
Phys 434

QUANTUM PHYSICS 3

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1 Review

1.1 Discrete Spectrum

States in quantum mechanics are vectors in Hilbert space \mathcal{H} . In Dirac notation, states are denoted as *kets* $|\psi\rangle$. Observables in quantum mechanics are operators $A : \mathcal{H} \rightarrow \mathcal{H}$ such that $|\psi\rangle \mapsto A|\psi\rangle$. Every operator A has a set of eigenkets $\{|a'\rangle\}$,

$$A|a'\rangle = a'|a'\rangle$$

The eigenvalue corresponding to the eigenket $|a'\rangle$ is denoted $a' \in \mathbb{R}$. The dual Hilbert space will be called the bra space and elements of the bra space will be denoted with a ket space $\langle\varphi|$.

We will denote the *inner product* (scalar product) to be $\langle\varphi|\psi\rangle$. By definition,

$$\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$$

$$\langle\psi|\psi\rangle = \|\psi\|^2 \geq 0$$

Every state in the Hilbert space can be normalized,

$$|\tilde{\psi}\rangle = \frac{1}{\sqrt{\langle\psi|\psi\rangle}}|\psi\rangle$$

In doing so, we have,

$$\langle\tilde{\psi}|\tilde{\psi}\rangle = \frac{\langle\psi|\psi\rangle}{\langle\psi|\psi\rangle} = 1$$

Evidently, if we have that $\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle$, then $\langle\varphi|\psi\rangle$ must be real. A bra $\langle\varphi|$ and ket $|\psi\rangle$ are said to be *orthogonal* if $\langle\varphi|\psi\rangle = 0$.

The dual of $A|\psi\rangle$ is $\langle\psi|A^\dagger$. Where A^\dagger is the Hermitian conjugate (adjoint) of A . We can act on the ket $A|\psi\rangle$ with the bra $\langle\varphi|$ and obtain,

$$\langle\varphi|A|\psi\rangle = \langle\psi|A^\dagger|\varphi\rangle^*$$

The operator A is *Hermitian* if and only if $A = A^\dagger$.

If A is a Hermitian operator, then A 's eigenvalues and eigenkets have particularly nice properties. Let $(a', |a'\rangle)$ and $(a'', |a''\rangle)$ be two eigen-pairs.

$$A|a'\rangle = a'|a'\rangle \tag{1.1}$$

$$A|a''\rangle = a''|a''\rangle \tag{1.2}$$

Let $\langle\varphi|$ be an arbitrary bra. By eq. (1.2) we have that,

$$\langle\varphi|A|a''\rangle = a''\langle\varphi|a''\rangle$$

The adjoint to this equation yields,

$$\langle a''|A|\varphi\rangle^* = a''\langle a''|\varphi\rangle^*$$

Conjugating each term,

$$\langle a''|A|\varphi\rangle = a''^*\langle a''|\varphi\rangle \tag{1.3}$$

Since eq. (1.3) is true for an arbitrary $\langle\varphi|$, it must be that

$$\langle a''|A = a''^*\langle a''| \tag{1.4}$$

Combining eqs. (1.4) and (1.1), and recognizing that A is Hermitian,

$$\underbrace{\langle a''|A|a'\rangle - \langle a''|A^\dagger|a'\rangle}_0 = a'\langle a''|a'\rangle = a''^*\langle a''|a'\rangle$$

Therefore,

$$(a' - a''^*)\langle a''|a'\rangle = 0 \quad (1.5)$$

As an example, we can chose $|a''\rangle = |a'\rangle$ to see that

$$(a' - a'^*)\langle a'|a'\rangle = 0 \implies a' = a'^*$$

Therefore all eigenvalues of Hermitian operators are always real. Since the spectrum of an operator represents all physical observables, this observation is in agreement with the fact that all physical quantities are real-valued.

Moreover returning to eq. (1.5) we can consider $|a'\rangle$ and $|a''\rangle$ to be different eigenkets that are non-degenerate (their eigenvalues differ). Then be eq. (1.5),

$$\langle a''|a'\rangle = 0$$

Therefore eigenkets of Hermitian operators are orthogonal (or can at least be orthogonalized). Since the norm of an eigenket is arbitrary, we will hence forth assert that all eigenkets are normalized. Each of these properties can be summarized with a Kronecker delta.

$$\langle a|a'\rangle = \delta_{a,a'} \quad (1.6)$$

In summary, the set of eigenkets of any Hermitian operator forms a complete orthonormal set of states. Effectively, the set of eigenkets form a basis for the Hilbert space. Consequently, we can write any ket $|\psi\rangle$ in terms of the eigenkets for any Hermitian operator A

$$|\psi\rangle = \sum_{a'} C_{a'} |a'\rangle \quad (1.7)$$

Where $C_{a'} \in \mathbb{C}$ are uniquely defined through acting with the dual eigenket $\langle a''|$,

$$\langle a''|\psi\rangle = \sum_{a'} C_{a'} \langle a''|a'\rangle = \sum_{a'} C_{a'} \delta_{a'',a'} = C_{a''} \implies C_{a'} = \langle a'|\psi\rangle \quad (1.8)$$

Physically, the coefficient $C_{a'}$ is called a *probability amplitude*. When a given system is in state $|\psi\rangle$, the probability of measuring the value a' when making the observation or measurement A is given by the square modulus of $C_{a'}$,

$$P_A(a') = |\langle a'|\psi\rangle|^2$$

We now have the luxury of re-writing eq. (1.7) as a spectral decomposition,

$$|\psi\rangle = \sum_{a'} |a'\rangle \langle a'|\psi\rangle \quad (1.9)$$

Since $|\psi\rangle$ is *arbitrary*, we obtain a closure relation (otherwise known as the resolution of identity).

$$\sum_{a'} |a'\rangle \langle a'| = \mathbb{I} \quad (1.10)$$

We define the projection operator $\Lambda_{a'} = |a'\rangle \langle a'|$.

$$\Lambda_{a''} |\psi\rangle = |a''\rangle \langle a''|\psi\rangle = \sum_{a'} |a'\rangle \underbrace{\langle a'|a''\rangle}_{\delta_{a',a''}} \langle a''|\psi\rangle = \langle a''|\psi\rangle |a''\rangle$$

As such, Λ_a *projects* $|\psi\rangle$ into the direction of $|a\rangle$. Using the closure operation eq. (1.10) and the spectral decomposition of a ket eq. (1.9) one can recover the spectral decomposition of an operator A . For each eigenket $|a'\rangle$, multiply eq. (1.1) by $\langle a'|$,

$$A|a'\rangle \langle a'| = a'|a'\rangle \langle a'|$$

And summing over all eigenkets,

$$A = \sum_{a'} a' |a'\rangle \langle a'|$$

Additionally consider another operator B ,

$$B = \mathbb{I} \cdot B \cdot \mathbb{I} = \sum_{a', a''} |a''\rangle \langle a''| B |a'\rangle \langle a'|$$

Where $\langle a''|B|a'\rangle$ can be interpreted as a matrix indexed by $|a''\rangle$ and $|a'\rangle$,

$$\langle a''|B|a'\rangle = B_{a'', a'}$$

Where refer to $B_{a'', a'}$ as the matrix elements of an operator B with respect to the a complete orthonormal set of eigenstates of a Hermitian operator A . The entries in $B_{a'', a'}$ have the following property,

$$\langle a''|B|a'\rangle = \langle a'|B^\dagger|a''\rangle^*$$

Therefore the matrix that corresponds to B^\dagger is the complex conjugate transposed of the matrix corresponding to B .

1.2 Continuous Spectrum

Of course, there exists operators with non-discrete spectrum. We will now generalize to operators with continuous spectrum. The two most important of such operators are position and momentum. Let $|\vec{x}'\rangle$ a position eigenket corresponding to the state of a particle at position \vec{x}' in space. Let \vec{x} be the position operator defined as,

$$\vec{x}|\vec{x}'\rangle = \vec{x}'|\vec{x}'\rangle$$

It is important not to get confused about notation:

- \vec{x} – Position operator
- \vec{x}' – Position eigenket

The wave function $\psi(\vec{x}')$ is the probability amplitude to find a particle in a state $|\psi\rangle$ at position \vec{x}' and is defined as,

$$\langle \vec{x}'|\psi\rangle = \psi(\vec{x}')$$

We also have the ability to generalize eq. (1.6) to a continuous spectrum. The continuous generalization of the Kronecker delta is the Dirac delta function.

$$\langle \vec{x}'|\vec{x}''\rangle = \delta(\vec{x}' - \vec{x}'')$$

Where $\delta\vec{x}'$ is defined as,

$$\int_{\mathbb{R}^3} d^3x' f(\vec{x}') \delta(\vec{x}') = f(\vec{0})$$

Where $f(\vec{x}') : \mathbb{R}^3 \rightarrow \mathbb{R}$ is a function on \mathbb{R}^3 .

The closure relation becomes,

$$\mathbb{I} = \int_{\mathbb{R}^3} d^3x' |\vec{x}'\rangle \langle \vec{x}'|$$

Therefore we have that,

$$|\psi\rangle = \mathbb{I} \cdot |\psi\rangle = \int_{\mathbb{R}^3} d^3x' |\vec{x}'\rangle \langle \vec{x}'|\psi\rangle$$

Now let $|\phi\rangle$ be another space in the same Hilbert space as $|\psi\rangle$,

$$\begin{aligned}\langle\phi|\psi\rangle &= \int_{\mathbb{R}^3} d^3x' \langle\phi|\vec{x}'\rangle \langle\vec{x}'|\psi\rangle \\ &= \int_{\mathbb{R}^3} d^3x' \langle\vec{x}'|\phi\rangle^* \langle\vec{x}'|\psi\rangle \\ &= \int_{\mathbb{R}^3} d^3x' \phi(\vec{x}')^* \psi(\vec{x}')\end{aligned}$$

1.3 Infinitesimal Translations

The operator of infinitesimal translations T is defined as,

$$T(d\vec{x}')|\vec{x}'\rangle = |\vec{x}' + d\vec{x}'\rangle$$

Where $d\vec{x}'$ is an infinitesimally small vector. Acting on an arbitrary state $|\psi\rangle$,

$$\begin{aligned}T(d\vec{x}')|\psi\rangle &= T(d\vec{x}') \left\{ \int_{\mathbb{R}^3} d^3x' |\vec{x}'\rangle \langle\vec{x}'|\psi\rangle \right\} \\ &= \int_{\mathbb{R}^3} d^3x' |\vec{x}' + d\vec{x}'\rangle \langle\vec{x}'|\psi\rangle \\ &= \int_{\mathbb{R}^3} d^3x' |\vec{x}'\rangle \langle\vec{x}' - d\vec{x}'|\psi\rangle \quad \vec{x}' \mapsto \vec{x}' - d\vec{x}'\end{aligned}$$

Next without loss of generality, let $|\psi\rangle$ be normalized $\langle\psi|\psi\rangle = 1$. Moreover, we may let $T(d\vec{x}')|\psi\rangle$ be normalized as well.

$$\langle\psi|T^\dagger(d\vec{x}')T(d\vec{x}')|\psi\rangle \quad (1.11)$$

If we wish for eq. (1.11) to hold for all states $|\psi\rangle$, it must be that $T(d\vec{x}')$ is *unitary*.

$$T^\dagger(d\vec{x}')T(d\vec{x}') = \mathbb{I} \implies T^\dagger(d\vec{x}') = T^{-1}(d\vec{x}') \quad (1.12)$$

Another desired property of translations $T(d\vec{x}')$ is that they are additive,

$$T(d\vec{x}')T(d\vec{x}'') = T(d\vec{x}' + d\vec{x}'') \quad (1.13)$$

Consequently,

$$T^{-1}(d\vec{x}') = T(-d\vec{x}') \quad T(\vec{0}) = \mathbb{I}$$

All of the above properties are satisfied if,

$$T(d\vec{x}') = \mathbb{I} - i\vec{K} \cdot d\vec{x}'$$

Where $\vec{K} = (K_x, K_y, K_z)$ is a vector operator that is Hermitian ($\vec{K}^\dagger = \vec{K}$) to be determined. First we demonstrate that such a $T(d\vec{x}')$ is unitary (eq. (1.12)),

$$\begin{aligned}T^\dagger(d\vec{x}')T(d\vec{x}') &= \left(\mathbb{I} + i\vec{K}^\dagger \cdot d\vec{x}'\right) \left(\mathbb{I} - i\vec{K} \cdot d\vec{x}'\right) \\ &= \mathbb{I} + \underbrace{i\vec{K}^\dagger \cdot d\vec{x}' - i\vec{K} \cdot d\vec{x}'}_0 + \mathcal{O}(|d\vec{x}'|^2) \xrightarrow{0} \\ &= \mathbb{I}\end{aligned}$$

Next we demonstrate additivity (eq. (1.13)),

$$T(d\vec{x}'')T(d\vec{x}') = \left(\mathbb{I} - i\vec{K} \cdot d\vec{x}''\right) \left(\mathbb{I} - i\vec{K} \cdot d\vec{x}'\right)$$

$$\begin{aligned}
&= \mathbb{I} - i\vec{K} \cdot d\vec{x}'' - i\vec{K} \cdot d\vec{x}' + \mathcal{O}(|d\vec{x}'|^2) \rightarrow 0 \\
&= \mathbb{I} - i\vec{K} \cdot (d\vec{x}'' + d\vec{x}') \\
&= T(d\vec{x}'' + d\vec{x}')
\end{aligned}$$

In order to illuminate the specific form of \vec{K} , we calculate the commutator $[\vec{x}, T(d\vec{x}')] ,$

$$\begin{aligned}
[\vec{x}, T(d\vec{x}')] &= [\vec{x}, \mathbb{I} - i\vec{K} \cdot d\vec{x}'] \\
&= -i\vec{x}\vec{K}d\vec{x}' + i\vec{K}d\vec{x}'\vec{x}
\end{aligned}$$

Choose $d\vec{x}' = dx'\hat{x}_j$ and $\vec{K} \cdot \hat{x}_j = K_j$ where \hat{x}_j is the unit vector in the direction of one of the basis vectors.

$$[\vec{x}, T(d\vec{x}')] = -i\vec{x}\vec{K}d\vec{x}' + i\vec{K}d\vec{x}'\vec{x}$$

Moreover $[X_i, K_j] = 0$ whenever $i \neq j$.

$$-ix_jK_j + iK_jx_j = 1 \implies -i[x_j, K_j] = 1 \implies [x_j, K_j] = i$$

Therefore,

$$[x_i, K_j] = i\delta_{ij} \implies \vec{K} = \frac{1}{\hbar}\vec{p}$$

Where \vec{p} is the generator of infinitesimal translations,

$$[x_i, p_j] = i\hbar\delta_{ij}$$

Such that,

$$T(d\vec{x}') = 1 - \frac{i}{\hbar}\vec{p} \cdot d\vec{x}'$$

1.4 Transformations Between Position and Momentum Representations

Calculate for a 1D system,

$$\begin{aligned}
T(\Delta x')|\psi\rangle &= \left(1 - \frac{i}{\hbar}p\Delta x'\right)|\psi\rangle \\
&= \int_{\mathbb{R}} dx' \left(1 - \frac{i}{\hbar}p\Delta x'\right)|x'\rangle\langle x'|\psi\rangle \\
&= \int_{\mathbb{R}} dx' T(\Delta x')|x'\rangle\langle x'|\psi\rangle \\
&= \int_{\mathbb{R}} dx' |x' + \Delta x'\rangle\langle x'|\psi\rangle \\
&= \int_{\mathbb{R}} dx' |x'\rangle\langle x' - \Delta x'|\psi\rangle
\end{aligned}$$

Examine $\langle x' - \Delta x'|\psi\rangle$,

$$\langle x' - \Delta x'|\psi\rangle \approx \langle x'|\psi\rangle - \Delta x' \frac{\partial}{\partial x'} \langle x'|\psi\rangle$$

Therefore,

$$\begin{aligned}
T(\Delta x')|\psi\rangle &= \int_{\mathbb{R}} dx' |x'\rangle \left[\langle x'|\psi\rangle - \Delta x' \frac{\partial}{\partial x'} \langle x'|\psi\rangle \right] \\
&= |\psi\rangle - \Delta x' \int_{\mathbb{R}} dx' |x'\rangle \left[\frac{\partial}{\partial x'} \langle x'|\psi\rangle \right]
\end{aligned}$$

Which in turn implies that,

$$p|\psi\rangle = \int_{\mathbb{R}} dx' |x'\rangle \left(-i\hbar \frac{\partial}{\partial x'} \right) \langle x'|\psi\rangle$$

Since a given ket $|\psi\rangle$ can be written in *any* basis or representation, we can transform $|\psi\rangle$ in the momentum basis. Recall the momentum eigenkets form a complete orthonormal set of states,

$$\vec{p}|\vec{p}'\rangle = \vec{p}'|\vec{p}'\rangle \quad \langle \vec{p}'|\vec{p}''\rangle = \delta(\vec{p}' - \vec{p}'')$$

Moreover we have the resolution of identity,

$$\mathbb{I} = \int d^3p' |\vec{p}'\rangle \langle \vec{p}'|$$

Therefore we have that,

$$|\psi\rangle = \mathbb{I} \cdot |\psi\rangle = \int d^3p' |\vec{p}'\rangle \langle \vec{p}'|\psi\rangle$$

So we define the wavefunction in momentum representation $\langle \vec{p}'|\psi\rangle = \psi(\vec{p}')$. We will now discover how to transform from $\psi(\vec{p}')$ to $\psi(\vec{x}')$ in 1D. By definition we have that,

$$\langle x'|p|\psi\rangle = -i\hbar \frac{\partial}{\partial x'} \langle x'|\psi\rangle$$

We now choose $|\psi\rangle = |p'\rangle$,

$$\langle x'|p|p'\rangle = -i\hbar \frac{\partial}{\partial x'} \langle x'|p'\rangle$$

But $|p'\rangle$ is an eigenket of p ,

$$p'\langle x'|p'\rangle = -i\hbar \frac{\partial}{\partial x'} \langle x'|p'\rangle$$

Therefore we have a differential equation for $f(x') = \langle x'|p'\rangle$,

$$p'f(x') = -i\hbar \frac{\partial f}{\partial x'} \tag{1.14}$$

Which has the well known solution,

$$f(x') = \langle x'|p'\rangle = Ne^{\frac{i}{\hbar}p'x'} \tag{1.15}$$

Where N is an arbitrary constant. To confirm eq. (1.14) check $\frac{\partial f}{\partial x'}$

$$\frac{\partial f}{\partial x'} = N \frac{i}{\hbar} p' e^{\frac{i}{\hbar}p'x'} = \frac{i}{\hbar} p' f(x')$$

As a quick trick notice that,

$$\langle x'|x''\rangle = \delta(x' - x'') = \langle x'|\mathbb{I}|x''\rangle = \int dp' \langle x'|p'\rangle \langle p'|x''\rangle$$

Substitute in eq. (1.15),

$$\delta(x' - x'') = N^2 \int dp' e^{\frac{i}{\hbar}p'x'} e^{-\frac{i}{\hbar}p'x''} = N^2 \int dp' e^{\frac{i}{\hbar}p'(x' - x'')} \tag{1.16}$$

Recall a integral representation of the Dirac-delta function,

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk = \delta(x) \tag{1.17}$$

Comparing eqs. (1.16) and (1.17) (and using $\mu_0 \pi a^2 n \dot{I}_s$) we have that,

$$N^2 = \frac{1}{2\pi\hbar} \implies N = \frac{1}{\sqrt{2\pi\hbar}}$$

This we have that,

$$\langle x' | p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p' x'} \quad (1.18)$$

Which refers to the usual plane wave wavefunction. Alternatively, one can obtain this result from the Schrödinger Equation $H\psi = E\psi$ and using a free Hamiltonian $H = \frac{p^2}{2m} = -\frac{\hbar^2 d^2}{2mdx^2}$. Generalizing eq. (1.18) to more than one dimension gives (say 3 dimensions),

$$\langle \vec{x}' | \vec{p}' \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar} \vec{p}' \cdot \vec{x}'}$$

This result allows us to convert from the momentum representation $\psi(\vec{p}')$ to the position representation $\psi(\vec{x}')$ and backward,

$$\begin{aligned} \langle x' | \psi \rangle &= \int dp' \langle x' | p' \rangle \langle p' | \psi \rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int dp' e^{\frac{i}{\hbar} p' x'} \langle p' | \psi \rangle \end{aligned}$$

Analogously we can rotate state space to give,

$$\langle p' | \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dx' e^{-\frac{i}{\hbar} p' x'} \langle x' | \psi \rangle$$

Which is nothing more than the **(Inverse) Fourier Transform**.

1.5 Time Dependence of Kets

Let $|\psi, t_0; t\rangle$ be the state which is $|\psi, t_0\rangle \equiv |\psi\rangle$ at time t_0 which becomes a different state $|\psi, t_0; t\rangle$ at a later time $t > t_0$. Of course, there must exist an operator that transforms initial states $|\psi, t_0\rangle$ into final state $|\psi, t_0; t\rangle$. Let $U(t, t_0)$ be this unknown operator,

$$|\psi, t_0; t\rangle = U(t, t_0) |\psi, t_0\rangle$$

Which we will now discover. To do so, we will demand some properties of $U(t, t_0)$. Consider some physical quantity with corresponding operator A with eigenkets $|a'\rangle$ and eigenvalues a' . Then we can write $|\psi, t_0\rangle$ in terms of the orthonormal set of states defined by $\{|a'\rangle\}$ ¹,

$$|\psi, t_0\rangle = \sum_{a'} C_{a'}(t_0) |a'\rangle$$

Analogously at time t ,

$$|\psi, t_0; t\rangle = \sum_{a'} C_{a'}(t) |a'\rangle$$

The coefficients $C_{a'}$ are determined by eq. (1.8),

$$\langle \psi, t_0 | \psi, t_0 \rangle = \sum_{a', a''} C_{a'}^*(t_0) C_{a''}(t_0) \underbrace{\langle a' | a'' \rangle}_{\delta_{a', a''}}$$

¹We will also assign all of the time evolution to the coefficients $C_{a'} = C_{a'}(t_0)$

Notice that normalization dictates that $\sum_{a'} |C_{a'}(t_0)|^2 = 1$. Therefore we can interpret $|C_{a'}(t_0)|$ as the probability that a measurement of a physical system A gives a' . Analogously at later times t ,

$$\sum_{a'} |C_{a'}(t)|^2 = 1$$

Therefore it must be that $U(t_0; t)$ is unitary.

$$\langle \psi, t_0; t | \psi, t_0; t \rangle = \langle \psi, t_0 | U^\dagger(t, t_0) U(t, t_0) | \psi, t_0 \rangle = \langle \psi, t_0 | \psi, t_0 \rangle$$

Which holds for all $|\psi\rangle$, thus,

$$U^\dagger(t, t_0) U(t, t_0) = \mathbb{I} \implies U^\dagger(t, t_0) = U^{-1}(t, t_0) \quad (1.19)$$

Another desired property of the time evolution operator $U(t; t_0)$ is *composition*. For $t_2 > t_1 > t_0$,

$$U(t_2, t_0) = U(t_2, t_1) U(t_1, t_0) \quad (1.20)$$

It turns out that eqs. (1.19) and (1.20) uniquely characterize $U(t, t_0)$. Consider an infinitesimal time evolution operator $U(t_0 + dt, t_0)$. We now prove that,

$$U(t_0 + dt, t_0) = \mathbb{I} - i\Omega dt$$

Where $\Omega = \Omega^\dagger$ is an unknown Hermitian operator. Consider,

$$\begin{aligned} U^\dagger(t_0 + dt, t_0) U(t_0 + dt, t_0) &= (\mathbb{I} + i\Omega^\dagger dt)(\mathbb{I} - i\Omega dt) \\ &= \mathbb{I} + i \left(\underbrace{\Omega^\dagger - \Omega}_0 \right) dt + \cancel{\mathcal{O}(dt^2)} \rightarrow 0 \\ &= \mathbb{I} \end{aligned}$$

Thus satisfying unitary properties. Next examine composition,

$$\begin{aligned} U(t_0 + dt_1 + dt_2, t_0 + dt_1) U(t_0 + dt_1, t_0) &= (\mathbb{I} - i\Omega dt_2)(\mathbb{I} - i\Omega dt_1) \\ &= \mathbb{I} - i\Omega(dt_1 + dt_2) + \mathcal{O}(dt_1 dt_2) \\ &= U(t_0 + dt_1 + dt_2, t_0) \end{aligned}$$

By dimensional analysis, Ω needs to have dimensions of inverse time or *frequency*. Of course the energy and frequency of a system are related by $E = \hbar\omega$. We conclude that,

$$\Omega = \frac{1}{\hbar} H$$

Where H is the usual Hamiltonian operator. This result is analogous to $\vec{K} = \frac{1}{\hbar} \vec{p}$. We have that,

$$U(t_0 + dt, t_0) = \mathbb{I} - \frac{i}{\hbar} H dt \quad (1.21)$$

Using this result, we will recover the Schrödinger equation. Consider the difference of two time evolution operators,

$$\begin{aligned} U(t + dt, t_0) - U(t, t_0) &= U(t + dt, t) U(t, t_0) - U(t, t_0) \\ &= \left(\mathbb{I} - \frac{i}{\hbar} H dt \right) U(t, t_0) - U(t, t_0) \\ &= -\frac{i}{\hbar} H dt U(t, t_0) \end{aligned}$$

Dividing both sides by dt and taking a limit,

$$\lim_{dt \rightarrow 0} \frac{U(t + dt, t_0) - U(t, t_0)}{dt} = -\frac{i}{\hbar} H U(t, t_0)$$

One obtains,

$$\frac{\partial}{\partial t} U(t, t_0) = -\frac{i}{\hbar} H U(t, t_0)$$

Which is identical to the Schrödinger equation for operators,

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H U(t, t_0)$$

We can also recover the more familiar Schrödinger equation for states through the following process,

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi, t_0\rangle = H U(t, t_0) |\psi, t_0\rangle \quad (1.22)$$

$$i\hbar \frac{\partial}{\partial t} |\psi, t_0; t\rangle = H |\psi, t_0; t\rangle \quad (1.23)$$

Now multiply by $\langle \vec{x}' |$,

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x}' | \psi, t_0; t\rangle = \langle \vec{x}' | H | \psi, t_0; t\rangle$$

Inserting resolution of identity,

$$\langle \vec{x}' | H | \psi, t_0; t\rangle = \int d^3x'' \langle \vec{x}' | H | \vec{x}'' \rangle \langle \vec{x}'' | \psi, t_0; t\rangle$$

Where $\langle \vec{x}' | H | \vec{x}'' \rangle$ is the Hamiltonian in terms of the position basis,

$$\langle \vec{x}' | H | \vec{x}'' \rangle = -\frac{\hbar^2}{2m} \vec{\nabla} \delta(\vec{x}' - \vec{x}'')$$

We will now attempt to solve eq. (1.22) in order to obtain the time evolution operator explicitly (not as in eq. (1.21)). As a reduction of complexity, we will consider the Hamiltonian H to be time independent $\frac{\partial H}{\partial t} = 0$ ². The solution to eq. (1.22) is then,

$$U(t, t_0) = e^{-\frac{i}{\hbar} H(t-t_0)} \quad (1.24)$$

Where ‘ e^A ’ is the operator exponential,

$$e^A = \sum_{n=1}^{\infty} \frac{A^n}{n!}$$

Therefore we have that,

$$e^{-\frac{i}{\hbar} H(t-t_0)} = \mathbb{I} - \frac{i}{\hbar} H(t-t_0) - \frac{1}{2\hbar^2} H^2(t-t_0)^2 + \mathcal{O}\left((t-t_0)^3\right)$$

Whose time derivative is,

$$\frac{\partial}{\partial t} e^{-\frac{i}{\hbar} H(t-t_0)} = -\frac{i}{\hbar} H - \frac{1}{\hbar^2} H^2(t-t_0) + \mathcal{O}\left((t-t_0)^2\right)$$

Moving the constant term $-\frac{i}{\hbar} H$ out,

$$\frac{\partial}{\partial t} e^{-\frac{i}{\hbar} H(t-t_0)} = -\frac{i}{\hbar} H \left[\mathbb{I} - \frac{i}{\hbar} H(t-t_0) + \mathcal{O}\left((t-t_0)^2\right) \right]$$

²As is common for a particle moving in a static potential.

Recognizing $e^{-\frac{i}{\hbar}H(t-t_0)}$,

$$\frac{\partial}{\partial t} e^{-\frac{i}{\hbar}H(t-t_0)} = -\frac{i}{\hbar}H \left[e^{-\frac{i}{\hbar}H(t-t_0)} \right]$$

Therefore we have that eq. (1.24) solves eq. (1.22). Also note that eq. (1.24) is consistent with eq. (1.21).

Recall that the eigen-system of the Hamiltonian is given by,

$$H|a'\rangle = E_{a'}|a'\rangle$$

Where $E_{a'}$ are the energy eigenvalues. Therefore $e^{-\frac{i}{\hbar}Ht}$ can be written as,

$$\mathbb{I}e^{-\frac{i}{\hbar}H(t-t_0)}\mathbb{I} = \sum_{a',a''} |a''\rangle\langle a''| e^{-\frac{i}{\hbar}H(t-t_0)} |a'\rangle\langle a'| \quad (1.25)$$

Where $\langle a''|e^{-\frac{i}{\hbar}H(t-t_0)}|a''\rangle$ is given by,

$$\begin{aligned} \langle a''|e^{-\frac{i}{\hbar}H(t-t_0)}|a''\rangle &= \langle a''| \sum_{n=1}^{\infty} \frac{-\frac{i}{\hbar}H(t-t_0)}{n!} |a'\rangle \\ &= \sum_{n=1}^{\infty} \frac{-\frac{i}{\hbar}\langle a''|H|a'\rangle(t-t_0)}{n!} \\ &= \sum_{n=1}^{\infty} \frac{-\frac{i}{\hbar}E_{a'}\langle a''|a'\rangle(t-t_0)}{n!} \\ &= \sum_{n=1}^{\infty} \frac{-\frac{i}{\hbar}E_{a'}\delta_{a'',a'}(t-t_0)}{n!} \\ &= \delta_{a'',a'} \sum_{n=1}^{\infty} \frac{-\frac{i}{\hbar}E_{a'}(t-t_0)}{n!} \\ &= \delta_{a'',a'} e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \end{aligned}$$

Therefore eq. (1.25) becomes,

$$\begin{aligned} e^{-\frac{i}{\hbar}H(t-t_0)} &= \sum_{a',a''} |a''\rangle\delta_{a'',a'} e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \langle a'| \\ &= \sum_{a'} e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} |a'\rangle\langle a'| \end{aligned} \quad (1.26)$$

Recall that,

$$|\psi, t_0 = 0\rangle = \sum_{a'} |a'\rangle\langle a'|\psi\rangle = \sum_{a'} C_{a'}(0)|a'\rangle$$

At some later time t ,

$$|\psi, t_0 = 0; t\rangle = e^{-\frac{i}{\hbar}Ht}|\psi, t_0 = 0\rangle$$

Subbing in eq. (1.26),

$$\begin{aligned} |\psi, t_0 = 0; t\rangle &= \sum_{a'} e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} |a'\rangle\langle a'|\psi, t_0 = 0\rangle \\ &= \sum_{a'} e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} |a'\rangle C_{a'}(t_0 = 0) \end{aligned}$$

Therefore it must be that,

$$C_{a'}(t) = e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} C_{a'}(t_0)$$

The coefficients evolve in the same way that $|\psi\rangle$ does.

1.6 Different Pictures for Quantum Mechanics

In the Schrödinger picture (as just discussed) the states depend on time, while operators do not. In contrast, the **Heisenberg picture** has operators depending on time while the states do not³. to illustrate the difference, consider an arbitrary unitary operator U ($U^\dagger = U^{-1}$),

$$|\psi\rangle \xrightarrow{U} U|\psi\rangle$$

Now consider an arbitrary Hermitian operator A ($A^\dagger = A$),

$$\langle\varphi|A|\psi\rangle \xrightarrow{U} \langle\varphi|U^\dagger A U|\psi\rangle$$

The Schrödinger picture would ascribe the evolution to the states,

$$\langle\varphi|A|\psi\rangle \xrightarrow{U} \{\langle\varphi|U^\dagger\} A \{U|\psi\rangle\}$$

While the Heisenberg picture applies the action to the operators,

$$\langle\varphi|A|\psi\rangle \xrightarrow{U} \langle\varphi|\{U^\dagger A U\}|\psi\rangle$$

Therefore instead of transforming states, we may transform operators:

$$A \xrightarrow{U} U^\dagger A U$$

As an example, if we take the time evolution operator exactly ($U(t) = e^{-\frac{i}{\hbar} H t}$). Let A under the Heisenberg picture as $A^{(H)}$,

$$A^{(H)}(t) = U^\dagger(t) A^{(S)} U(t) \quad (1.27)$$

We have the useful identities,

$$A^{(H)}(0) = A^{(S)}$$

$$|\psi; t\rangle^{(H)} = |\psi; t_0\rangle$$

$$|\psi; t\rangle^{(S)} = U(t)|\psi; t_0\rangle$$

As a final consistency check, observables should be independent of the *picture* used,

$$\begin{aligned} \langle A \rangle^{(S)} &= {}^{(S)}\langle\psi; t| A^{(S)} |\psi; t\rangle^{(S)} \\ &= \langle\psi; t_0| U^\dagger(t) A^{(S)} U(t) |\psi; t_0\rangle \\ &= {}^{(H)}\langle\psi; t_0| A^{(H)} |\psi; t_0\rangle^{(H)} \\ &= \langle A \rangle^{(H)} \end{aligned}$$

Next we find an equation of motion for $A^{(H)}(t)$,

$$\begin{aligned} \frac{d}{dt} e^{\frac{i}{\hbar} H t} A^{(S)} e^{-\frac{i}{\hbar} H t} &= \frac{i}{\hbar} H e^{\frac{i}{\hbar} H t} A^{(S)} e^{-\frac{i}{\hbar} H t} - e^{\frac{i}{\hbar} H t} A^{(S)} \frac{i}{\hbar} H e^{-\frac{i}{\hbar} H t} \\ &= \frac{i}{\hbar} H e^{\frac{i}{\hbar} H t} A^{(S)} e^{-\frac{i}{\hbar} H t} - e^{\frac{i}{\hbar} H t} A^{(S)} \frac{i}{\hbar} e^{-\frac{i}{\hbar} H t} H \quad \text{Commuting } [f(H), H] = 0 \\ &= \frac{i}{\hbar} H A^{(H)}(t) - \frac{i}{\hbar} A^{(H)}(t) H \\ &= \frac{i}{\hbar} [H, A^{(H)}(t)] \end{aligned}$$

³The *interaction picture* shares evolution between states and operators.

Therefore,

$$\frac{dA^{(H)}}{dt} = \frac{i}{\hbar} [H, A^{(H)}] \quad (1.28)$$

Notice that the Hamiltonian itself is the same in either picture,

$$e^{\frac{i}{\hbar}Ht} H e^{-\frac{i}{\hbar}Ht} = e^{\frac{i}{\hbar}Ht} e^{-\frac{i}{\hbar}Ht} H = H$$

Which is simply a manifestation of the conservation of energy.

1.6.1 Conserved Quantities

To solve eq. (1.28), consider the situation of a free particle with no external potential. Then,

$$H = \frac{\vec{p}^2}{2m} \quad \frac{dp_i}{dt} = \frac{i}{\hbar} [H, p_i]$$

But for a free particle $[H, p_i] = 0$. Therefore $\frac{dp_i}{dt} = 0$ and the momentum of a free particle is conserved. In general, any operator A such that $[H, A] = 0$ represents a conserved physical quantity of the system with Hamiltonian H . Next consider the position operator \vec{x} which does not commute with H ,

$$\frac{dx_i}{dt} = \frac{i}{\hbar} [H, x_i] \quad (1.29)$$

First recall that $[x_i, p_i] = i\hbar$.

$$\vec{p}^2 = \sum_{i=x,y,z} p_i^2$$

Thus,

$$\begin{aligned} [p_i^2, x_i] &= p_i^2 x_i - x_i p_i^2 \\ &= p_i^2 x_i - (i\hbar + p_i x_i) p_i \\ &= p_i^2 x_i - i\hbar p_i - p_i x_i p_i \\ &= \cancel{p_i^2 x_i} - i\hbar p_i - \cancel{p_i^2 x_i} - i\hbar p_i \\ &= -2i\hbar p_i \end{aligned} \quad (1.30)$$

Which solves eq. (1.29) to be,

$$\frac{dx_i}{dt} = \frac{i}{\hbar} \left(-\frac{2i\hbar}{2m} \right) p_i = \frac{p_i}{m}$$

Which acts as a classical velocity. Since p_i is time-independent for a free particle, we can easily integrate to solve this DE,

$$x_1(t) = x_1(0) + \frac{p_1}{m} t$$

In more generality, let us consider a particle interacting with some external potential.

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

Therefore,

$$\frac{dp_i}{dt} = \frac{i}{\hbar} [V(\vec{x}), p_i]$$

Which by a similar approach to eq. (1.30) we compute $[x_i^2, p_i]$,

$$\begin{aligned} [x_i^2, p_i] &= x_i^2 p_i - p_i x_i^2 \\ &= x_i^2 p_i - (x_i p_i - i\hbar) x_i \end{aligned}$$

$$\begin{aligned}
&= x_i^2 p_i - x_i p_i x_i - i\hbar x_i \\
&= x_i^2 p_i - x_i (x_i p_i - i\hbar) - i\hbar x_i \\
&= 2i\hbar x_i
\end{aligned}$$

By extension,

$$[x_i, p_i] = i\hbar \quad [x_i^2, p_i] = 2i\hbar x_i \quad \dots$$

We arrive at⁴,

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

Which yields **Ehrenfest's Theorem**,

$$\frac{dp_i}{dt} = -\frac{\partial}{\partial x_i} V(\vec{x})$$

We can further look at the acceleration,

$$\begin{aligned}
\frac{d^2 x_i}{dt^2} &= \frac{i}{\hbar} \left[H, \frac{dx_i}{dt} \right] \\
&= \frac{i}{\hbar} \left[H, \frac{p_i}{m} \right] \\
&= -\frac{1}{m} \frac{\partial}{\partial x_i} V(\vec{x})
\end{aligned}$$

Therefore we recover Newton's law,

$$m \frac{d^2 x_i}{dt^2} = -\frac{\partial}{\partial x_i} V(\vec{x})$$

Similarly,

$$i\hbar \frac{\partial}{\partial t} |\psi, t_0; t\rangle = H |\psi, t_0; t\rangle$$

Hences by multiplying by $\langle \vec{x}' |$,

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x}' | \psi, t_0; t \rangle = \langle \vec{x}' | H | \psi, t_0; t \rangle$$

Which requires us to solve,

$$\left\langle \vec{x}' \left| \frac{\vec{p}^2}{2m} \right| \psi \right\rangle = \langle \vec{x}' | V(\vec{x}') | \psi \rangle$$

The details are left as an exercise but,

$$\begin{aligned}
\langle \vec{x}' | \vec{p} | \psi \rangle &= -i\hbar \vec{\nabla}' \langle \vec{x}' | \psi \rangle \\
\left\langle \vec{x}' \left| \frac{\vec{p}^2}{2m} \right| \psi \right\rangle &= -\frac{\hbar^2}{2m} \vec{\nabla}'^2 \langle \vec{x}' | \psi \rangle
\end{aligned}$$

Therefore we arrive at the Schrödinger equation for a wavefunction,

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x}' | \psi, t_0; t \rangle = -\frac{\hbar^2}{2m} \vec{\nabla}'^2 \langle \vec{x}' | \psi, t_0; t \rangle + V(\vec{x}') \langle \vec{x}' | \psi, t_0; t \rangle$$

Which in terms of wavefunctions is simply,

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}', t) = -\frac{\hbar^2}{2m} \vec{\nabla}'^2 \psi(\vec{x}', t) + V(\vec{x}') \psi(\vec{x}', t)$$

⁴This also follows directly from the construction of the momentum operator; being the dual to x_i , a derivative in position representation. $[V(\vec{x}), p_i]|\psi\rangle = V(\vec{x})p_i|\psi\rangle - p_i(V(\vec{x})|\psi\rangle) = V(\vec{x})p_i|\psi\rangle - (p_i V(\vec{x}))|\psi\rangle - V(\vec{x})(p_i|\psi\rangle)$

2 Rotations and Angular Momentum

To begin, let us remind ourselves about the algebra of rotations in 3D space. Suppose one has a Cartesian coordinate system $\{x, y, z\}$. To retain some consistency, we always rotate the physical system with respect to fixed coordinates (i.e. the *active* view of rotations, not the *passive* view).

As an example, consider rotating the system \vec{r} about the z -axis to the vector \vec{r}' . Let the vector perpendicular to \vec{r} be denoted $\hat{z} \times \vec{r}$. Then one can write the vector \vec{r}' as,

$$\vec{r}' = \vec{r} \cos \varphi + \hat{z} \times \vec{r} \sin \varphi$$

In terms of components (considering \vec{r} in the x, y -plane),

$$\begin{aligned} \vec{r}' &= (x\hat{x} + y\hat{y}) \cos \varphi + \hat{z} \times (x\hat{x} + y\hat{y}) \sin \varphi \\ &= (x\hat{x} + y\hat{y}) \cos \varphi + (x\hat{y} - y\hat{x}) \sin \varphi \\ &= (y \cos \varphi + x \sin \varphi)\hat{y} + (x \sin \varphi - y \cos \varphi)\hat{x} \end{aligned}$$

The rotated components are given by,

$$\begin{aligned} x' &= x \cos \varphi - y \sin \varphi \\ y' &= x \sin \varphi + y \cos \varphi \\ z &= z' \end{aligned}$$

Which can be written as a matrix,

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R_z(\varphi) \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Where the **rotation matrix** about the z -axis is given by,

$$R_z(\varphi) = \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Analogously one can define,

$$\begin{aligned} R_x(\varphi) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \varphi & -\sin \varphi \\ 0 & \sin \varphi & \cos \varphi \end{pmatrix} \\ R_y(\varphi) &= \begin{pmatrix} \cos \varphi & 0 & -\sin \varphi \\ 0 & 1 & 0 \\ \sin \varphi & 0 & \cos \varphi \end{pmatrix} \end{aligned}$$

Next consider the transpose of a rotation matrix,

$$R_z^\top(\varphi) = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Which gives,

$$R_z^\top(\varphi) R_z(\varphi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Therefore $R_z^\top(\varphi) = R_z^{-1}(\varphi)$. Due to this property we say that $R_z(\varphi)$ is an **orthogonal matrix**.

Moreover we have that,

$$R_x(\varphi_1) R_y(\varphi_2) \neq R_y(\varphi_2) R_x(\varphi_1)$$

Therefore the commutation is,

$$[R_x, R_y] \neq 0$$

Much like we did with translations, consider the infinitesimal rotation ($\varphi = \epsilon \ll 1$).

$$R_z(\epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & -\epsilon & 0 \\ \epsilon & 1 - \frac{\epsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

We can now compute the commutation between two infinitesimal rotations.

$$R_x(\epsilon)R_y(\epsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 - \frac{\epsilon^2}{2} & -\epsilon \\ 0 & \epsilon & 1 - \frac{\epsilon^2}{2} \end{pmatrix} \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & 0 & -\epsilon \\ 0 & 1 & 0 \\ \epsilon & 0 & 1 - \frac{\epsilon^2}{2} \end{pmatrix}$$

Which gives,

$$R_x(\epsilon)R_y(\epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & 0 & \epsilon \\ \epsilon^2 & 1 - \frac{\epsilon^2}{2} & -\epsilon \\ -\epsilon & \epsilon & 1 - \epsilon^2 \end{pmatrix}$$

Similarly,

$$R_y(\epsilon)R_x(\epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & \epsilon^2 & \epsilon \\ 0 & 1 - \frac{\epsilon^2}{2} & -\epsilon \\ -\epsilon & \epsilon & 1 - \epsilon^2 \end{pmatrix}$$

Thus,

$$[R_x(\epsilon), R_y(\epsilon)] = \begin{pmatrix} 0 & \epsilon^2 & 0 \\ \epsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Notice that,

$$[R_x(\epsilon), R_y(\epsilon)] = R_x(\epsilon^2) - \mathbb{I}$$

2.1 Rotations in Quantum Mechanics

Let the rotation be some operator $D \in \mathcal{B}(\mathcal{H})$ be,

$$|\psi\rangle_R = D(R)|\psi\rangle$$

Where $D(R)$ represents the **rotation operator** associated with the rotation R . $|\psi\rangle_R$ is the rotated version of $|\psi\rangle$. Say for example, R represents the rotation by an infinitesimal small angle $d\varphi$ about an axis \hat{n} . Evidently $D(R)$ *should* maintain the same properties (eqs. (1.13) and (1.12)) as the translation operator $T(d\vec{x}')$. Therefore it is acceptable to postulate that,

$$D(\hat{n}, d\varphi) = \mathbb{I} - \frac{i}{\hbar} \vec{J} \cdot \hat{n} d\varphi$$

By dimensional analysis, \vec{J} is the angular momentum of the system. We saw that \vec{J} is the generator of rotations.

Again we can find the rotation about any angle φ (not just $d\varphi$) using,

$$D(\hat{n}, \varphi) = \lim_{N \rightarrow \infty} \left[\mathbb{I} - \frac{i}{\hbar} \vec{J} \cdot \hat{n} \frac{\varphi}{N} \right]^N$$

Which gives the familiar result,

$$D(\hat{n}, \varphi) = e^{-\frac{i}{\hbar} \vec{J} \cdot \hat{n} \varphi}$$