_a|\psi\rangle = \langle\psi|A|\psi\rangle$.

Example:

For a pure state $\rho = |\psi\rangle\langle\psi|$,

$$\langle A\rangle_\rho = \langle\psi|A|\psi\rangle = Tr(\rho A)$$

For a mixed state $\rho = \sum_j p_j P_j, \quad P_j|\psi_j\rangle\langle\psi_j|$,

$$\langle A\rangle_\rho = \sum_j p_j \langle A\rangle_{\psi_j} = \sum_j p_j Tr(P_j A) = Tr(\rho A)$$

Classical Composite

$$(x, p) \in \Gamma$$

, $\dim(\Gamma) = 2$

$$(x_a, p_a) \in \Gamma_a$$

$$(x_b, p_b) \in \Gamma_b$$

$(x_a x_b, p_a p_b) \in \Gamma_a \times \Gamma_b$,

$$\dim(\Gamma_a \times \Gamma_b) = \dim\Gamma_a + \dim\Gamma_b$$

Quantum Composite

$$\mathcal{H}_a, \mathcal{H}_b \to \mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$$

$$|a\rangle \in \mathcal{H}_a,\ |b\rangle \in \mathcal{H}_b \to |a\rangle \otimes |b\rangle \in \mathcal{H}_{ab}$$

(Product State)

$$\dim\mathcal{H}_a \otimes \mathcal{H}_b = \dim\mathcal{H}_a \cdot \dim\mathcal{H}_b$$

For a basis $\{|a_j\rangle\}$ and $\{|b_k\rangle\}$ for $\mathcal{H}_a$ and $\mathcal{H}_b$, we can choose a basis $\{|a_j\rangle \otimes |b_k\rangle\}$ for $\mathcal{H}_{ab}$. To simplify notation, $|a_j\rangle \otimes |b_k\rangle = |j\rangle_a \otimes |k\rangle_b = |j\rangle_a|k\rangle_b = |jk\rangle$.

For a system with two spin-1/2 particles, the standard basis is $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$.

Spinor Particle Spinors are used to describe particles with position and spin.

Position: $\psi(\vec{r}) = \langle \vec{r}|\psi\rangle$

Spin: $\alpha|+\rangle + \beta|-\rangle$

Product state: $(\alpha|+\rangle + \beta|-\rangle) \cdot \psi(\vec{r})$

General state is a sum of product states:

$$|\omega\rangle = \sum_j (\alpha_j|+\rangle + \beta_j|-\rangle)\psi_j(\vec{r}) = \begin{bmatrix} \omega_+(r) \\ \omega_-(r) \end{bmatrix}$$

$\omega_+(\vec{r}) = \langle \vec{r}+|\omega\rangle$, \

$$\omega_-(\vec{r}) = \langle \vec{r}-|\omega\rangle$$

$$\omega_+(\vec{r}) = \sum_j \alpha_j \psi_j(\vec{r})$$

$$\omega_-(\vec{r}) = \sum_j \beta_j \psi_j(\vec{r})$$

Toy Models

Example 1 Say we have a 1D line upon which a particle can move, and suppose this is a discrete space, where the position is given by $m = 0, 1, 2, 3$ (in solid state this is a tight-binding model). $\dim(\mathcal{H}_m) = 4$ since there are four possible place the particle can be.

Add a detector with two states, $n = 0$ and $n = 1$. If the detector finds a particle in the detector space, it is in state 1, otherwise

$$n = 0$$

. $\dim(\mathcal{H}_n) = 2$

For the combined particle + detector space, $\dim(\mathcal{H}_{mn}) = 8$.

Example 2 Eight positions, four for spin up and four for spin down. A particle with spin has $dim = 8$ also.

Example 3 Suppose we have four possible positions in the x-direction and two in the y-direction. This is a particle in 2D. There are eight possible positions for the particle, so the dimension of the product space is 8.

All of these spaces are isomorphic.

Notation:

$$|\psi\rangle \in \mathcal{H}_{mn}$$

$$\psi_n(m) = \langle mn|\psi\rangle$$

Entangled States We know that any $|\psi\rangle \in \mathcal{H}_{ab}$ can be expanded in a basis $\{|j\rangle_a \otimes |k\rangle_b\}$:

$|\psi\rangle = \sum_{jk} \Psi_{jk} |jk\rangle$ where Ψ is just the coefficient of the basis.

$$\Psi = (\dim \mathcal{H}_a) \times (\dim \mathcal{H}_b)$$

The "rank" of an array is the number of independent rows which is equivalent to the number of independent columns.

Rank = 1 $\exists\ |a\rangle \in \mathcal{H}_a,\ |b\rangle \in \mathcal{H}_b$ such that $|\psi\rangle = |a\rangle \otimes |b\rangle$

This is a product state

Rank > 1 There is no such state. This is an entangled state.

$|a\rangle = \alpha_+ |+\rangle_a + \alpha_- |-\rangle_a$,

$$|b\rangle = \beta_+ |+\rangle_b + \beta_- |-\rangle_b$$

$$|\psi\rangle = |a\rangle \otimes |b\rangle = \alpha_+\beta_+ |++\rangle + \alpha_+\beta_- |+-\rangle + \alpha_-\beta_+ |-+\rangle + \alpha_-\beta_- |--\rangle$$

Here, $\Psi_{++} = \alpha_+\beta_+$, $\Psi_{+-} = \alpha_+\beta_-$, etc.

Note, $\Psi_{++}\Psi_{--} = \alpha_+\beta_+\alpha_-\beta_- = \Psi_{-+}\Psi_{+-}$, so $\det\{\Psi\} = 0$. If the determinant vanishes, the state is a product state, otherwise it is an entangled state. For example,

$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$ (EPR State)

$\Psi_{++} = \Psi_{--} = 0$ while $\Psi_{+-} = \frac{1}{\sqrt{2}} = -\Psi_{-+}$ so $\det\{\Psi\} = \frac{1}{2}$.

Tensor Product Spaces

Review

$$|\psi\rangle = |a\rangle \otimes |b\rangle = |ab\rangle \in \mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$$

$$(|a\rangle \otimes |b\rangle)^\dagger = \langle ab| \in \mathcal{H}_{ab}^\dagger = \mathcal{H}_a^\dagger \otimes \mathcal{H}_b^\dagger$$

$$|\psi'\rangle = |a'\rangle \otimes |b'\rangle$$

$$\langle\psi|\psi'\rangle = \langle a|a'\rangle \cdot \langle b|b'\rangle$$

Suppose we have an operator A acting in $\mathcal{H}_a$ and B acting in $\mathcal{H}_b$. Then $A \otimes B$ acts on states in $\mathcal{H}_{ab}$. In this case, the tensor product is equivalent to $\sum_{jk} A_j \otimes B_k$.

We can also have products of tensor products of operators:

$(A \otimes B)(A' \otimes B') = (AA') \otimes (BB')$. Additionally $(A \otimes I_b)(I_a \otimes B) = A \otimes B$.

Example: Spin in a two-particle space $A = [z+]_a = |+\rangle_a\langle+|_a$, $I_b = |+\rangle_b\langle+|_b + |-\rangle_b\langle-|_b$.

$$(A \otimes I_b) = |++\rangle_{ab}\langle++|_{ab} + |+-\rangle_{ab}\langle+-|_{ab} = [z_a+]$$

You can check that this is in fact an operator by squaring it.

Recitation $|\psi_0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$ "EPR State"

$$[\psi_0] = \frac{1}{2}([++] + [--] + |+-\rangle\langle-+| - |-+\rangle\langle+-|)$$

$$[z_a+] \equiv [z+]_a \otimes I_b = [++] + |+-\rangle\langle-+|$$

$$[\psi_0][z_a+] = \frac{1}{2}(|+-\rangle\langle+-| - |+-\rangle\langle-+|)$$

$$[z_a+][\psi_0] = \frac{1}{2}(|+-\rangle\langle+-| - |-+\rangle\langle+-|)$$

What can we say about this system? Are the spins the same?

$$P = [++] + [--]$$

$$Q = [+-] + [-+]$$

$P[\psi_0] = [\psi_0]P = 0$ implies the spins are not the same.

Let's work with the "GHZ" state, a state of three particles.

$$|\phi\rangle = |(z_1+)(z_2+)(z_3+)\rangle - |(z_1-)(z_2-)(z_3-)\rangle$$

Define $\sigma_x = \frac{2}{\hbar}S_x$ such that $\sigma_x|x+\rangle = |x+\rangle$, and $\sigma_x|x-\rangle = -|x-\rangle$. It can also be shown that:

$$\sigma_x|z+\rangle = |z-\rangle$$

and

$\sigma_y|z-\rangle = -\imath|z+\rangle$, and

$$\sigma_y|z+\rangle = \imath|z-\rangle$$

Define $X_1 = \sigma_x^1\sigma_y^2\sigma_y^2$, $X_2 = \sigma_y^1\sigma_x^2\sigma_y^3$, and $X_3 = \sigma_y^1\sigma_y^2\sigma_x^3$.

$X_1|z+z+z+\rangle = \imath^2|z-z-z-\rangle = -|z-z-z-\rangle$.

The GHZ state is an eigenstate of X_1, X_2 and X_3. Suppose we measure S_x^1, yielding ±1. Likewise, we could measure other components of other particles.

$X_1|\phi\rangle = |\phi\rangle \Rightarrow m_x^1m_y^2m_y^2 = +1$ (and similar for other the other two operators). Additionally, we can take the product of these three results to claim $m_x^1m_x^2m_x^3 = +1$. We claim this is an eigenvalue of an operator called $X_{123} = \sigma_x^1\sigma_x^2\sigma_x^3$. The associated eigenvalue is $-1 = m_x^1m_x^2m_x^3 = +1$. The error is trying to apply the three operators at the same time. We cannot simultaneously attribute x and y values of the spin of a particle. We can measure them, but we can't claim they are preexisting "real" quantities.

The Schrödinger Equation

Classical Phase Space
Given an initial condition, $\vec{F} = m\vec{a}$ implies the system evolves along some unique path which does not cross any other p $\frac{d}{dt}\vec{\gamma}(t) = \bar{J}\frac{\partial H}{\partial \vec{\gamma}}$, where $\bar{J} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$.

The Unitary Time-Development Operator

$$\frac{d}{dt}\langle\phi_t|\psi_t\rangle = \langle\phi_t|\frac{d}{dt}\psi_t\rangle + \left(\frac{d}{dt}\langle\phi_t|\right)|\psi_t\rangle = 0$$

because

$$\frac{d}{dt}\langle\phi_t| = \left(\frac{d}{dt}|\phi_t\rangle\right)^\dagger = \left(-\frac{\imath}{\hbar}H|\phi_t\rangle\right)^\dagger$$

and $|\frac{d}{dt}\psi_t\rangle = \left(-\frac{\imath}{\hbar}H|\psi_t\rangle\right)$. This implies the inner product is invariant under time evolution given the same Hamiltonian. This also implies $\frac{d}{dt}\||\psi_t\rangle\| = \frac{d}{dt}\langle\psi|\psi\rangle = 0$. This is an analog of the Classical Liouville theorem involving preservation of phase space volume with time evolution.

Consider a mapping T (the time-evolution operator) which takes a state from an earlier time to a later time. This mapping should be independent of initial condition, mapping the entire Hilbert space to itself. Additionally, it should be linear to maintain completeness.

$|\psi_t\rangle = T(t,t')|\psi_{t'}\rangle$ for any state.

$$\langle\phi_t|\psi_t\rangle = \langle\phi_{t'}|T^\dagger(t,t')T(t,t')|\psi_{t'}\rangle$$

takes both the ket and bra vector from $t' \to t$. The inner product tells us that this is equal to $\langle\phi_{t'}|\psi_{t'}\rangle$, and this holds for any pair of vectors. This tells us that $T^\dagger T = I$, so T must be a unitary operator.

Say we knew how the system evolves from $t' \to t$, and we knew how things evolved from $t'' \to t'$ (here $t > t' > t''$). We can compose these operators to figure out how to get from $t'' \to t$.

> N.B. The Hamiltonian could be time-dependent, so the time evolution operator at later times might be different than the operator at earlier times (for example, a magnetic field switched on at a later time).

$$T(t,t')T(t',t'') = T(t,t'')$$

Also, if we look at the adjoint, $T^\dagger(t,t') = T^{-1}(t,t')$. If we say that T is a map from earlier times to later times, and we know the map is one-to-one, then $T^\dagger(t,t') = T^{-1}(t,t') = T(t',t)$.

Additionally, $T(t,t) = I$

> For a general unitary operator U, we can introduce an orthonormal basis $\{|b_j\rangle\}$. We can find the matrix elements from $\langle b_j|U|b_k\rangle = U_{jk}$ and $U = \sum_{jk}|b_j\rangle U_j k\langle b_k|$. Additionally, $UU^\dagger = U^\dagger U = I$. This tells us that the rows and columns of U form a set of orthonormal vectors.
>
> For a general 2x2 unitary matrix, $U = \begin{bmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{bmatrix}$ where $|\alpha|^2 + |\beta|^2 = 1$. There could have been other choices which preserve orthogonality, but that could violate normalization (unless

our choice had unitary magnitude). Therefore, U is unique up to a phase, $U = e^{\imath\phi}\begin{bmatrix}\alpha & \beta \\ -\beta^* & \alpha^*\end{bmatrix}$.
In general, we can represent U as $U = e^{\imath K} = I + \imath K + \sum_{n=1}^{\infty} \frac{1}{n!}\imath^n K^n$, where $K^\dagger = K$ is also unitary.

$\imath\hbar\frac{d}{dt}|\psi_t\rangle = \imath\hbar\frac{d}{dt}T(t,t')|\psi_{t'}\rangle = H|\psi_t\rangle = HT(t,t')|\psi_{t'}\rangle$. Therefore

$\imath\hbar\frac{\partial}{\partial t}T(t,t') = HT(t,t')$. This is a first-order linear differential equation, so there is an exact formal solution. It can be evaluated if H is time dependent, but let's focus on the special case where it isn't.

$\frac{1}{T}\frac{\partial T}{\partial t} = -\frac{\imath}{\hbar}H = \frac{\partial}{\partial t}\ln T,$

where $S = \ln T \Rightarrow e^S = T$. If H is time-independent,

$\ln T = \frac{-\imath}{\hbar}H \cdot (t-t')$, imposing the initial condition where $T(t,t) = I$. Therefore, $T(t,t') = T(t-t') = e^{-\frac{\imath}{\hbar}H\,\cdot\,(t-t')}$.

Suppose we knew the eigenvectors and eigenvalues of the Hamiltonian. We could then take the spectral decomposition of the Hamiltonian,

$H = \sum_j E_j P_j$, where $P_j = |\psi_j\rangle\langle\psi_j|$.

$H^2 = \sum_{jk} E_j E_k P_j P_k = \sum_{jk} E_j E_k \delta_{jk} P_j$, so

$T(t-t') = \sum_j e^{-\frac{\imath}{\hbar}E_j\,\cdot\,(t-t')}P_j$.

$$e^{-\frac{\imath}{\hbar}H\,\cdot\,(t-t')}|\psi_j\rangle = (I - \frac{\imath}{\hbar}H\cdot(t-t') - \frac{1}{2}\frac{1}{\hbar^2}H^2\cdot(t-t')^2 + \cdots)|\psi_j\rangle = (I - \frac{\imath}{\hbar}E_j\cdot(t-t') - \cdots)|\psi_j\rangle$$

Multi-time Born Rule $Pr(P_t \mid |\psi_{t'}\rangle) = Pr(P_t \mid |\psi_t\rangle)$ where $|\psi_t\rangle = T(t-t')|\psi'_t\rangle$. This is equivalent to $||P_t T(t,t')|\psi'_t\rangle||^2$.

N.B.
$$Pr(|\psi_t\rangle \mid |\psi_{t'}\rangle) = ||\langle\psi_t|T(t,t')|\psi_{t'}\rangle||^2 = ||\langle\psi_t|\psi_{t'}\rangle||^2 = 1$$
assuming we are working with normalized vectors. This is a demonstration of the determinism of time-evolution.

Bloch Sphere

"A handy way to relate ket vectors in Hilbert space to spin orientations in physical space" - Dr. Widom

General spin-$\frac{1}{2}$:
$$|\psi\rangle = \alpha|z+\rangle + \beta|z-\rangle$$

Normalize: $|\alpha|^2 + |\beta|^2 = 1$

We can use a phase choice: $\alpha \geq 0$

This gives us another way to write the general ket vector:

$$|\psi\rangle = \cos\frac{\theta}{2}|z+\rangle + \sin\frac{\theta}{2}e^{\imath\phi}|z-\rangle$$

with $0 \leq \theta \leq \pi,\ 0 \leq \phi \leq 2\pi$. Define $\cos\theta = z_c$, $\sin\theta\cos\phi = x_c$, and $\sin\theta\sin\phi = y_c$. If we do this, $|\alpha|^2 + |\beta|^2 = x_c^2 + y_c^2 + z_c^2 = 1$, so we can represent spin vectors as locations on a sphere (the Bloch sphere).

The vector $|z+\rangle$ sits at the top of the sphere and

$$|z-\rangle$$

on the bottom. $|x\pm\rangle$ and $|y\pm\rangle$similarly sit on their corresponding axes.

$\langle z - |z+\rangle = 0$, but on the Bloch sphere, these points are not perpendicular.

Pauli Matrices

$S_x = \frac{\hbar}{2}\sigma_x$, where σ_x is now a dimensionless spin operator, called a Pauli matrix.

$S_x|x\pm\rangle = \pm\frac{\hbar}{2}|x\pm\rangle$, so $\sigma_x|x\pm\rangle = \pm|x\pm\rangle$, therefore

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}$, and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

The Pauli matrices with the identity form a basis of any 2×2 matrix. If we choose $M = a_0 I + a_X\sigma_x + a_y\sigma_y + a_z\sigma_z$, we find that $M = \begin{pmatrix} a_0 + a_z & a_x - \imath a_y \\ a_x + \imath a_y & a_0 - a_z \end{pmatrix} = a_0 I + \vec{a}\cdot\vec{\sigma}$.

Hermitian Matrices

$$M^\dagger = M \implies a_j \in \mathbb{R}$$

Let us define $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, so $S_n \equiv \hat{n}\cdot\vec{S} = \frac{\hbar}{2}\hat{n}\cdot\vec{\sigma} = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta e^{-\imath\phi} \\ \sin\theta e^{\imath\phi} & -\cos\theta \end{pmatrix}$.

You can apply trig identities to show that $S_n|\hat{n}\pm\rangle = \pm\frac{\hbar}{2}|\hat{n}\pm\rangle$.

Other Useful Facts $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$, and $\sigma_j\sigma_k = \imath\epsilon_{jul}\sigma_l$. We can also exponentiate the matrices:

$e^{\imath\theta\hat{n}\cdot\vec{\sigma}} = I + \imath\theta\hat{n}\cdot\vec{\sigma} + \frac{1}{2}(\imath\theta)^2(\hat{n}\cdot\vec{\sigma})^2 + \cdots = I\cos\theta + \imath\hat{n}\cdot\vec{\sigma}\sin\theta$. This is a generalization of the De Moivre formula to the space of operators.

Density Operator

$$Tr\rho = 1$$

For pure states, $Tr\rho^2 = 1$, and for mixed states, it is < 1.

General spin-$\frac{1}{2}$:

$$\rho = \frac{1}{2}(I + \rho_x\sigma_x + \rho_y\sigma_y + \rho_z\sigma_z)$$

The trace of this must be less than or equal to 1 if we want it to be a density matrix.

$\langle S_x\rangle = \frac{\hbar}{2}Tr(\rho\sigma_x) = \frac{\hbar}{2}\frac{1}{2}2\rho_x = \frac{\hbar}{2}\rho_x$, so $\langle\vec{S}\rangle = \frac{\hbar}{2}\vec{\rho}$

Is ρ a pure or mixed state?

$$Tr\rho^2 = Tr\frac{1}{4}(I^2 + \rho_x I\sigma_x + \rho_y I\sigma_y + \rho_z I\sigma_z + \rho_x\sigma_x I + \rho_x^2\sigma_x^2 + \cdots)$$

This is just $\frac{1}{2}(1+\rho_x^2+\rho_y^2+\rho_z^2) \leq 1$.

If a single $\rho_j = 1$, the others are zero, so you would have a pure state. On the other hand, if multiple ρ_j are nonzero, this would be a mixed state. Pure states are on the surface of the Bloch sphere, whereas mixed states are points in its interior.

Spin-1/2 in a Constant Magnetic Field

$$\vec{B} = B\hat{n}$$

$$H = -\vec{\mu} \cdot \vec{B}$$

$$\vec{\mu} = \gamma\vec{S} = \frac{1}{2}\hbar\gamma\vec{\sigma}$$

Define Armor frequency $\omega = -\gamma B$

Let $\vec{B} = B\hat{z}$:

$$H = \frac{1}{2}\hbar\omega\sigma_z = \frac{1}{2}\hbar\omega \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$T(t) = e^{-\imath tH/\hbar} = \begin{bmatrix} e^{-\imath t\omega/2} & 0 \\ 0 & e^{\imath t\omega/2} \end{bmatrix}$$

Let's start with the state $|\psi_0\rangle = \begin{pmatrix} 1 \\ \beta \end{pmatrix}$. Acting with the time operator, we see that $|\psi_t\rangle = e^{-\imath\omega t/2}\begin{pmatrix} 1 \\ \beta e^{\imath\omega t} \end{pmatrix}$. We can see that the spin-up component stays constant in time relative to the phase, but the other component rotates around the Bloch sphere at the Larmor frequency.

Take an arbitrary magnetic field in direction $\hat{n}$. Now $T(t) = e^{\imath\hat{n}\cdot\vec{\sigma}\omega t/2} = \cos\frac{\omega t}{2} I - \imath\sin\frac{\omega t}{2}\hat{n}\cdot\vec{\sigma}$.

Now suppose $\hat{n} = \hat{y}$, and $\sigma_y = \begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix}$, so $T(t) = \begin{bmatrix} \cos\frac{\omega t}{2} & -\sin\frac{\omega t}{2} \\ \sin\frac{\omega t}{2} & \cos\frac{\omega t}{2} \end{bmatrix}$. Starting in the state $|\psi_0\rangle = |z+\rangle$, we find $|\psi_t\rangle = \begin{pmatrix} \cos\frac{\omega t}{2} \\ \sin\frac{\omega t}{2} \end{pmatrix}$. Let's calculate $Pr([z+]_t \mid |\psi_t\rangle) = \langle\psi_t|z+\rangle\langle z+|\psi_t\rangle = \cos^2\frac{\omega t}{2}$. We can also see that $Pr([x+]_t \mid |\psi_t\rangle) = \frac{1}{2}\cos\frac{\omega t}{2}\sin\frac{\omega t}{2}$. The spin projection is rotating around the $\hat{y}$ axis at the Larmor frequency.

Generalization of Time-Dependent Spin Hamiltonian

$$H = \frac{1}{2}\hbar\vec{\omega}(t)\cdot\vec{\sigma}$$

$$\vec{\omega}(t) = \omega(t)\hat{n}(t)$$

$$T(t+\Delta t, t) \approx e^{-\imath(\omega(t)\hat{n}(t)\cdot\vec{\sigma}/2)\Delta t}$$

If $|\vec{\omega}|$ is constant and $\hat{n}$ rotates around a fixed axis at a fixed rate, we can find the exact solution. For instance, we could have $\vec{\omega}(t) = \omega_z \hat{z} + \omega_p(\cos(\omega_r t)\hat{x} + \sin(\omega_r t)\hat{y})$. In NMR, ω_z is related to the large polarizing magnet while ω_p is related to the RF pulse.

Let us now look at this in a co-rotating coordinate system.

$$|\psi\rangle = \sum_j \langle b_j|\psi\rangle|b_j\rangle = \sum_j |b_j\rangle\langle b_j|)|\psi\rangle$$

$$\{|b_j\rangle\} \to \{|\bar{b}_j\rangle\}$$

$$\langle\bar{b}_k|\psi\rangle = \langle\bar{b}_k \sum_j |b_j\rangle\langle b_j|\psi\rangle = \sum_j U_{kj}\langle b_j|\psi\rangle$$

For our system, suppose

$$|\psi\rangle \to |\bar{\psi}\rangle = S(t)|\psi\rangle$$

so

$$\imath\frac{d}{dt}|\bar{\psi}\rangle = \imath\dot{S}|\psi\rangle + S\imath\frac{d}{dt}|\psi\rangle = \imath\dot{S}S^\dagger|\bar{\psi}\rangle + SHS^\dagger|\bar{\psi}\rangle$$

is the equation of motion in our rotating coordinate system. We can re-characterize this as the combination of two Hamiltonians, $\bar{H}_1 = \imath\dot{S}S^\dagger$ and $\bar{H}_0 = SH_0S^\dagger$. Our old Hamiltonian was

$$H_0 = \frac{1}{2}\omega_z\sigma_z + \frac{1}{2}\omega_p\begin{pmatrix} 0 & \cos\omega_r t - \imath\sin\omega_r t \\ \cos\omega_r t + \imath\sin\omega_r t & 0 \end{pmatrix}$$

$$S(t) = \begin{pmatrix} e^{\imath\omega_r t/2} & 0 \\ 0 & e^{-\imath\omega_r t/2} \end{pmatrix}$$

$\bar{H}_1 = -\frac{1}{2}\omega_r\sigma_z$ and

$$\bar{H}_0 = \frac{1}{2}\omega_z\sigma_z + \frac{1}{2}\omega_p\sigma_x$$

The net result

$$\bar{H} = \bar{H}_0 + \bar{H}_1 = \frac{1}{2}(\omega_z - \omega_r)\sigma_z + \frac{1}{2}\omega_p\sigma_x$$

This is time-independent so we can use our solution from earlier. Note that if $\omega_z = \omega_r$, the effective field in the z-direction can be eliminated, meaning that if we match the frequency of our RF signal to the effect of the large super-conducting magnet, we can cancel its effect. Now the states will progress in the order

$$|\bar{z}+\rangle \to |\bar{y}-\rangle \to |\bar{z}-\rangle \to |\bar{y}+\rangle \to -|\bar{z}+\rangle$$

where we pick up a phase after one complete rotation. The first motion is a "$\pi/2$ pulse", where the characteristic time scale is $t = \frac{\pi}{2}\frac{1}{\omega_p}$. If we start with the state $|\bar{z}+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, we can write the other states as column vectors, $|\bar{y}-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -\imath \end{pmatrix}$, $|\bar{z}-\rangle = \begin{pmatrix} 1 \\ -\imath \end{pmatrix}$, $|\bar{y}+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ -\imath \end{pmatrix}$. The motion from $|\bar{z}+\rangle \to |\bar{z}-\rangle$ is a "π pulse" with characteristic time scale $t = \frac{\pi}{\omega_p}$. The time evolution operator is $T = e^{-\imath\frac{1}{2}\omega_p t\sigma_x}$.

This was in the "on resonance" condition, where $\omega_r = \omega_z$. In the "off resonance" condition, let's call the distance off of the resonant condition $\delta = \omega_z - \omega_r$.

Now,

$$H = \frac{1}{2}\delta\sigma_z + \frac{1}{2}\omega_p\sigma_x = \frac{1}{2}\begin{pmatrix} \delta & \omega_p \\ \omega_p & -\delta \end{pmatrix}$$

Eigenstates and eigenvalues are:

$$|\phi\rangle = (\cdots)\begin{pmatrix} \delta \pm \sqrt{\delta^2 + \omega_p^2} \\ -\omega_p \end{pmatrix}$$

$$\lambda = \pm\frac{1}{2}\Omega = \pm\frac{1}{2}\sqrt{\delta^2 + \omega_p^2}$$

$$\bar{T} = e^{-\imath\bar{H}t} = e^{\imath\Omega t/2}|\phi_+\rangle\langle\phi_+| + e^{\imath\Omega t/2}|\phi_-\rangle\langle\phi_-|$$

$$Pr([z-]_t) = \|[\bar{z}-]_t\bar{T}(t)|\bar{z}+\rangle_0\|^2$$

So the maximum probability of being flipped into the $|z-\rangle$ state decreases the further off-resonance you are.

Sample Spaces

Take some space of samples $\mathcal{S}$ with samples $s \in \mathcal{S}$ with probability p_s of occurring. For some random variable on the samples $V(s)$, we can find the average value of the outcome as

$\langle V\rangle = \sum_s p_s V(s)$.

For some indicator $E(s)$, we are defining a subspace of the sample space (all the dice rolls that turn up even, for example). The probability of getting a state with that particular indicator is

$Pr(E) = \sum_{s\in E} p_s$.

Say we have two random variables $V(s)$ and $W(s)$. We can now talk about joint probabilities. For instance, let's create two events, E is the event where $V = v$ and F is the event where $W = w$:

$Pr(V = v, W = w) = \sum_{s\in E\cap F} p_s = \langle EF\rangle$.

Example: Fair 6-sided Die

$$\mathcal{S} = \{1, 2, 3, 4, 5, 6\}$$

, $p_s = \frac{1}{6}$

$V(s) =$ "parity"

$$W(s) = (s - 3)^2$$

v\w	$w = 0$	$w = 1$	$w = 4$	$w = 9$	TOTALS
$v =$ even	0	2/6	0	1/6	1/2
$v =$ odd	1/6	0	2/6	0	1/2
TOTALS	1/6	2/6	2/6	1/6	1

Marginal probabilities: If you start with the joint probabilities for many variables and sum over all the probabilities for one of them, you get the marginal probability (the probabilities in the "TOTALS" rows and columns).

Conditional Probability $Pr(A \mid B) = Pr(A, B)/Pr(B)$ reads as "the probability of 'A' given 'B'"

Examples

$$Pr(v = \text{odd} \mid w = 4) = Pr(\text{odd}, 4)/Pr(4) = \frac{1}{3}/\frac{1}{3} = 1$$

$$Pr(w = 4 \mid v = \text{odd}) = Pr(4, \text{odd})/Pr(\text{odd}) = \frac{2}{6}/\frac{1}{2} = \frac{4}{6}$$

Statistical Independence If we have a joint probability of two events,

$$Pr(A, B) = Pr(A) \cdot Pr(B)$$

and

$Pr(\neg A, B) = Pr(\neg A) \cdot Pr(B)$ etc.

are conditions which must be met for the events to be statistically independent.

Example

$$Pr(s = 1 \text{ or } 6, s = \text{even}) = \sum_{s \in \{1,6\} \cap \{2,4,6\}} p_s = p_6 = \frac{1}{6}$$

$$Pr(s = 1 \text{ or } 6) = \frac{2}{6}$$

$$Pr(s = \text{even}) = \frac{3}{6}$$

We can continue through the other conditions to show that these events are independent. However, if we had the probability of rolling 2 or 6 instead of 1 or 6, we would find that these conditions are not satisfied, since all 2 and 6 rolls will also be even rolls.

Quantum Statistics We want this to be the same as the Classical case. However, there must be some differences (for instance, non-commuting operators). Our method to avoid these difficulties is called the "single framework rule". Suppose $V = v_1 P_1 + v_2 P_2 + v_3 P_3$ and $W = w_1 P_1 + w_2 Q_2 + w_3 Q_3$. Let's imagine $P_2 Q_2 \neq Q_2 P_2$ and $P_3 Q_3 \neq Q_3 P_3$. If we were to talk about values of V and W, we are forbidden from making statements about joint probabilities for all values of the operators. However, some statements can still be made. For example, if we took, as our sample space, $\mathcal{P} = \{P_1, I - P_1\}$ (note $I - P_1 = P_2 + P_3 = Q_2 + Q_3$) we can say things like $Pr(v_1, w_1)$, $Pr(v_1, \neg w_1)$, etc. as long as we only talk about things in commuting subspaces.

Can we say that $\neg(V = v_1) = (V = v_2)$ or $(V = v_3)$? No, we cannot interpret this in such a way if we include W in our space of operators.

Sequences of Outcomes Suppose we have a sequence of values $\{s_0, s_1, \cdots s_f\}$ in a particular order. We can write this as a vector $\vec{s}$ if we want.

$$\vec{s} \in \mathcal{S} \times \mathcal{S} \times \cdots \times \mathcal{S} = S^f$$

is a cartesian product. We could use different sample spaces if we want. We require $0 \leq Pr(\vec{S}) \leq 1$ and $\sum_{\vec{s}} Pr(\vec{s}) = 1$.

We can also calculate marginal probabilities

$$Pr_j(s_j) = \sum_{s_0, s_1 \cdots s_{j-1}} \sum_{s_j+1\cdots} Pr(s_0 s_1 \cdots s_{j-1} s_j s_{j+1} \cdots s_f)$$

These can tell us about any particular instance, but they won't tell us anything about correlations.

Markov Process This occurs when s_{j+1} is correlated with s_j but not s_{j-i} where $i > 0$. In this case, $Pr(s_0, s_1) = Pr(s_1 \mid s_0)Pr(s_0)$, $Pr(s_0, s_1, s_2) = Pr(s_2 \mid s_1)Pr(s_0, s_1)$. This is sometimes true in general cases but it is always true in Markov processes.
