1.1 Dirac Notation and rules of Quantum Mechanics

1.1.1 States and operators

A quantum state is represented by the ket $|\psi\rangle$. The Hermitian conjugate is the bra $\langle\psi|$. The inner product is

$$\langle\phi|\psi\rangle = c \text{ (a number)}. \tag{1.1}$$

If $c = \langle\phi|\psi\rangle$ then the complex conjugate is $c^* = \langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$. Kets and bras exist in a Hilbert space which is a generalization of the three dimensional linear vector space of Euclidean geometry to a complex valued space with possibly infinitely many dimensions.
The inner product is linear

$$\langle\phi|\left(a_1|\psi_1\rangle + a_2|\psi_2\rangle\right) = a_1\langle\phi|\psi_1\rangle + a_2\langle\phi|\psi_2\rangle. \tag{1.2}$$

Operators are denoted by a hat $\hat{A}$.

$$\hat{A}\left(c_1|\psi_1\rangle + c_2|\psi_2\rangle\right) = c_1\hat{A}|\psi_1\rangle + c_2\hat{A}|\psi_2\rangle.$$

The matrix element of an operator is

$$\langle\phi|\hat{A}|\psi\rangle = \langle\phi|\left(\hat{A}|\psi\rangle\right) = \left(\langle\phi|\hat{A}\right)|\psi\rangle = c \text{ (a number)}. \tag{1.3}$$

The expectation value of an operator for a system in state $|\psi\rangle$ is

$$\langle\hat{A}\rangle = \langle a\rangle = \langle\psi|\hat{A}|\psi\rangle. \tag{1.4}$$

The complex conjugate of the matrix element is

$$\langle\phi|\hat{A}|\psi\rangle^* = \langle\psi|\hat{A}^\dagger|\phi\rangle = c^* \tag{1.5}$$

where $\hat{A}^\dagger$ is the Hermitian conjugate of $\hat{A}$. When $\hat{A}$ is represented by a matrix the Hermitian conjugate is found by transposing the matrix and then taking the complex conjugate of each matrix element. The operation of taking the Hermitian conjugate of a combination of numbers, states, and operators involves changing $c \to c^*$, $|\psi\rangle \to \langle\psi|$, $\langle\psi| \to |\psi\rangle$, $\hat{A} \to \hat{A}^\dagger$ and reversing the order of all elements. For example

$$\left(c_1\hat{A}^\dagger\langle\phi|\hat{B}|\psi\rangle\langle\xi|\right)^\dagger = c_1^*|\xi\rangle\langle\psi|\hat{B}^\dagger|\phi\rangle\hat{A}.$$

1.1.2 Observables

Observables are represented by Hermitian operators which satisfy $\hat{A}^\dagger = \hat{A}$. The expectation value of a Hermitian operator is real:

$$a^* = \langle\hat{A}\rangle^* = \langle\psi|\hat{A}|\psi\rangle^* = \langle\psi|\hat{A}^\dagger|\psi\rangle = \langle\psi|\hat{A}|\psi\rangle = a. \tag{1.6}$$

Denote the eigenstates of a Hermitian operator by $|n\rangle$. The eigenvalues are real since

$$\langle m|\hat{A}|m\rangle = \langle m|a_m|m\rangle = a_m\langle m|m\rangle = a_m$$

and

$$a_m^* = \langle m|\hat{A}|m\rangle^* = \langle m|\hat{A}^\dagger|m\rangle = \langle m|\hat{A}|m\rangle = a_m.$$

States corresponding to different eigenvalues are orthogonal. We assume the states are normalized so that $\langle m|n\rangle = \delta_{mn}$. To prove orthogonality we calculate

$$\langle m|\hat{A}|n\rangle = \langle m|a_n|n\rangle = a_n\langle m|n\rangle$$

and

$$\langle m|\hat{A}|n\rangle = \left(\langle m|\hat{A}\right)|n\rangle = \left(\hat{A}^\dagger|m\rangle\right)^\dagger|n\rangle = (a_m|m\rangle)^\dagger|n\rangle = a_m^*\langle m|n\rangle = a_m\langle m|n\rangle.$$

Thus

$$(a_m - a_n)\langle m|n\rangle = 0$$

so $\langle m|n\rangle = 0$ if $m \neq n$.

The eigenstates $|n\rangle$ of a Hermitian operator form a complete set. Therefore for an arbitrary ket $|\psi\rangle$

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle \tag{1.7}$$

where

$$\langle n|\psi\rangle = \langle n|\sum_{j=0}^{\infty} c_j|j\rangle = \sum_{j=0}^{\infty} c_j\langle n|j\rangle = \sum_{j=0}^{\infty} c_j\delta_{nj} = c_n.$$

Thus

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle = \sum_{n=0}^{\infty}\langle n|\psi\rangle|n\rangle = \sum_{n=0}^{\infty}|n\rangle\langle n|\psi\rangle = \left(\sum_{n=0}^{\infty}|n\rangle\langle n|\right)|\psi\rangle.$$

Since this is true for arbitrary $|\psi\rangle$ we can write the identity operator as

$$\hat{I} = \sum_{n=0}^{\infty}|n\rangle\langle n|. \tag{1.8}$$

A component of $|\psi\rangle$ can be found by operating with the projection operator $\hat{P}_n = |n\rangle\langle n|$. We have

$$\hat{P}_n|\psi\rangle = |n\rangle\langle n|\sum_{j=0}^{\infty} c_j|j\rangle = |n\rangle\sum_{j=0}^{\infty} c_j\langle n|j\rangle = |n\rangle\sum_{j=0}^{\infty} c_j\delta_{nj} = c_n|n\rangle. \tag{1.9}$$

The projection operator is idempotent:

$$(\hat{P}_n)^2 = \hat{P}_n\hat{P}_n = (|n\rangle\langle n|)(|n\rangle\langle n|) = |n\rangle(\langle n|n\rangle)\langle n| = |n\rangle\langle n| = \hat{P}_n. \tag{1.10}$$

The inner product of two states can be expressed in terms of the coefficients of their decomposition. We write $|\psi\rangle = \sum_n c_n|n\rangle$, $|\phi\rangle = \sum_n b_n|n\rangle$. Then

$$\langle\phi|\psi\rangle = \sum_m b_m^*\langle m|\sum_n c_n|n\rangle = \sum_m\sum_n b_m^* c_n\delta_{mn} = \sum_n b_n^* c_n. \tag{1.11}$$

The spectral representation of an operator is found from

$$\begin{aligned}\hat{A} &= \hat{I}\hat{A}\hat{I} = \left(\sum_m |m\rangle\langle m|\right)\hat{A}\left(\sum_n |n\rangle\langle n|\right) = \sum_m\sum_n |m\rangle\langle m|a_n|n\rangle\langle n| \\ &= \sum_m\sum_n a_n|m\rangle\delta_{mn}\langle n| = \sum_n a_n|n\rangle\langle n|.\end{aligned}$$

Thus

$$\hat{A} = \sum_n a_n|n\rangle\langle n|. \tag{1.12}$$

The representation (1.12) is diagonal since we have expressed $\hat{A}$ in a basis of the eigenvectors of $\hat{A}$. If we choose some other set of basis vectors $\{|m\rangle\}$ (not the eigenvectors of $\hat{A}$) then the representation will not be diagonal. Thus

$$\begin{aligned}\hat{A} &= \sum_n a_n|n\rangle\langle n| \\ &= \sum_n a_n\left(\sum_m |m\rangle\langle m|\right)|n\rangle\langle n|\left(\sum_{m'}|m'\rangle\langle m'|\right) \\ &= \sum_{n,m,m'} a_n|m\rangle c_{mn}c_{nm'}\langle m'| \\ &= \sum_{m,m'} u_{mm'}|m\rangle\langle m'|.\end{aligned}$$

where $c_{mn} = \langle m|n\rangle$ and $u_{mm'} = \sum_n a_n c_{mn} c_{nm'}$.

1.1.3 Degeneracy

Each eigenvalue a_α may be associated with a subspace of dimension $n_\alpha > 1$. The n_α degenerate eigenvectors can be orthonormalized to span the subspace. In this case we label the eigenvectors with an additional parameter r as $|\alpha, r\rangle$ where $r = 1, 2...n_\alpha$ and $\langle\beta, s|\alpha, r\rangle = \delta_{\alpha\beta}\delta_{rs}$. The eigenvalue relation is then

$$\hat{A}|\alpha, r\rangle = a_\alpha|\alpha, r\rangle \text{ for } r = 1, ...n_\alpha. \tag{1.13}$$

The identity operator can be written as

$$\hat{I} = \sum_{\alpha=0}^{\infty}\sum_{r=1}^{n_\alpha}|\alpha, r\rangle\langle\alpha, r|. \tag{1.14}$$

The spectral decomposition of the operator is

$$\hat{A} = \sum_{\alpha=0}^{\infty}\sum_{r=1}^{n_\alpha}a_\alpha|\alpha, r\rangle\langle\alpha, r|. \tag{1.15}$$

1.1.4 Continuous Basis

A Dirac ket $|\psi\rangle$ should be thought of as an abstract symbol for a quantum state. It is not tied to any particular representation. By taking inner products we can find a representation in terms of a discrete set of basis states as in Eq. (1.7). This can also be generalized to a continuous basis $|\xi\rangle$ using the orthogonality condition

$$\langle\xi'|\xi\rangle = \delta(\xi - \xi')$$

and the representation of the unit operator

$$\hat{I} = \int d\xi\, |\xi\rangle\langle\xi|.$$

An arbitrary state $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\int d\xi\, |\xi\rangle\langle\xi|\right)|\psi\rangle = \int d\xi\, \langle\xi||\psi\rangle|\xi\rangle = \int d\xi\, \psi(\xi)|\xi\rangle$$

where we have introduced the wavefunction $\psi(\xi) = \langle\xi|\psi\rangle$. The wavefunction $\psi(\xi)$ gives the amplitude of the decomposition of the state $|\psi\rangle$ into the basis ket $|\xi\rangle$.

Using a continuous basis we can calculate the matrix elements of operators as follows. Consider a general operator $\hat{A}(\hat{\xi}, \frac{\partial}{\partial\hat{\xi}})$ that is some function of $\hat{\xi}$ and $\frac{\partial}{\partial\hat{\xi}}$. For arbitrary states $|\psi\rangle, |\phi\rangle$ we have

$$\langle\phi|\hat{A}|\psi\rangle = \int d\xi'' d\xi' \langle\phi|\xi''\rangle\langle\xi''|\hat{A}(\hat{\xi}, \frac{\partial}{\partial\hat{\xi}})|\xi'\rangle\langle\xi'|\psi\rangle. \tag{1.16}$$

Now the matrix element in the middle of the last expression is

$$\langle\xi''|\hat{A}(\hat{\xi}, \frac{\partial}{\partial\hat{\xi}})|\xi'\rangle = \langle\xi''|A(\xi', \frac{\partial}{\partial\xi'})|\xi'\rangle \equiv \delta(\xi'' - \xi')A(\xi', \frac{\partial}{\partial\xi'}).$$

Thus (1.16) becomes

$$\begin{aligned}\langle\phi|\hat{A}|\psi\rangle &= \int d\xi'' d\xi'\, \langle\phi|\xi''\rangle\delta(\xi'' - \xi')A(\xi', \frac{\partial}{\partial\xi'})\langle\xi'|\psi\rangle \\ &= \int d\xi'\, \langle\phi|\xi'\rangle A(\xi', \frac{\partial}{\partial\xi'})\langle\xi'|\psi\rangle \\ &= \int d\xi\, \phi^*(\xi)A(\xi, \frac{\partial}{\partial\xi})\psi(\xi). \end{aligned} \tag{1.17}$$

Equation (1.17) gives the general formula for evaluating a matrix element in terms of an expansion in a continuous basis.

1.1.5 Representation of Derivatives

Given a ket $|\psi\rangle$ we can define another ket $|d\psi/d\xi\rangle$ whose representation is the derivative of the original one. This new ket is the result of transforming the original one with an operator and we write the transforming operator as $\frac{d}{d\hat{\xi}}$ so

$$\frac{d}{d\hat{\xi}}|\psi\rangle = |\frac{d\psi}{d\hat{\xi}}\rangle.$$

The matrix element of the differential operator is

$$\langle\phi|\frac{d}{d\hat{\xi}}|\psi\rangle = \int d\xi'\, \langle\phi|\frac{d}{d\hat{\xi}}|\xi'\rangle\langle\xi'|\psi\rangle = \int d\xi'\, \langle\phi|\frac{d}{d\hat{\xi}}|\xi'\rangle\psi(\xi') = \int d\xi'\, \phi^*(\xi')\frac{d\psi(\xi')}{d\xi'}. \tag{1.18}$$

Assuming the wavefunctions vanish at infinity an integration by parts gives

$$\int d\xi'\, \phi^*(\xi')\frac{d\psi(\xi')}{d\xi'} = -\int d\xi'\, \frac{d\phi^*(\xi')}{d\xi'}\psi(\xi'). \tag{1.19}$$

Comparing (1.18) and (1.19) we get

$$\langle\phi|\frac{d}{d\hat{\xi}}|\xi'\rangle = -\frac{d\phi^*(\xi')}{d\xi'} = -\langle\frac{d\phi}{d\hat{\xi}}|\xi'\rangle$$

so

$$\langle\phi|\frac{d}{d\hat{\xi}} = -\langle\frac{d\phi}{d\hat{\xi}}| \tag{1.20}$$

and $\left(d/d\hat{\xi}\right)^\dagger = -d/d\hat{\xi}$. Thus $\left(id/d\hat{\xi}\right)^\dagger = id/d\hat{\xi}$ and e.g. the momentum operator $-i\hbar d/d\hat{x}$ is a Hermitian operator.

If you find the steps from (1.18) - (1.20) unnecessarily complicated an alternative is to simply note that

$$\begin{aligned}
\langle\phi|\frac{d}{d\hat{\xi}}|\psi\rangle &= \langle\phi|\left(\frac{d}{d\hat{\xi}}|\psi\rangle\right)\\
&= \int d\xi\, \phi^*\frac{d\psi}{d\xi}\\
&= -\int d\xi\, \frac{d\phi^*}{d\xi}\psi\\
&= -\langle\frac{d\phi}{d\xi}|\psi\rangle\\
&= \left(\langle\phi|\frac{d}{d\hat{\xi}}\right)|\psi\rangle.
\end{aligned}$$

Thus

$$\langle\phi|\frac{d}{d\hat{\xi}} = -\langle\frac{d\phi}{d\hat{\xi}}|.$$

1.1.6 Position and momentum representations

We can use the above results for a continuous basis to find the relation between the position and momentum wavefunctions $\psi(x)$ and $\phi(p)$. Consider position and momentum eigenkets: $\hat{x}|x\rangle = x|x\rangle$ and $\hat{p}|p\rangle = p|p\rangle$. The matrix element of $\hat{p}$ between different basis kets is

$$\langle x|\hat{p}|p\rangle = \langle x|p|p\rangle = p\langle x|p\rangle.$$

Using the position representation of the momentum operator we can also write this as

$$\langle x|\hat{p}|p\rangle = \langle x|\left(-i\hbar\frac{\partial}{\partial\hat{x}}\right)|p\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle. \tag{1.21}$$

This follows also from the general expression for matrix elements Eq. (1.17) [1].

Comparing we see that

$$\frac{\partial}{\partial x}\langle x|p\rangle = \frac{ip}{\hbar}\langle x|p\rangle$$

which has solution

$$\langle x|p\rangle = Ne^{\imath px/\hbar}$$

with N a normalization constant.

We then observe that

$$\psi(x) = \langle x|\psi\rangle = \langle x|\left(\int dp\,|p\rangle\langle p|\right)|\psi\rangle = N\int dp\, e^{\imath px/\hbar}\psi(p)$$

and

$$\psi(p) = \langle p|\psi\rangle = \langle p|\left(\int dx\,|x\rangle\langle x|\right)|\psi\rangle = N^*\int dp\, e^{-\imath px/\hbar}\psi(x).$$

Requiring that $\int dx\,|\psi(x)|^2 = \int dp\,|\psi(p)|^2$ gives $|N|^2 = 1/h$. We choose N to be real and obtain

$$\begin{aligned}\psi(x) &= \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{\imath px/\hbar}\psi(p)\\ \psi(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int dx\, e^{-\imath px/\hbar}\psi(x),\end{aligned}$$

which demonstrates that $\psi(x)$ and $\psi(p)$ are related by a Fourier transform. For clarity we will sometimes write $\phi(p)$ instead of $\psi(p)$.

1.1.7 Commuting observables

If a state $|\psi\rangle$ is an eigenstate of two observables $\hat{A}$ and $\hat{B}$ with eigenvalues α and β then

$$\hat{A}\hat{B}|\psi\rangle = \alpha\beta|\psi\rangle = \beta\alpha|\psi\rangle = \hat{B}\hat{A}|\psi\rangle. \tag{1.22}$$

A necessary and sufficient condition for $\hat{A}$ and $\hat{B}$ to have a common complete set of eigenstates is that $\hat{A}$ and $\hat{B}$ commute:

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0. \tag{1.23}$$

The uncertainty (variance) of an operator is

$$\langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2. \tag{1.24}$$

[1] To see this use $|x\rangle = \int d\xi\,|\xi\rangle\langle\xi|x\rangle = \int d\xi\,\delta(\xi-x)|\xi\rangle$, so (1.17) gives $\langle x|\hat{p}|p\rangle = -i\hbar\langle x|\frac{\partial}{\partial\hat{x}}|p\rangle = -i\hbar\int d\xi\,\delta(\xi-x)\frac{\partial}{\partial\xi}\langle\xi|p\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle$.

The generalized uncertainty relation for two noncommuting observables is

$$(\Delta A)(\Delta B) \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle| \tag{1.25}$$

where $\Delta A = \sqrt{\langle(\Delta\hat{A})^2\rangle}$, $\Delta B = \sqrt{\langle(\Delta\hat{B})^2\rangle}$.

There are many ways to prove this, see for example the proof in Zettili p. 95 which invokes the Schwarz inequality. Here is an alternative approach. Define $\hat{A}' = \hat{A} - \langle\hat{A}\rangle$ so $\langle\hat{A}'\rangle = 0$,

$$\langle(\Delta\hat{A}')^2\rangle = \langle\hat{A}'^2\rangle = (\Delta A)^2$$

and similarly for $\hat{B}' = \hat{B} - \langle\hat{B}\rangle$. We note that $[\hat{A}', \hat{B}'] = [\hat{A}, \hat{B}]$.

Consider an arbitrary ket $|\psi\rangle$ and the quantity $(\hat{A}' + i\lambda\hat{B}')|\psi\rangle$ with λ real. The square of the norm is

$$\begin{aligned}
||(\hat{A}' + i\lambda\hat{B}')|\psi\rangle||^2 &= \langle\psi|(\hat{A}' - i\lambda\hat{B}')(\hat{A}' + i\lambda\hat{B}')|\psi\rangle \\
&= \langle\psi|\hat{A}'^2|\psi\rangle + \lambda^2\langle\psi|\hat{B}'^2|\psi\rangle + i\lambda\langle\psi|[\hat{A}', \hat{B}']|\psi\rangle \\
&= \lambda^2(\Delta B)^2 + i\lambda\langle\psi|[\hat{A}, \hat{B}]|\psi\rangle + (\Delta A)^2 \\
&\geq 0.
\end{aligned}$$

The last term is the commutator of two Hermitian operators which is anti-Hermitian (it has imaginary eigenvalues), so i times the commutator is a Hermitian operator. The above expression is therefore a quadratic function of λ with real coefficients, and is therefore strictly real. It is non-negative for all values of λ, and therefore must not have two different real roots, since if that were the case the expression would have to change sign and be somewhere negative. For this to be so the discriminant must be negative or zero which corresponds to

$$(\Delta A)(\Delta B) \geq \frac{1}{2}|\langle\psi|[\hat{A}, \hat{B}]|\psi\rangle|.$$

Since this is true for any $|\psi\rangle$ we can write

$$(\Delta A)(\Delta B) \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle|$$

as desired.

As an example of application of the commutation relation (1.25) consider $\hat{x}$ and $\hat{p}$. Their commutator can be evaluated in the position representation as

$$\begin{aligned}
\langle\psi|[\hat{x}, \hat{p}]|\psi\rangle &= \langle\psi|(\hat{x}\hat{p} - \hat{p}\hat{x})|\psi\rangle \\
&= -i\hbar\int dx\,\psi^*\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)\psi \\
&= -i\hbar\int dx\,\psi^*\left(x\frac{\partial\psi}{\partial x} - \psi - x\frac{\partial\psi}{\partial x}\right) \\
&= i\hbar\int dx\,\psi^*\psi \\
&= \langle\psi|i\hbar|\psi\rangle.
\end{aligned}$$

Since $|\psi\rangle$ is an arbitrary ket we have $[\hat{x}, \hat{p}] = i\hbar$ and using (1.25)

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2}$$

which is the usual position-momentum form of the uncertainty relation.

1.1.8 Measurements

An arbitrary state is $|\psi\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$. The result of a measurement of the observable A is

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \sum_m c_m^* \langle m | \hat{A} \sum_n c_n |n\rangle = \sum_m \sum_n c_m^* c_n a_n \langle m|n\rangle = \sum_n |c_n|^2 a_n. \tag{1.26}$$

The probability of the measurement result being the eigenvalue a_n is

$$P(a_n) = |c_n|^2 = |\langle n|\psi\rangle|^2 = ||\hat{P}_n|\psi\rangle||^2 = \langle \psi|\hat{P}_n|\psi\rangle. \tag{1.27}$$

After $\hat{A}$ has been measured and given the result a_n the new state of the system is

$$|\psi'\rangle = \frac{\hat{P}_n|\psi\rangle}{||\hat{P}_n|\psi\rangle||} = \frac{c_n}{|c_n|}|n\rangle. \tag{1.28}$$

A subsequent measurement of $\langle \hat{A} \rangle$ will return a_n with unit probability.

1.1.9 Evolution in time

Time evolution is governed by the Hamiltonian $\hat{H}$ and

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. \tag{1.29}$$

For a particle of mass m in the coordinate representation $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$ and we get the Schrödinger equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r})\psi(\mathbf{r}, t). \tag{1.30}$$

The formal solution for time evolution is

$$|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle$$

where the time evolution operator is

$$\hat{U}(t, t_0) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \hat{H}(t')\right]_+ \tag{1.31}$$

and $[....]_+$ indicates time ordering of operator products: $\left[\hat{A}(t_1)...\hat{A}(t_n)\right]_+ = \hat{A}(t_1)...\hat{A}(t_n)$ when $t_1 \geq t2 \geq ... \geq t_n$.

When $\hat{H}$ is not explicitly time dependent this simplifies to

$$\hat{U}(t,t_0) = \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right]. \tag{1.32}$$

The time evolution operator is unitary which means $\hat{U}^\dagger = \hat{U}^{-1}$ so

$$\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{I}. \tag{1.33}$$

The time evolution of an initial state $|\psi(t_0)\rangle$ can be determined explicitly by expanding in energy eigenfunctions $\hat{H}|n\rangle = E_n|n\rangle$. Assume the initial state

$$|\psi(t_0)\rangle = \sum_n \langle n|\psi(t_0)\rangle|n\rangle = \sum_n c_{n0}|n\rangle$$

and the time dependent state

$$|\psi(t)\rangle = \sum_n \langle n|\psi(t)\rangle|n\rangle = \sum_n c_n(t)|n\rangle.$$

Plugging in to the Schrödinger equation gives

$$i\hbar\sum_n \frac{dc_n}{dt}|n\rangle = \sum_n \hat{H}c_n|n\rangle = \sum_n E_n c_n|n\rangle.$$

Projecting out the $m^{\rm th}$ component by operating on both sides with $\langle m|$ gives

$$i\hbar\frac{dc_m}{dt} = E_m c_m$$

which is solved by

$$c_m(t) = c_{m0}e^{-\imath E_m(t-t_0)/\hbar}.$$

Thus

$$|\psi(t)\rangle = \sum_n c_n(t)|n\rangle = \sum_n c_{n0}e^{-\imath E_n(t-t_0)/\hbar}|n\rangle.$$

1.1.10 Schrödinger and Heisenberg pictures

There are several different ways of working with time evolution.

In the Schrödinger picture the state $|\psi(t)\rangle_S$ is a function of time while all observables $\hat{A}_S$ are constant. The state vector evolves according to the Schrödinger equation $i\hbar\frac{d|\psi\rangle_S}{dt} = \hat{H}_S|\psi\rangle_S$ and the expectation value of an operator at time t is

$$\begin{aligned} a(t) &= \langle\hat{A}_S\rangle \\ &= {}_S\langle\psi(t)|\hat{A}_S|\psi(t)\rangle_S. \end{aligned}$$

Here the subscripts S refer to the Schrödinger picture.

We can cast this in a different form as follows. The expectation value of an operator at time t is

$$\begin{aligned} a(t) &= \langle \hat{A}_S \rangle \\ &= {}_S\langle \psi(t)|\hat{A}_S|\psi(t)\rangle_S \\ &= \langle \psi(0)|\hat{U}^\dagger(t)\hat{A}_S\hat{U}(t)|\psi(0)\rangle. \end{aligned}$$

We can define a time dependent operator by $\hat{A}_H = \hat{U}^\dagger(t)\hat{A}_S\hat{U}(t)$, and time independent states by $|\psi\rangle_H = |\psi(0)\rangle$ such that

$$a(t) = {}_H\langle \psi|\hat{A}_H|\psi\rangle_H.$$

This is the Heisenberg picture in which the kets are stationary but the operators evolve in time. The equation of motion for the operator is found from

$$\begin{aligned} \frac{d\hat{A}_H(t)}{dt} &= \frac{d}{dt}\left(\hat{U}^\dagger(t)\hat{A}_S\hat{U}(t)\right) + \frac{\partial \hat{A}_H}{\partial t} \\ &= \frac{d\hat{U}^\dagger(t)}{dt}\hat{A}_S\hat{U}(t) + \hat{U}^\dagger(t)\hat{A}_S\frac{d\hat{U}(t)}{dt} + \frac{\partial \hat{A}_H}{\partial t} \\ &= \left(\frac{i}{\hbar}\hat{U}^\dagger\hat{H}\right)\hat{A}_S\hat{U}(t) + \hat{U}^\dagger(t)\hat{A}_S\left(\frac{-i}{\hbar}\hat{H}\hat{U}(t)\right) + \frac{\partial \hat{A}_H}{\partial t} \\ &= \frac{i}{\hbar}[\hat{H}, \hat{A}_H] + \frac{\partial \hat{A}_H}{\partial t} \end{aligned}$$

where the last lines follows from $[\hat{U}, \hat{H}] = 0$, and for completeness we have included the possibility of an explicit time dependence (not due to $\hat{U}(t)$) in $\hat{A}_H$. Thus

$$\frac{d\hat{A}_H}{dt} = -\frac{i}{\hbar}[\hat{A}_H, \hat{H}] + \frac{\partial \hat{A}_H}{\partial t}, \tag{1.34}$$

which is referred to as the Heisenberg equation (although it was first written down by Dirac). This equation is usually more difficult to solve than the Schrödinger equation. However, it provides a clear picture of the correspondence between quantum and classical mechanics.

1.1.11 Quantum - Classical correspondence and Ehrenfest's theorem

In classical mechanics we can describe a dynamical system by coordinates q_j and momenta p_j. The Hamiltonian of the system is a function $H(q_j, p_j)$ of the coordinates and momenta which satisfy Hamilton's equations

$$\frac{\partial q_j}{\partial t} = \frac{\partial H}{\partial p_j}, \qquad \frac{\partial p_j}{\partial t} = -\frac{\partial H}{\partial q_j}.$$

For a particle in a potential $V(\mathbf{r})$, $H = \mathbf{p}^2/2m + V(\mathbf{r})$ so Hamilton's equations give $d\mathbf{r}/dt = \mathbf{p}/m$ and $d\mathbf{p}/dt = -\nabla V(\mathbf{r})$.

For any two dynamical quantities A, B we define the Poisson bracket $\{A, B\}$ by

$$\{A,B\} = \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} \right).$$

Clearly $\{A, B\} = -\{B, A\}$.

The time derivative of the quantity A is

$$\begin{aligned} \frac{dA}{dt} &= \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial q_j}{\partial t} + \frac{\partial A}{\partial p_j}\frac{\partial p_j}{\partial t} \right) + \frac{\partial A}{\partial t} \\ &= \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial H}{\partial q_j} \right) + \frac{\partial A}{\partial t} \\ &= \{A, H\} + \frac{\partial A}{\partial t}. \end{aligned} \tag{1.35}$$

The similarity between the quantum equation (1.34) and the classical equation (1.35) is remarkable. We see that the quantum equation of motion for the operator $\hat{A}$ can be found by writing down the classical equation for the dynamical variable A in terms of Poisson brackets and making the substitution

$$\{A, H\} \to -\frac{i}{\hbar}[\hat{A}_H, \hat{H}]. \tag{1.36}$$

Alternatively, we may think of quantum mechanics as the more fundamental theorem which classical mechanics is an approximation to. In the limit of $\hbar \to 0$ the transformation

$$-\frac{i}{\hbar}[\hat{A}_H, \hat{H}] \to \{A, H\} \tag{1.37}$$

reveals the limiting classical equation of motion. Note that while (1.36) should always lead to a valid quantum equation, the substitution (1.37) may be meaningless since there are quantum problems for which no classical analog exists. A prime example is the spin of an electron.

Finally, we note that the time evolution of the expectation value of a quantum variable has a close analogy with the time evolution of the corresponding classical quantity. This analogy is already apparent in equations (1.34,1.35), which when written in terms of expectation values is referred to as Ehrenfest's theorem.

To see this note that for any differentiable operator function $\hat{F} = F(\hat{q}_j, \hat{p}_j)$ we have the following commutators

$$[\hat{q}_j, \hat{F}] = i\hbar \frac{\partial \hat{F}}{\partial \hat{p}_j}, \qquad [\hat{p}_j, \hat{F}] = -i\hbar \frac{\partial \hat{F}}{\partial \hat{q}_j}.$$

From (1.34)with $\hat{F} = \hat{H}$ we obtain

$$\frac{d}{dt}\langle \hat{q}_j \rangle = \left\langle \frac{\partial \hat{H}}{\partial \hat{p}_j} \right\rangle, \qquad \frac{d}{dt}\langle \hat{p}_j \rangle = -\left\langle \frac{\partial \hat{H}}{\partial \hat{q}_j} \right\rangle.$$

Thus for a particle in potential $V(\hat{\mathbf{r}})$ with $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}})$ we get

$$\frac{d}{dt}\langle\hat{\mathbf{r}}\rangle = \frac{\langle\hat{\mathbf{p}}\rangle}{m}, \qquad \frac{d}{dt}\langle\hat{\mathbf{p}}\rangle = -\langle\nabla V(\hat{\mathbf{r}})\rangle. \tag{1.38}$$

The first of Eqs. (1.38) is identical to the corresponding classical equation obtained by putting $\langle\hat{\mathbf{r}}\rangle \to \mathbf{r}$, $\langle\hat{\mathbf{p}}\rangle \to \mathbf{p}$. However, the second equation differs from the corresponding classical equation since, in general,

$$\langle\nabla V(\hat{\mathbf{r}})\rangle \neq \nabla V(\mathbf{r})|_{\mathbf{r}=\langle\hat{\mathbf{r}}\rangle}.$$

The difference betweens these two expressions is negligible provided the potential is close to constant over the extent of the deBroglie wave packet of the particle. This condition must be satisfied for the evolution of the expectation values of the quantum variables to agree with the results of a classical description.

1.2 Principles of quantum mechanics

We can summarize the formalism given above in a small set of principles.

1. A physical system is associated with a Hilbert space $\mathcal{E}_{\mathrm{H}}$ containing ket vectors. At time t the physical state is completely described by a ket $|\psi(t)\rangle$ residing in $\mathcal{E}_{\mathrm{H}}$.

2. Any physical quantity A is associated with a Hermitian operator $\hat{A}$ that acts on kets in $\mathcal{E}_{\mathrm{H}}$. The result of a measurement of A is always one of the eigenvalues a_n of $\hat{A}$. The probability of measuring a_n is $P(a_n) = ||\hat{P}_n|\psi\rangle||^2$ where $\hat{P}_n = |n\rangle\langle n|$ is the projector onto the ket $|n\rangle$. After the measurement the system will be in the new state $|\psi'\rangle = \frac{\hat{P}_n|\psi\rangle}{||\hat{P}_n|\psi\rangle||}$.

3. Time evolution is governed by the Hamiltonian according to $i\hbar\frac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle$.

How to translate these simple rules into explicit procedures is often far from obvious, and learning how to do so constitutes a course in Quantum Mechanics.