Supplementary information I
Hilbert Space, Dirac Notation, and Matrix Mechanics

Properties of Vector Spaces

- Unit vectors $\vec{x}_i$ form a basis which spans the space and which are orthonormal

$$\vec{x}_i \cdot \vec{x}_j = \delta_{ij} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ otherwise} \end{cases}$$

- Column vectors

$$\vec{z} = |z\rangle = z_1\vec{x}_1 + z_2\vec{x}_2 + \cdots + z_n\vec{x}_N = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{pmatrix}$$

- Row vectors $\vec{v} = \langle v| = \begin{pmatrix} v_1^* & v_2^* & \dots & v_N^* \end{pmatrix}$
- Inner product can be defined

$$\vec{v} \cdot \vec{z} = \langle v|z\rangle = v_1^* z_1 + v_2^* z_2 + \cdots + v_N^* z_N$$

Quantum States as Vectors: Dirac Notation

- The mathematical structure of QM is based on vector spaces.
- In QM, states correspond to vectors. For each state ψ, we associate a "ket" $|\psi\rangle$ and "bra" $\langle\psi|$ with it (analogous to column and row vectors).
- We can define the inner product between different states ψ and ϕ as $\langle\psi|\phi\rangle$.
- In the case where the states can be represented as functions of position $\psi(x)$ and $\phi(x)$, $\langle\psi|\phi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\phi(x)dx$.
- Note that if $|\psi\rangle$ and $|\phi\rangle$ are distinct, $\langle\psi|\phi\rangle$ may be complex.

Quantum States as Vectors

- Bras and kets obey the following rules (where a is a scalar):

$$\begin{aligned}
\langle \psi | a\phi \rangle &= a \langle \psi | \phi \rangle \\
\langle a\psi | \phi \rangle &= a^* \langle \psi | \phi \rangle \\
\langle \psi | \phi \rangle^* &= \langle \phi | \psi \rangle \\
\langle \phi + \psi | &= \langle \phi | + \langle \psi | \text{ and } | \phi + \psi \rangle = | \phi \rangle + | \psi \rangle
\end{aligned}$$

- Therefore

$$\langle \psi_1 + \psi_2 | \phi_1 + \phi_2 \rangle = \langle \psi_1 | \phi_1 \rangle + \langle \psi_1 | \phi_2 \rangle + \langle \psi_2 | \phi_1 \rangle + \langle \psi_2 | \phi_2 \rangle$$

Hilbert Spaces

The vector spaces of interest in QM are *Hilbert spaces*.
A Hilbert space $\mathcal{H}$ is a linear vector space whose elements are functions or vectors $|\psi\rangle$ with a positive-definite scalar product (i.e., $\langle\psi|\psi\rangle > 0$ and is finite). The dimensionality N of the Hilbert space is the number of linearly independent vectors/states needed to span it (may be finite or infinite).

Properties:

1. Linearity: if $|\psi\rangle$ and $|\phi\rangle$ are elements of $\mathcal{H}$, so is $a\psi + b\phi$.
2. Inner product: $\langle\psi|\phi\rangle$ exists and $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$.
3. Every element $|\psi\rangle$ has a norm/length $\|\psi\|$ such that $\langle\psi|\psi\rangle = \|\psi\|^2$.
4. Completeness: every Cauchy series of functions in $\mathcal{H}$ converges to an element in $\mathcal{H}$.

Basis States of Hilbert Spaces

For a Hilbert space of dimension N, we can choose N orthonormal states (basis states) $|\phi_1\rangle, |\phi_2\rangle, \cdots |\phi_N\rangle$ which span the space, such that any state $|\psi\rangle$ in $\mathcal{H}$ can be decomposed into

$$|\psi\rangle = \sum_{n=1}^{N} b_n |\phi_n\rangle$$

where b_n are scalars.
This definition holds in infinite dimensions $N \to \infty$ provided $\sum_{n=1}^{N} |b_n|^2 < \infty$.

Orthonormality of Basis

- Orthonormal basis: a set of basis vectors ϕ_i of unit norm, which are pairwise orthogonal.
- Two vectors/states are orthogonal if $\langle \phi_m | \phi_n \rangle = 0$ for $m \neq n$.
- Normalization: vector/state is normalized if $\langle \phi_m | \phi_m \rangle = 1$.

We postulate that the set of eigenstates of <u>any</u> observable is orthonormal and hence is a possible basis for the Hilbert space (provable for finite dimensions, axiomatic for infinite dimensions).

Basis Expansion and the Born Rule

Suppose we express an arbitrary state $|\psi\rangle$ in terms of the orthonormalized eigenstates ϕ_i of an observable A such that

$$|\psi\rangle = \sum_n b_n |\phi_n\rangle$$

Then let us examine the inner product

$$\langle\phi_i|\psi\rangle = \sum_n b_n \langle\phi_i|\phi_n\rangle = \sum_n b_n \delta_{i,n} = b_i$$

The Born rule ("generalized statistical interpretation") states that a measurement of A performed on $|\psi\rangle$ has probability $|\langle\phi_i|\psi\rangle|^2$ of returning the eigenvalue a_i, leaving the system in the eigenstate $|\phi_i\rangle$ of $\hat{A}$.
Therefore the coefficients b_n are the probability amplitudes of observing $|\phi_n\rangle$ upon measurement!

Dual Space

- We define a dual space composed of "bra" states $\langle\psi|$ adjoint to the original "ket" Hilbert space. This allows us to perform operations between vectors/states.
- The analogy between column and row vectors is useful. If we write the coefficients of state ψ as $|\psi\rangle = \begin{pmatrix} b_1 \\ b_2 \\ \dots \\ b_N \end{pmatrix}$ then the corresponding "bra" is a row vector $\langle\psi| = \begin{pmatrix} b_1^* & b_2^* & \dots & b_N^* \end{pmatrix}$.
- If $\langle\psi|$ is the adjoint of $|\psi\rangle$, the adjoint of $a\,|\psi\rangle$ (where a is a scalar) is given by

$$a\,|\psi\rangle = |a\psi\rangle \iff \langle a\psi| = \langle\psi|\,a^*$$

Operators in Dirac notation

Operators transform one state (ket vector) into another state in $\mathcal{H}$

$$\hat{A}\left|\psi\right\rangle = \left|\theta\right\rangle$$

We can define an adjoint operator $\hat{A}^\dagger$ that acts on the adjoint vector (bra):

$$\left\langle\psi\right|\hat{A}^\dagger = \left\langle\theta\right|$$

For linear operators and scalar a:

$$\hat{A}a\left|\psi\right\rangle = a\hat{A}\left|\psi\right\rangle$$

$$(\hat{A}+\hat{B})\left|\psi\right\rangle = \hat{A}\left|\psi\right\rangle + \hat{B}\left|\psi\right\rangle$$

$$\hat{A}(\left|\psi\right\rangle + \left|\phi\right\rangle) = \hat{A}\left|\psi\right\rangle + \hat{A}\left|\phi\right\rangle$$

Projection and Identity Operators

- The projection operator $\hat{P}_i$ picks out ("projects") a particular component of a state vector $\hat{P}_i = |\phi_i\rangle \langle\phi_i|$.
- For any $|\psi\rangle = \sum_n b_n |\phi_n\rangle$,
  $\hat{P}_i |\psi\rangle = |\phi_i\rangle \langle\phi_i| \sum_n b_n |\phi_n\rangle = |\phi_i\rangle \sum_n b_n \langle\phi_i|\phi_n\rangle =$
  $|\phi_i\rangle \sum_n b_n \delta_{in} = b_i |\phi_i\rangle$
- The identity operator $\hat{I}$ always returns the state it is applied to
  $\hat{I} |\psi\rangle = |\psi\rangle$ and $\langle\psi| \hat{I} = \langle\psi|$
- Note that $\hat{I} = \sum_n |\phi_n\rangle \langle\phi_n| = \sum_n \hat{P}_n$ (a very useful result)
- If the eigenvalues indexed by n range over a continuous set of values, the summation becomes an integration
  $\hat{I} = \int |\phi_n\rangle \langle\phi_n| \, dn$

An Infinite-Dimensional Hilbert Space: $\mathcal{L}_2$

- The Hilbert space $\mathcal{L}_2(a, b)$ is the set of all square-integrable functions $f(x)$ on the interval $[a, b]$, *i.e.*, $f(x)$ such that $\int_a^b f^*(x)f(x)dx < \infty$
- The inner product in $\mathcal{L}_2(a, b)$ is defined as

$$\langle\psi|\phi\rangle = \int_a^b \psi^*(x)\phi(x)dx$$

- Examples include $\mathcal{L}_2(0, a)$ for the infinite square well and $\mathcal{L}_2(-\infty, \infty)$ for the free particle. Note the infinite dimensionality of the Hilbert spaces (evidenced by the infinite number of energy eigenfunctions, which comprise possible bases for these spaces).

Interregnum: The Dirac Delta Function

- We define the Dirac delta function via

$$\delta(x) \equiv \begin{cases} \infty \text{ for } x = 0 \\ 0 \text{ otherwise} \end{cases}$$

$$\int\limits_{-\infty}^{\infty} \delta(x)dx = 1$$

- Note the units of $\delta(x)$ are x^{-1}.
- The Dirac delta function picks out the origin. Operationally, for any function $f(x)$,

$$f(x)\delta(x-a) = f(a)\delta(x-a)$$

because for any integral

$$\int\limits_{-\infty}^{\infty} f(x)\delta(x-a)dx = f(a)\int\limits_{-\infty}^{\infty} \delta(x-a)dx = f(a)$$

The Dirac Delta Function cont'ed

- The Dirac delta function is not a traditional mathematical function, though it can be seen as the limit of a variety of sharply peaked well-defined functions, for instance

$$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{\pi x} \sin\left(\frac{x}{\epsilon}\right)$$

- Note that if we take $f(x) = x$, we obtain

$$x\delta(x - x_0) = x_0\delta(x - x_0)$$

- This looks like an eigenvalue equation for the operator $\hat{x}$. The implication is that the eigenfunctions of the position operator are Dirac delta functions centered at particular eigenvalues x_0.

The Dirac Delta Function cont'ed

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk \Leftrightarrow F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

If $f(x) = \delta(x - x_0)$, then $F(k) = \frac{\exp(-ikx_0)}{\sqrt{2\pi}}$. This implies

$$\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x_0)} dk$$

The Fourier transform of a delta function has constant magnitude $|F(k)|^2 = \frac{1}{2\pi}$. A function completely localized in position space is completely delocalized in momentum space, and vice versa.

Basis States for Position/Momentum Space

- For the Hilbert space $\mathcal{L}_2$, we can choose real space x or momentum space p as our basis. For $\hat{x}$, the eigenfunctions/eigenvalues are $\delta(x - x_0)$ for all x_0 in the range of $\mathcal{L}_2$. For $\hat{p}$, we can define the eigenfunctions $\frac{1}{\sqrt{2\pi\hbar}} \exp(ipx/\hbar)$ with definite momentum $p = \hbar k$.
- Relationships between basis states:

$$\langle p_1 | p_2 \rangle = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{i(p_2 - p_1)x/\hbar} dx = \delta(p_1 - p_2)$$

$$\langle x_1 | x_2 \rangle = \int_{-\infty}^{\infty} \delta(x - x_1)\delta(x - x_2) dx = \delta(x_1 - x_2)$$

$$\langle x_1 | p_1 \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \delta(x - x_1) e^{ip_1 x/\hbar} dx = \frac{1}{\sqrt{2\pi\hbar}} \exp(ip_1 x_1/\hbar)$$

Position and Momentum Space, cont'd

- Note that though the position and momentum eigenfunctions are not square-integrable (and hence technically outside the Hilbert space), they are orthonormal in the Dirac sense.
- This is generally the case for operators whose eigenvalues are continuous.
- However, it is still extremely useful to use these states as basis functions, so we can write a general state ψ as

$$\begin{aligned} |\psi\rangle &= \int dx\, |x\rangle \langle x|\psi\rangle \\ &= \int dp\, |p\rangle \langle p|\psi\rangle \end{aligned}$$

- Note that because we are dealing with a continuous rather than discrete range of eigenvalues, we integrate rather than sum over all possible eigenvalues.

Position and Momentum Space cont'ed

$$|\psi\rangle = \int dx\,|x\rangle\langle x|\psi\rangle = \int dp\,|p\rangle\langle p|\psi\rangle$$

- $\langle x|\psi\rangle = \psi(x)$, i.e., the value of the wave function at position x is simply the projection of the state $|\psi\rangle$ onto the position eigenstate $|x\rangle$.
- This makes our original interpretation of $|\psi(x)|^2$ as the probability of measurement of x consistent with and subordinate to the Born rule that the probability $= |\langle x|\psi\rangle|^2$.
- Likewise we can interpret $\psi(p) = \langle p|\psi\rangle$ as the momentum space wave function, i.e., probability amplitude for measurement of p.
- Complete information about the state can be obtained from $\psi(p)$ or $\psi(x)$; they are simply projections of $|\psi\rangle$ onto different bases.
- Consistency of inner product definitions: using $\hat{I} = \int |x\rangle\langle x|\,dx$

$$\langle\phi|\psi\rangle = \langle\phi|(\int |x\rangle\langle x|\,dx)\psi\rangle = \int \langle\phi|x\rangle\langle x|\psi\rangle\,dx = \int \phi^*(x)\psi(x)dx$$

Position and Momentum - Fourier Transforms

- Conversion between $\psi(x)$ and $\psi(p)$:

$$\psi(p) = \langle p|\psi\rangle = \int \langle p|x\rangle \langle x|\psi\rangle \, dx$$
$$= \int e^{-ipx/\hbar}\psi(x)\frac{dx}{\sqrt{2\pi\hbar}}$$

- Similarly $\psi(x) = \int e^{ipx/\hbar}\psi(p)\frac{dp}{\sqrt{2\pi\hbar}}$.
- The conversion between position and momentum space is mathematically a Fourier transform because $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(ipx/\hbar)$.

Discrete vs. Continuous Spectra

Let $\hat{A}\,|a_n\rangle = a_n\,|a_n\rangle$ (where the eigenvalues a_n are discrete) and $\hat{B}\,|b_n\rangle = b_n\,|b_n\rangle$ (where the eigenvalues b_n are continuous)

Discrete	**Continuous**
$\langle a_m \vert a_n\rangle = \delta_{mn}$	$\langle b_m \vert b_n\rangle = \delta(b_m - b_n)$
$\sum_m \vert a_m\rangle\langle a_m\vert = 1$	$\int db_m\,\vert b_m\rangle\langle b_m\vert = 1$
$\vert\alpha\rangle = \sum_m \vert a_m\rangle\langle a_m\vert\alpha\rangle$	$\vert\beta\rangle = \int db_m\,\vert b_m\rangle\langle b_m\vert\beta\rangle$
$\sum_m \vert\langle a_m\vert\alpha\rangle\vert^2 = 1$	$\int db_m \vert\langle b_m\vert\beta\rangle\vert^2 = 1$
$\langle a_m\vert A\vert a_n\rangle = a_n\delta_{mn}$	$\langle b_m\vert B\vert b_n\rangle = b_n\delta(b_m - b_n)$

where δ_{mn} is the Kronecker delta function and $\delta(b_m - b_n)$ is the Dirac delta function.

Operators - Matrix Formulation

- We have seen that quantum states can be represented as vectors in a vector space of dimension N.
- A linear operator can be represented by an $N \times N$ matrix that operates on bra and ket vectors.
- It is completely defined by its actions on the basis vectors.
- If we know $\hat{A}\,|\phi_n\rangle = |\phi_n'\rangle$ for each n we can write

$$\hat{A}\,|\psi\rangle = \hat{A}\sum_n b_n\,|\phi_n\rangle = \sum_n b_n \hat{A}\,|\phi_n\rangle = \sum_n b_n\,|\phi_n'\rangle = |\psi'\rangle$$

- Here the set of states $|\phi_n\rangle$ is some orthonormal basis (not necessarily eigenstates of $\hat{A}$), while the set $|\phi_n'\rangle$ is generally <u>not</u> orthonormal.

Operators - Matrix Formulation cont'ed

Let us express $|\psi'\rangle = \sum_m b'_m |\phi_m\rangle$ by projecting it back onto the original basis. We can find each amplitude b'_m of the new state

$$\begin{aligned} b'_m = \langle \phi_m | \psi' \rangle &= \langle \phi_m | \left(\sum_n b_n |\phi'_n\rangle \right) \\ &= \langle \phi_m | \left(\sum_n b_n \hat{A} |\phi_n\rangle \right) \\ &= \sum_n \langle \phi_m | \hat{A} | \phi_n \rangle \, b_n \\ \therefore b'_m &= \sum_n A_{mn} b_n \end{aligned}$$

We have N^2 scalars $A_{mn} = \langle \phi_m | \hat{A} | \phi_n \rangle$ which depend only on the basis states $\{|\phi_m\rangle\}$, not $|\psi\rangle$ or $|\psi'\rangle$.

Operators - Matrix Formulation cont'ed

We can therefore write $|\psi'\rangle = \hat{A}\,|\psi\rangle$ as a matrix equation.

$$|\psi'\rangle = \begin{pmatrix} b'_1 \\ b'_2 \\ \vdots \\ b'_N \end{pmatrix} = \begin{pmatrix} \langle\phi_1|\hat{A}|\phi_1\rangle & \langle\phi_1|\hat{A}|\phi_2\rangle & \cdots \\ \langle\phi_2|\hat{A}|\phi_1\rangle & \langle\phi_2|\hat{A}|\phi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \\ \langle\phi_N|\hat{A}|\phi_1\rangle & \langle\phi_N|\hat{A}|\phi_2\rangle & \cdots \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$$

The scalars $A_{mn} = \langle\phi_m|\hat{A}|\phi_n\rangle$ are the matrix elements of $\hat{A}$ in the basis set ϕ_i.
In Dirac notation, we can write $\hat{A} = \sum_{m,n} A_{mn}\,|\phi_m\rangle\,\langle\phi_n|$.

Adjoint Operators

For scalars we have $a\,|\psi\rangle = |a\psi\rangle \longleftrightarrow \langle a\psi| = \langle\psi|\,a^*$
For adjoint operators: $\hat{A}\,|\psi\rangle = |\hat{A}\psi\rangle \longleftrightarrow \langle\hat{A}\psi| = \langle\psi|\,\hat{A}^\dagger$
If $\hat{A}\,|\psi\rangle = |\psi'\rangle \longleftrightarrow \langle\psi|\,\hat{A}^\dagger = \langle\psi'|$
If $A_{mn} = \langle\phi_m|\hat{A}|\phi_n\rangle$ then

$$\begin{aligned}
\hat{A}^\dagger_{mn} &= \langle\phi_m|\hat{A}^\dagger|\phi_n\rangle \\
&= \langle\hat{A}\phi_m|\phi_n\rangle \\
&= \langle\phi_n|\hat{A}\phi_m\rangle^* \\
&= \langle\phi_n|\hat{A}|\phi_m\rangle^*
\end{aligned}$$

Therefore $A^\dagger_{mn} = A^*_{nm}$. Adjoints are the transpose conjugate of the operator matrix.

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \longleftrightarrow A^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}$$

Adjoints cont'ed

It can be shown that $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$.

In general, to find the adjoint of bras, kets, operators, or scalars:
Reverse order of all factors
$\hat{A} \longleftrightarrow \hat{A}^\dagger$
$|\rangle \longleftrightarrow \langle|$
$a \longleftrightarrow a^*$.
Note that in an quantity like $\langle\alpha|\hat{A}|\beta\rangle$, $\hat{A}$ can operate to the right (as $\hat{A}$ on the ket) or to the left (as $\hat{A}^\dagger$ on the bra). The same result will be obtained in either case.

Hermitian Operators and Observables

- Hermitian operators $\hat{A}$ have the property that $\hat{A}^\dagger = \hat{A}$:
- This implies $\langle \phi | \hat{A} \psi \rangle = \langle \hat{A} \phi | \psi \rangle$.
- In matrix notation, $A_{mn} = A_{nm}^*$. Any Hermitian matrix will be of the form

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{12}^* & A_{22} & A_{23} & \cdots \\ A_{13}^* & A_{23}^* & A_{33} & \cdots \\ \vdots & \vdots & & \ddots \end{bmatrix}$$

- All eigenvalues of Hermitian operators are real. Therefore, (by postulate), all operators for physical observables are Hermitian (because measured quantities are real numbers).
- An operator is anti-Hermitian if $\hat{A}^\dagger = -\hat{A}$.

Hermitian Operators: Reality

Proof of the reality of eigenvalues of Hermitian operators:

If $|\phi_n\rangle$ and a_n are the sets of eigenvectors and eigenvalues of $\hat{A}$, then $\hat{A}\,|\phi_n\rangle = a_n\,|\phi_n\rangle$ and $\langle\phi_n|\,\hat{A} = \langle\phi_n|\,a_n^*$.
Then $\langle\phi_n|\hat{A}|\phi_n\rangle = a_n\,\langle\phi_n|\phi_n\rangle = a_n^*\,\langle\phi_n|\phi_n\rangle$ depending on whether $\hat{A}$ operates to the left or right. Therefore $a_n = a_n^*$, so a_n must be real.

Hermitian Operators: Orthogonality

Proof of the orthogonality of eigenvectors of Hermitian operators:

$\langle \phi_m | \hat{A} | \phi_n \rangle = a_n \langle \phi_m | \phi_n \rangle$ (operating to the right)
and
$\langle \phi_m | \hat{A} | \phi_n \rangle = a_m^* \langle \phi_m | \phi_n \rangle$ (operating to the left)
Therefore $a_n \langle \phi_m | \phi_n \rangle = a_m^* \langle \phi_m | \phi_n \rangle$
If $a_n \neq a_m$ then $\langle \phi_m | \phi_n \rangle = 0$, i.e., $\langle \phi_m | \phi_n \rangle = \delta_{mn}$.
Nondegenerate eigenstates of Hermitian operators are necessarily orthogonal.
If different eigenstates are degenerate (i.e., share the same eigenvalue), we can always construct linear combinations of them which are orthonormal (for example using the Gram-Schmidt procedure).

Commutators

- Commutators between two operators are defined as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.
- Clearly $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$.
- Two operators $\hat{A}, \hat{B}$ commute (or are compatible) if $[\hat{A}, \hat{B}] = 0$.
- To figure out commutation relations, apply the operators on a test function and look at the end result (sans test function).
- Example: the canonical commutation relation $[\hat{x}, \hat{p}] = i\hbar$.

The Uncertainty Principle (again)

Consider two operators $\hat{A}, \hat{B}$ which don't commute, and whose commutator $[\hat{A}, \hat{B}] = i\hat{C}$ where $\hat{A}, \hat{B}, \hat{C}$ are Hermitian.

From linear algebra, the Schwarz inequality for any two vectors $|\alpha\rangle, |\beta\rangle$ states that

$$\langle\alpha|\alpha\rangle \langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

Take $|\alpha\rangle = (\hat{A} - \langle A\rangle)|\psi\rangle$ and $|\beta\rangle = (\hat{B} - \langle B\rangle)|\psi\rangle$ where $\langle A\rangle, \langle B\rangle$ are expectation values over $|\psi\rangle$ and must be real.
$\langle\alpha|\alpha\rangle = \langle\psi|(\hat{A} - \langle A\rangle)^2|\psi\rangle = \sigma_A^2$
$\langle\beta|\beta\rangle = \langle\psi|(\hat{B} - \langle B\rangle)^2|\psi\rangle = \sigma_B^2$
For any complex z

$$|z|^2 = [\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2 \geq [\mathrm{Im}(z)]^2 = \left[\frac{1}{2i}(z - z^*)\right]^2$$

The Uncertainty Principle, cont'ed

For $z = \langle\alpha|\beta\rangle$ this implies

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}[\langle\alpha|\beta\rangle - \langle\beta|\alpha\rangle]\right)^2$$

$$\begin{aligned}\langle\alpha|\beta\rangle &= \langle\psi|(\hat{A} - \langle A\rangle)(\hat{B} - \langle B\rangle)|\psi\rangle \\ &= \langle\psi|\hat{A}\hat{B}|\psi\rangle - \langle B\rangle\langle\psi|\hat{A}|\psi\rangle - \langle A\rangle\langle\psi|\hat{B}|\psi\rangle + \langle A\rangle\langle B\rangle\langle\psi|\psi\rangle \\ &= \langle\hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle\end{aligned}$$

By similar reasoning $\langle\beta|\alpha\rangle = \langle\hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle$

$$\langle\alpha|\beta\rangle - \langle\beta|\alpha\rangle = \langle\hat{A}\hat{B}\rangle - \langle\hat{B}\hat{A}\rangle = \langle[\hat{A},\hat{B}]\rangle = i\hat{C}$$

$$\therefore \sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2 = |\langle C\rangle|^2$$

The Uncertainty Principle, cont'd

Example: $[\hat{x}, \hat{p}] = i\hbar$

$$\sigma_x^2 \sigma_p^2 \geq \left(\frac{\hbar}{2}\right)^2$$
$$\therefore \sigma_x \sigma_p \geq \frac{\hbar}{2}$$

Note that if two operators commute (are compatible), it is possible that the same state will be an eigenfunction of both operators. Then the two corresponding observables can be simultaneously specified for that state.
The eigenvalues of the observables are "good quantum numbers" of the state.

Some Equivalences

Wave Functions	Vectors	Dirac Notation
ψ	$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$	$\lvert\psi\rangle$
ψ^*	$\begin{pmatrix} b_1^* & b_2^* & \cdots & b_N^* \end{pmatrix}$	$\langle\psi\rvert$
$\psi(\vec{r})$	$\begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \end{pmatrix}$	$\langle r\lvert\psi\rangle$
$\int \psi^* \psi d\vec{r}$	$\begin{pmatrix} b_1^* & b_2^* & \cdots & b_N^* \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$	$\langle\psi\lvert\psi\rangle$
$\hat{A}\psi = \phi$	$[A] \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$	$\hat{A}\lvert\psi\rangle = \lvert\phi\rangle$

Some Equivalences cont'ed

Wave Functions	Vectors	Dirac Notation
$\langle A \rangle = \int \psi^* \hat{A} \psi dr$	$\begin{pmatrix} b_1^* & b_2^* & \cdots & b_N^* \end{pmatrix} [A] \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$	$\langle \psi \| A \| \psi \rangle$
$\hat{A}\phi_n(x) = a_n \phi_n(x)$	$\begin{pmatrix} a_1 & 0 & & 0 \\ 0 & a_2 & & 0 \\ & & \ddots & \\ 0 & 0 & & a_N \end{pmatrix}$ in ϕ_n basis	$\hat{A} \|\phi_n\rangle = a_n \|\phi_n\rangle$
$\int \phi_m^* \phi_n d\vec{r} = \delta_{mn}$	$\begin{pmatrix} 0 & \cdots & 1 & \cdots & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} = \delta_{mn}$	$\langle \phi_m \| \phi_n \rangle = \delta_{mn}$

Unitary Operators

- Unitary operators $\hat{U}$ are such that $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$.
- This implies $\hat{U}^\dagger = \hat{U}^{-1}$.
- Note that unitary operators are not in general Hermitian and vice versa. The application of an unitary operator on a state leaves the norm unchanged.
- Unitary operators are useful because they transform between different choices of basis states in $\mathcal{H}$.

$\hat{H}$ as the Generator of Time Evolution

Let $|\psi(t_0)\rangle = \sum_i |\phi_i\rangle \langle\phi_i|\psi(t_0)\rangle = \sum_i b_i(t_0)|\phi_i\rangle$ where $\{\phi_i\}$ are eigenstates of $\hat{H}$ with corresponding energies $\{\hbar\omega_i\}$. From the time-dependent SE, the state at some later time t is

$$\begin{aligned} |\psi(t)\rangle = \hat{U}(t-t_0)|\psi(t_0)\rangle &= \exp\left(-\frac{i\hat{H}(t-t_0)}{\hbar}\right)|\psi(t_0)\rangle \\ &= \exp\left(-\frac{i\hat{H}(t-t_0)}{\hbar}\right)\sum_i b_i(t_0)|\phi_i\rangle \\ &= \sum_i b_i(t_0)e^{-i\omega_i(t-t_0)}|\phi_i\rangle \end{aligned}$$

Here we define

$$\hat{U}(t-t_0) \equiv \exp\left(-\frac{i\hat{H}(t-t_0)}{\hbar}\right) = 1 - \frac{i(t-t_0)}{\hbar}\hat{H} + \frac{1}{2!}\left(\frac{i(t-t_0)}{\hbar}\right)^2 \hat{H}^2 + \ldots$$

The Hamiltonian "generates" the time evolution of states. $\hat{U}(t-t_0)$ is unitary.

Momentum as the Generator of Spatial Translation

Define the translation operator $\hat{T}(a)$ such that
$\hat{T}(a)f(x) = f(x+a)$. ($\hat{T}$ translates a state by distance a.)

$$\hat{T}(a) = \exp\left(\frac{i\hat{p}a}{\hbar}\right) = \exp\left(a\frac{d}{dx}\right) = 1 + \frac{d}{dx}a + \frac{1}{2!}\frac{d^2}{dx^2}a^2 \ldots$$

$$\hat{T}(a)f(x) = f(x) + \frac{df(x)}{dx}a + \frac{1}{2!}\frac{d^2f(x)}{dx^2}a^2 \cdots = f(x+a)$$

Note the similarity between $\hat{T}(a)$ and the time evolution operator $\hat{U}(t') = \exp\left(-\frac{i\hat{H}t'}{\hbar}\right)$. Both are unitary operators.

We say momentum "generates" spatial translations.

Ehrenfest Theorem

What is the time dependence of expectation values?

$$
\begin{aligned}
\frac{d\langle A\rangle}{dt} &= \frac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle = \int \frac{d}{dt}\Big(\psi^*(x,t)\hat{A}\psi(x,t)\Big)\,dx \\
&= \left(\frac{\partial}{\partial t}\langle\psi(t)|\right)\hat{A}\,|\psi(t)\rangle + \left\langle \psi \,\middle|\, \frac{\partial\hat{A}}{\partial t} \,\middle|\, \psi \right\rangle + \langle\psi(t)|\,\hat{A}\left(\frac{\partial}{\partial t}|\psi(t)\rangle\right) \\
&= -\frac{1}{i\hbar}\Big(\langle\hat{H}\psi|\hat{A}|\psi\rangle - \langle\psi|\hat{A}|\hat{H}\psi\rangle\Big) + \left\langle \psi \,\middle|\, \frac{\partial\hat{A}}{\partial t} \,\middle|\, \psi \right\rangle \\
&= \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle + \left\langle \frac{\partial\hat{A}}{\partial t} \right\rangle
\end{aligned}
$$

If $\hat{A}$ has no explicit time dependence, then $\frac{d\langle A\rangle}{dt} = \frac{i}{\hbar}\left\langle[\hat{H},\hat{A}]\right\rangle$.

Ehrenfest Theorem, cont'ed

Consider a Hamiltonian $\hat{H} = -\frac{\hat{p}^2}{2m} + V(x)$.

$$
\begin{aligned}
\frac{d\langle p\rangle}{dt} &= \frac{i}{\hbar}\langle[\hat{H},\hat{p}]\rangle = \frac{i}{\hbar}\left\langle\left[V(x), -i\hbar\frac{d}{dx}\right]\right\rangle \\
&= \left[\int \psi^*(x,t)V(x)\frac{\partial\psi(x,t)}{\partial x}dx - \int \psi^*(x,t)\frac{\partial}{\partial x}(V(x)\psi(x,t))dx\right] \\
&= -\int \psi^*(x,t)\frac{dV(x)}{dx}\psi(x,t)dx
\end{aligned}
$$

Therefore

$$
\frac{d\langle p\rangle}{dt} = -\left\langle\frac{dV(x)}{dx}\right\rangle
$$

The quantum expectation values reproduce classical mechanics.

Symmetry and Conservation Laws

Any generator that leaves the Hamiltonian of a system invariant corresponds to a conserved quantity of that system (Noether's theorem).

Examples:
Translational invariance implies **momentum conservation**: $[\hat{H}, \hat{p}] = 0$ for free particle ($\hat{H} = \hat{p}^2/2m$) implies $\frac{d\langle p \rangle}{dt} = 0$.
Temporal invariance implies **energy conservation**: $[\hat{H}, \hat{H}] = 0$ for time-independent $\hat{H}$ implies $\frac{d\langle E \rangle}{dt} = 0$.
Rotational invariance implies **angular momentum conservation**: $[\hat{H}, \vec{J}] = 0$ for angular momentum $\vec{L}$ implies $\frac{d\langle \vec{L} \rangle}{dt} = 0$.