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 $A : \mathcal{H} \to \mathcal{H}$ 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 bra $\langle\varphi|$.

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

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

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

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 the *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,

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

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) be 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,

$$\underbrace{\langle a''|A|a'\rangle - \left\langle a''\middle|A^\dagger\middle|a'\right\rangle}_{0} = a'\langle a''|a'\rangle - a''^*\langle a''|a'\rangle$$

Therefore,

$$(a' - a''^*)\langle a''|a'\rangle = 0 \tag{1.5}$$

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.

$$\langle a|a'\rangle = \delta_{a,a'} \tag{1.6}$$

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

$$|\psi\rangle = \sum_{a'} C_{a'}|a'\rangle \tag{1.7}$$

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

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

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,

$$|\psi\rangle = \sum_{a'}|a'\rangle\langle a'|\psi\rangle \tag{1.9}$$

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

$$\sum_{a'}|a'\rangle\langle a'| = \mathbb{1} \tag{1.10}$$

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,

$$B = \mathbb{1} \cdot B \cdot \mathbb{1} = \sum_{a',a''} |a''\rangle\langle a''|B|a'\rangle\langle a'|$$

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,

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

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,

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

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

The closure relation becomes,

$$\mathbb{1} = \int_{\mathbb{R}^3} \mathrm{d}^3x' |\vec{x}\,'\rangle\langle \vec{x}\,'|$$

Therefore we have that,

$$|\psi\rangle = \mathbb{1} \cdot |\psi\rangle = \int_{\mathbb{R}^3} \mathrm{d}^3x' |\vec{x}\,'\rangle\langle \vec{x}\,'|\psi\rangle$$

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

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

1.3 Infinitesimal Translations

The operator of infinitesimal translations T is defined as,

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

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

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

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

$$\langle\psi|T^\dagger(\mathrm{d}\vec{x}\,')T(\mathrm{d}\vec{x}\,')|\psi\rangle = 1 \tag{1.11}$$

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

$$T^\dagger(\mathrm{d}\vec{x}\,')T(\mathrm{d}\vec{x}\,') = \mathbb{1} \implies T^\dagger(\mathrm{d}\vec{x}\,') = T^{-1}(\mathrm{d}\vec{x}\,') \tag{1.12}$$

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

$$T(\mathrm{d}\vec{x}\,')T(\mathrm{d}\vec{x}\,'') = T(\mathrm{d}\vec{x}\,' + \mathrm{d}\vec{x}\,'') \tag{1.13}$$

Consequently,

$$T^{-1}(\mathrm{d}\vec{x}\,') = T(-\mathrm{d}\vec{x}\,') \qquad T(\vec{0}) = \mathbb{1}$$

All of the above properties are satisfied if,

$$T(\mathrm{d}\vec{x}\,') = \mathbb{1} - i\vec{K}\cdot\mathrm{d}\vec{x}\,'$$

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 $T(\mathrm{d}\vec{x}\,')$ is unitary (eq. (1.12)),

$$\begin{aligned}T^\dagger(\mathrm{d}\vec{x}\,')T(\mathrm{d}\vec{x}\,') &= \left(\mathbb{1} + i\vec{K}^{\,\dagger}\cdot\mathrm{d}\vec{x}\,'\right)\left(\mathbb{1} - i\vec{K}\cdot\mathrm{d}\vec{x}\,'\right) \\ &= \mathbb{1} + \underbrace{i\vec{K}^{\,\dagger}\cdot\mathrm{d}\vec{x}\,' - i\vec{K}\cdot\mathrm{d}\vec{x}\,'}_{0} + \cancelto{0}{\mathcal{O}\left(|\mathrm{d}\vec{x}\,'|^2\right)} \\ &= \mathbb{1}\end{aligned}$$

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

$$T(\mathrm{d}\vec{x}\,'')T(\mathrm{d}\vec{x}\,') = \left(\mathbb{1} - i\vec{K}\cdot\mathrm{d}\vec{x}\,''\right)\left(\mathbb{1} - i\vec{K}\cdot\mathrm{d}\vec{x}\,'\right)$$

$$
\begin{aligned}
&= \mathbb{1} - i\vec{K}\cdot \mathrm{d}\vec{x}'' - i\vec{K}\cdot \mathrm{d}\vec{x}' + \cancelto{0}{\mathcal{O}\Big(|\mathrm{d}\vec{x}'|^2\Big)} \\
&= \mathbb{1} - i\vec{K}\cdot (\mathrm{d}\vec{x}'' + \mathrm{d}\vec{x}') \\
&= T(\mathrm{d}\vec{x}'' + \mathrm{d}\vec{x}')
\end{aligned}
$$

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

$$[\vec{x}, T(\mathrm{d}\vec{x}')]|\vec{x}'\rangle = \vec{x}T(\mathrm{d}\vec{x}')|\vec{x}'\rangle - T(\mathrm{d}\vec{x}')\vec{x}|\vec{x}'\rangle = \mathrm{d}\vec{x}'|\vec{x}' + \mathrm{d}\vec{x}'\rangle \approx \mathrm{d}\vec{x}'|\vec{x}'\rangle$$

Alternatively we have,

$$
\begin{aligned}
[\vec{x}, T(\mathrm{d}\vec{x}')] &= \left[\vec{x}, \mathbb{1} - i\vec{K}\cdot \mathrm{d}\vec{x}'\right] \\
&= -i\vec{x}\vec{K}\cdot \mathrm{d}\vec{x}' + i\vec{K}\cdot \mathrm{d}\vec{x}'\vec{x} \\
&= \mathrm{d}\vec{x}'
\end{aligned}
$$

Choose $\mathrm{d}\vec{x}' = \mathrm{d}x'\hat{x}_j$ 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.

$$[\vec{x}, T(\mathrm{d}\vec{x}')]_i = -ix_iK_j\mathrm{d}x' + iK_j\mathrm{d}x'x_i = \delta_{ij}\mathrm{d}x'$$

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,

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

1.4 Transformations Between Position and Momentum Representations

Calculate for a 1D system,

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

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,

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

Which in turn implies that,

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

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,

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

Moreover we have the resolution of identity,

$$\mathbb{1} = \int \mathrm{d}^3p'|\vec{p}\,'\rangle\langle\vec{p}\,'|$$

Therefore we have that,

$$|\psi\rangle = \mathbb{1}\cdot|\psi\rangle = \int \mathrm{d}^3p'|\vec{p}\,'\rangle\langle\vec{p}\,'|\psi\rangle$$

So we define the wave-function 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,

$$\langle x'|x''\rangle = \delta(x' - x'') = \langle x'|\mathbb{1}|x''\rangle = \int \mathrm{d}p'\langle x'|p'\rangle\langle p'|x'\rangle$$

Substitute in eq. (1.15),

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

Recall a integral representation of the Dirac-delta function,

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

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,

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

Which refers to the usual plane wave wave-function. Alternatively, one can obtain this result from the Schrödinger Equation $H\psi = E\psi$ and using a free Hamiltonian $H = \frac{p^2}{2m} = -\frac{\hbar^2 \mathrm{d}^2}{2m\mathrm{d}x^2}$ 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,

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

Analogously we can rotate state space to give,

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

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),

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

[1] We 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,

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

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

$$U(t_2, t_0) = U(t_2, t_1) U(t_1, t_0) \tag{1.20}$$

In turns out that eqs. (1.19) and (1.20) uniquely characterize $U(t, t_0)$. Consider an infinitesimal time evolution operator $U(t_0 + \mathrm{d}t, t_0)$. We now prove that,

$$U(t_0 + \mathrm{d}t, t_0) = \mathbb{1} - i\Omega \mathrm{d}t$$

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

$$\begin{aligned} U^\dagger(t_0 + \mathrm{d}t, t_0) U(t_0 + \mathrm{d}t, t_0) &= \left(\mathbb{1} + i\Omega^\dagger \mathrm{d}t\right)(\mathbb{1} - i\Omega \mathrm{d}t) \\ &= \mathbb{1} + i\left(\underbrace{\Omega^\dagger - \Omega}_{0}\right)\mathrm{d}t + \cancelto{0}{\mathcal{O}(\mathrm{d}t^2)} \\ &= \mathbb{1} \end{aligned}$$

Thus satisfying unitary properties. Next examine composition,

$$\begin{aligned} U(t_0 + \mathrm{d}t_1 + \mathrm{d}t_2, t_0 + \mathrm{d}t_1) U(t_0 + \mathrm{d}t_1, t_0) &= (\mathbb{1} - i\Omega \mathrm{d}t_2)(\mathbb{1} - i\Omega \mathrm{d}t_1) \\ &= \mathbb{1} - i\Omega(\mathrm{d}t_1 + \mathrm{d}t_2) + \mathcal{O}(\mathrm{d}t_1 \mathrm{d}t_2) \\ &= U(t_0 + \mathrm{d}t_1 + \mathrm{d}t_2, t_0) \end{aligned}$$

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,

$$U(t_0 + \mathrm{d}t, t_0) = \mathbb{1} - \frac{i}{\hbar} H \mathrm{d}t \tag{1.21}$$

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

$$\begin{aligned} U(t + \mathrm{d}t, t_0) - U(t, t_0) &= U(t + \mathrm{d}t, t) U(t, t_0) - U(t, t_0) \\ &= \left(\mathbb{1} - \frac{i}{\hbar} H \mathrm{d}t\right) U(t, t_0) - U(t, t_0) \\ &= -\frac{i}{\hbar} H \mathrm{d}t U(t, t_0) \end{aligned}$$

Dividing both sides by dt and taking a limit,

$$\lim_{\mathrm{d}t\to 0}\frac{U(t+\mathrm{d}t,t_0)-U(t,t_0)}{\mathrm{d}t} = -\frac{i}{\hbar}HU(t,t_0)$$

One obtains,

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

Which is identical to the Schrödinger equation for operators,

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

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

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

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

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,

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

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,

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

Where 'e^A' is the operator exponential,

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

Therefore we have that,

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

Whose time derivative is,

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

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

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

[2] As 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,
$$\mathbb{1}e^{-\frac{i}{\hbar}H(t-t_0)}\mathbb{1} = \sum_{a',a''}|a''\rangle\langle a''|e^{-\frac{i}{\hbar}H(t-t_0)}|a'\rangle\langle a'| \tag{1.25}$$
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,
$$e^{-\frac{i}{\hbar}H(t-t_0)} = \sum_{a',a''}|a''\rangle\delta_{a'',a'}e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}\langle a'|$$
$$e^{-\frac{i}{\hbar}H(t-t_0)} = \sum_{a'}e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}|a'\rangle\langle a'| \tag{1.26}$$
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),
$$|\psi, t_0 = 0; t\rangle = \sum_{a'}e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}|a'\rangle\langle a'|\psi, t_0 = 0\rangle$$
$$|\psi, t_0 = 0; t\rangle = \sum_{a'}e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}|a'\rangle C_{a'}(t_0 = 0)$$
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 not[3]. 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 ($A^\dagger = A$),

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

The Schrödinger picture would ascribe the evolution to the states,

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

While the Heisenberg picture applies the action to the operators,

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

Therefore instead of transforming states, we may transform operators:

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

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

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

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 $A^{(H)}(t)$,

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

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

Therefore,

$$\frac{\mathrm{d}A^{(H)}}{\mathrm{d}t} = \frac{i}{\hbar}\left[H, A^{(H)}\right] \tag{1.28}$$

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

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

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,

$$H = \frac{\vec{p}^2}{2m} \qquad \frac{\mathrm{d}p_i}{\mathrm{d}t} = \frac{i}{\hbar}[H, p_i]$$

But for a free particle $[H, p_i] = 0$. Therefore $\frac{\mathrm{d}p_i}{\mathrm{d}t} = 0$ 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,

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \frac{i}{\hbar}[H, x_i] \tag{1.29}$$

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

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

Thus,

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

Which solves eq. (1.29) to be,

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \frac{i}{\hbar}\left(-\frac{2i\hbar}{2m}\right)p_i = \frac{p_i}{m}$$

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,

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \frac{i}{\hbar}[V(\vec{x}), p_i]$$

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

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

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

By extension,

$$[x_i, p_i] = i\hbar \quad \left[x_i^2, p_i\right] = 2i\hbar x_i \quad \cdots$$

We arrive at[4],

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

Which yields **Ehrenfest's Theorem**,

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial}{\partial x_i} V(\vec{x})$$

We can further look at the acceleration,

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

Therefore we recover Newton's law,

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

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,

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

The details are left as a exercise but,

$$\langle \vec{x}\,'|\vec{p}|\psi\rangle = -i\hbar \vec{\nabla}\,'\langle \vec{x}\,'|\psi\rangle$$

$$\left\langle \vec{x}\,' \middle| \frac{\vec{p}^{\,2}}{2m} \middle| \psi \right\rangle = -\frac{\hbar^2}{2m}\vec{\nabla}\,'^2\langle \vec{x}\,'|\psi\rangle$$

Therefore we arrive at the Schrödinger equation for a wave-function,

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

Which in terms of wave-functions is simply,

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

[4]This 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,

$$x' = x\cos\varphi - y\sin\varphi$$

$$y' = x\sin\varphi + y\cos\varphi$$

$$z = z'$$

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,

$$R_z(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2.1}$$

Analogously one can define,

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

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

Next consider the transpose of a rotation matrix,

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

Which gives,

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

Therefore $R_z^{\intercal}(\varphi) = R_z^{-1}(\varphi)$. 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,

$$[R_x(\epsilon), R_y(\epsilon)] = R_z\left(\epsilon^2\right) - \mathbb{1} \tag{2.2}$$

2.1 Rotations in Quantum Mechanics

Let the rotation be some operator $D(R) \in \mathcal{B}(\mathcal{H})$ 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 $\mathrm{d}\varphi$ about an axis $\hat{n}$. Evidently $D(R)$ *should* maintain the same properties (eqs. (1.13) and (1.12)) as the translation operator $T(\mathrm{d}\vec{x}\,')$. Therefore is is acceptable to postulate that,

$$D_{\hat{n}}(\mathrm{d}\varphi) = \mathbb{1} - \frac{i}{\hbar}\vec{J} \cdot \hat{n}\mathrm{d}\varphi$$

By dimensional analysis, $\vec{J}$ is the angular momentum of the system. We sat that $\vec{J}$ is the generator of rotations.
Again we can find the rotation about any angle φ (not just $\mathrm{d}\varphi$) using,

$$D_{\hat{n}}(\varphi) = \lim_{N\to\infty}\left[\mathbb{1} - \frac{i}{\hbar}\vec{J} \cdot \hat{n}\frac{\varphi}{N}\right]^N$$

Which gives the familiar result,

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

The rotation operator *must* have the same multiplicative properties of the rotation matrices. If for example $R_3 = R_1 \cdot R_2$, then it must be that,

$$R_3 = R_1 \cdot R_2 \implies D(R_3) = D(R_1) \cdot D(R_2)$$

Recall the commutation relation for the rotation matrices from eq. (2.2). Thus,

$$[D_x(\epsilon), D_y(\epsilon)] = D_z\left(\epsilon^2\right) - \mathbb{1}$$

To demonstrate this, consider $D_x(\epsilon), D_y(\epsilon)$,

$$\begin{aligned} D_x(\epsilon) &= \mathbb{1} - \frac{i}{\hbar} J_x \epsilon - \frac{1}{2\hbar^2} J_x^2 \epsilon^2 + \mathcal{O}\left(\epsilon^3\right) \\ D_y(\epsilon) &= \mathbb{1} - \frac{i}{\hbar} J_y \epsilon - \frac{1}{2\hbar^2} J_y^2 \epsilon^2 + \mathcal{O}\left(\epsilon^3\right) \\ D_z\left(\epsilon^2\right) &= \mathbb{1} - \frac{i}{\hbar} J_z \epsilon^2 + \mathcal{O}\left(\epsilon^3\right) \end{aligned}$$

Keeping only first orders of ϵ,

$$\begin{aligned} &[D_x(\epsilon), D_y(\epsilon)] \\ &= D_x(\epsilon) D_y(\epsilon) - D_y(\epsilon) D_x(\epsilon) \\ &= \left(\mathbb{1} - \frac{i}{\hbar} J_x \epsilon - \frac{1}{2\hbar^2} J_x^2 \epsilon^2\right)\left(\mathbb{1} - \frac{i}{\hbar} J_y \epsilon - \frac{1}{2\hbar^2} J_y^2 \epsilon^2\right) - \left(\mathbb{1} - \frac{i}{\hbar} J_y \epsilon - \frac{1}{2\hbar^2} J_y^2 \epsilon^2\right)\left(\mathbb{1} - \frac{i}{\hbar} J_x \epsilon - \frac{1}{2\hbar^2} J_x^2 \epsilon^2\right) \\ &= \cancel{\mathbb{1}} - \cancel{\frac{i}{\hbar} J_y} \epsilon - \cancel{\frac{1}{2\hbar^2} J_y^2 \epsilon^2} - \cancel{\frac{i}{\hbar} J_x} \epsilon - \cancel{\frac{1}{2\hbar^2} J_x^2 \epsilon^2} - \frac{1}{\hbar^2} J_x J_y \epsilon^2 - \cancel{\mathbb{1}} + \cancel{\frac{1}{\hbar} J_x} \epsilon + \cancel{\frac{1}{2\hbar^2} J_x^2} \epsilon + \cancel{\frac{1}{\hbar} J_y} \epsilon + \cancel{\frac{1}{2\hbar^2} J_y^2} \epsilon + \frac{1}{\hbar^2} J_y J_x \epsilon^2 \\ &= -\frac{1}{\hbar^2}[J_x, J_y]\epsilon^2 = D_z\left(\epsilon^2\right) - \mathbb{1} = -\frac{i}{\hbar} J_z \epsilon^2 \end{aligned}$$

In general,

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k \tag{2.3}$$

Where ϵ_{ijk} is the fully symmetric tensor,

$$\begin{aligned} \epsilon_{xyz} = \epsilon_{zxy} = \epsilon_{yzx} = +1 \\ \epsilon_{xzy} = \epsilon_{zyx} = \epsilon_{yxz} = -1 \end{aligned} \tag{2.4}$$

The commutation relation is in contrast to the commutation of the momentum operator,

$$[p_x, p_y] = 0$$

Since linear momentum is the generator of translations, different components of momentum commute. We say that the group of translations is **abelian**, while the group of rotations is **non-abelian** because generators of rotations do not commute.

2.2 Spin-1/2 Operators

Consider the spin operators $S_{\hat{n}}$ with the commutation relation,

$$[S_i, S_j] = i\hbar \epsilon_{ijk} S_k \tag{2.5}$$

Where,

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

Where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the **Pauli matrices**,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Notice that the Pauli matrices have the following nice property,

$$\sigma_i^2 = \mathbb{1} \quad \forall i \in x, y, z \tag{2.6}$$

We can also write the spin operators in a different way.

$$S_i = \frac{\hbar}{2} \sum_{a,b} |a\rangle \sigma_{ab} \langle b| \tag{2.7}$$

Where $|a\rangle, |b\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$. Expanding out eq. (2.7),

$$\begin{aligned} S_x &= \frac{\hbar}{2}(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|) \\ S_y &= \frac{i\hbar}{2}(-|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|) \\ S_z &= \frac{\hbar}{2}(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|) \end{aligned}$$

2.3 Rotations of Operators

Expectations of the spin operator are transformed by rotations,

$$\begin{aligned} \langle S_x \rangle_R &= {}_R\langle \psi | S_x | \psi \rangle_R \\ &= \langle \psi | D_z^\dagger(\varphi) S_x D_z(\varphi) | \psi \rangle \end{aligned}$$

Where the "rotated" spin operator $D_z^\dagger(\varphi) S_x D_z(\varphi)$ can be computed directly,

$$\begin{aligned} D_z^\dagger(\varphi) S_x D_z(\varphi) &= e^{\frac{i}{\hbar} S_z \varphi} S_x e^{-\frac{i}{\hbar} S_z \varphi} \\ &= \frac{\hbar}{2} e^{\frac{i}{2}\sigma_z \varphi} \sigma_x e^{-\frac{i}{2}\sigma_z\varphi} \end{aligned} \tag{2.8}$$

Making use of the Taylor series,

$$e^{-\frac{i}{2}\sigma_z\varphi} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{2}\sigma_z\varphi\right)^n$$

Breaking up even and odd powers of this series,

$$e^{-\frac{i}{2}\sigma_z\varphi} = \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left(-\frac{i}{2}\sigma_z\varphi\right)^{2n} + \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left(-\frac{i}{2}\sigma_z\varphi\right)^{2n+1}$$

Using eq. (2.6),

$$e^{-\frac{i}{2}\sigma_z\varphi} = \mathbb{1} \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left(-\frac{i}{2}\varphi\right)^{2n} + \sigma_z \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left(-\frac{i}{2}\varphi\right)^{2n+1}$$

Reorganizing yields,

$$e^{-\frac{i}{2}\sigma_z\varphi} = \mathbb{1} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \left(\frac{\varphi}{2}\right)^{2n} - i\sigma_z \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} \left(\frac{\varphi}{2}\right)^{2n+1}$$

Recognizing the Taylor series for $\sin x, \cos x$ where $x = \varphi/2$ we have that,

$$e^{-\frac{i}{2}\sigma_z\varphi} = \cos\left(\frac{\varphi}{2}\right)\mathbb{1} - i\sin\left(\frac{\varphi}{2}\right)\sigma_z$$

This result holds for any Pauli by eq. (2.6),

$$e^{-\frac{i}{2}\vec{\sigma}\cdot\hat{n}\varphi} = \cos\left(\frac{\varphi}{2}\right)\mathbb{1} - i\sin\left(\frac{\varphi}{2}\right)\vec{\sigma}\cdot\hat{n}$$

Therefore returning to eq. (2.8),

$$\begin{aligned}
e^{\frac{i}{2}\sigma_z\varphi}\sigma_x e^{-\frac{i}{2}\sigma_z\varphi} &= \left(\cos\left(\frac{\varphi}{2}\right)\mathbb{1} + i\sin\left(\frac{\varphi}{2}\right)\sigma_z\right)\sigma_x\left(\cos\left(\frac{\varphi}{2}\right)\mathbb{1} - i\sin\left(\frac{\varphi}{2}\right)\sigma_z\right) \\
&= \cos^2\frac{\varphi}{2}\sigma_x - i\cos\frac{\varphi}{2}\sin\frac{\varphi}{2}\sigma_x\sigma_z + i\cos\frac{\varphi}{2}\sin\frac{\varphi}{2}\sigma_z\sigma_x + \sin^2\frac{\varphi}{2}\sigma_z\sigma_x\sigma_z \\
&= \cos^2\frac{\varphi}{2}\sigma_x + i\cos\frac{\varphi}{2}\sin\frac{\varphi}{2}[\sigma_z,\sigma_x] + \sin^2\frac{\varphi}{2}\sigma_z\sigma_x\sigma_z \\
&= \cos^2\frac{\varphi}{2}\sigma_x + \frac{i}{2}\sin\varphi[\sigma_z,\sigma_x] + \sin^2\frac{\varphi}{2}\sigma_z\sigma_x\sigma_z
\end{aligned}$$

In order to determine the commutation relations for the Pauli matrices, make use of eq. (2.5),

$$\frac{\hbar^2}{4}[\sigma_i,\sigma_j] = i\hbar\frac{\hbar}{2}\epsilon_{ijk}\sigma_k$$

Therefore,

$$[\sigma_i,\sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

Where ϵ_{ijk} is the fully antisymmetric symbol seen previously in eq. (2.4). We say that Pauli matrices anti-commute. By hand,

$$\begin{aligned}
\sigma_x\sigma_z &= \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} = -i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = -i\sigma_y \\
\sigma_z\sigma_x &= \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = i\sigma_y
\end{aligned}$$

Therefore $\sigma_x\sigma_z = -\sigma_z\sigma_x$. Therefore we must have,

$$\begin{aligned}
e^{\frac{i}{2}\sigma_z\varphi}\sigma_x e^{-\frac{i}{2}\sigma_z\varphi} &= \cos^2\frac{\varphi}{2}\sigma_x + \frac{i}{2}\sin\varphi[\sigma_z,\sigma_x] - \sin^2\frac{\varphi}{2}\underbrace{\sigma_z\sigma_z}_{\mathbb{1}}\sigma_x \\
&= \left\{\cos^2\frac{\varphi}{2} - \sin^2\frac{\varphi}{2}\right\}\sigma_x + \frac{i}{2}\sin\varphi[\sigma_z,\sigma_x] \\
&= \cos\varphi\sigma_x + \frac{i}{2}\sin\varphi[\sigma_z,\sigma_x] \\
&= \cos\varphi\sigma_x - \sin\varphi\sigma_y
\end{aligned}$$

Thus,

$$D_z^\dagger(\varphi)S_x D_z(\varphi) = S_x\cos\varphi - S_y\sin\varphi$$

Which was expected when considering the classical action of eq. (2.1). This result also allows us to also state that,

$$\langle S_x\rangle_R = \langle S_x\rangle\cos\varphi - \langle S_y\rangle\sin\varphi$$

Both the operator $\vec{S}$ and its expectation value transform under rotation as an ordinary vector. As a useful exercise, we can also determine how kets themselves transform under rotations.

2.4 Rotations of Kets

Any ket that represents a spin-1/2 system can be written as a linear combination of the eigenvalues of S_z,

$$S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle \qquad S_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$$

Therefore,

$$\sigma_z|\uparrow\rangle = |\uparrow\rangle \qquad \sigma_z|\downarrow\rangle = -|\downarrow\rangle$$

Representation theory allows us to write $|\uparrow\rangle$ and $|\downarrow\rangle$ as,

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix} \tag{2.9}$$

We call eq. (2.9) **spinors**. Therefore an arbitrary state $|\psi\rangle$ can be written as,

$$|\psi\rangle = \psi_\uparrow|\uparrow\rangle + \psi_\downarrow|\downarrow\rangle$$

Where $\psi_\uparrow$ and $\psi_\downarrow$ are arbitrary complex numbers such that they normalize $|\psi\rangle$.

$$\langle\psi|\psi\rangle = |\psi_\uparrow|^2 + |\psi_\downarrow|^2 = 1$$

Therefore we can also represent,

$$|\psi\rangle = \begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix}$$

We can then find a particular $|\psi\rangle$ that is an eigenstate of $\vec{\sigma}\cdot\hat{n}$ where $\hat{n}$ is an arbitrary unit direction in space (and has eigenvalue $+1$).

$$\vec{\sigma}\cdot\hat{n}|\psi\rangle = |\psi\rangle$$

In spherical coordinates, we can express $\hat{n}$ in terms of θ, φ. To rotate the system from $\vec{z}$ to $\hat{n}$, we may first rotate by angle θ about the y-axis and then by φ about the z-axis. Therefore,

$$\begin{aligned}
|\psi\rangle &= e^{-\frac{i}{2}\sigma_z\varphi}e^{-\frac{i}{2}\sigma_y\theta}|\uparrow\rangle \\
&= \begin{pmatrix}\cos\frac{\varphi}{2} - i\sin\frac{\varphi}{2} & 0 \\ 0 & \cos\frac{\varphi}{2} + i\sin\frac{\varphi}{2}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}1 \\ 0\end{pmatrix} \\
&= \begin{pmatrix}e^{-i\frac{\varphi}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{\varphi}{2}}\sin\frac{\theta}{2}\end{pmatrix}
\end{aligned} \tag{2.10}$$

Next let's check if this result makes sense. Consider the expectation value of S_x,

$$\begin{aligned}
\langle\psi|S_x|\psi\rangle &= \frac{\hbar}{2}\langle\psi|\sigma_x|\psi\rangle \\
&= \frac{\hbar}{2}\left\{\psi_\uparrow^*\langle\uparrow| + \psi_\downarrow^*\langle\downarrow|\right\}\sigma_x\left\{\psi_\uparrow|\uparrow\rangle + \psi_\downarrow|\downarrow\rangle\right\} \\
&= \frac{\hbar}{2}\left(\psi_\uparrow^*\psi_\downarrow\langle\uparrow|\sigma_x|\downarrow\rangle + \psi_\downarrow^*\psi_\uparrow\langle\downarrow|\sigma_x|\uparrow\rangle\right) \\
&= \frac{\hbar}{2}\left(\psi_\uparrow^*\psi_\downarrow + \psi_\downarrow^*\psi_\uparrow\right) \\
&= \frac{\hbar}{2}\left(e^{i\varphi}\frac{1}{2}\sin\theta + e^{-i\varphi}\frac{1}{2}\sin\theta\right) \\
&= \frac{\hbar}{2}\sin\theta\cos\varphi
\end{aligned}$$

Similarly,

$$\begin{aligned}
\langle\psi|S_y|\psi\rangle &= -\frac{i\hbar}{2}\langle\psi|\sigma_y|\psi\rangle \\
&= -\frac{i\hbar}{2}\left\{\psi_\uparrow^*\langle\uparrow| + \psi_\downarrow^*\langle\downarrow|\right\}\sigma_y\left\{\psi_\uparrow|\uparrow\rangle + \psi_\downarrow|\downarrow\rangle\right\} \\
&= -\frac{i\hbar}{2}\left(\psi_\uparrow^*\psi_\downarrow\langle\uparrow|\sigma_y|\downarrow\rangle + \psi_\downarrow^*\psi_\uparrow\langle\downarrow|\sigma_y|\uparrow\rangle\right) \\
&= -\frac{i\hbar}{2}\left(\psi_\uparrow^*\psi_\downarrow - \psi_\downarrow^*\psi_\uparrow\right) \\
&= -\frac{i\hbar}{2}\left(e^{i\varphi}\frac{1}{2}\sin\theta - e^{-i\varphi}\frac{1}{2}\sin\theta\right) \\
&= \frac{\hbar}{2}\sin\theta\sin\varphi
\end{aligned}$$

Also,

$$\langle\psi|S_z|\psi\rangle = \cdots = \frac{\hbar}{2}\cos\theta$$

In summary we have the following,

$$\langle\psi|\vec{S}|\psi\rangle = \frac{\hbar}{2}(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) = \frac{\hbar}{2}\hat{n}$$

We write an arbitrary direction as,

$$\hat{n} = \sum_{a,b}\psi_a^*\vec{\sigma}_{ab}\psi_b$$

Where $a, b = \uparrow, \downarrow$ such that $|\psi_\uparrow|^2 + |\psi_\downarrow|^2 = 1$.

2.5 Euler Angles

The way we have represented rotations so far was using a unit vector $\vec{n}$ and a rotation about that axis of an amount φ. Generally, we need 3 angles to specific the most arbitrary of rotations in $\mathbb{R}^3$. Another choice different from $\{\hat{n}, \varphi\}$ are called **Euler Angles** α, β, γ.

$$R(\alpha,\beta,\gamma) = R_{z'}(\gamma)R_{y'}(\beta)R_z(\alpha)$$

1. Rotate about the z axis an angle α creating new x, y axises denoted x', y'
2. Rotate about the y' axis an angle β creating new z, x' axises denoted z', x''
3. Rotate about the z' axis an angle γ creating new x'', y' axises denoted x''', y''

How can be re-write $R(\alpha,\beta,\gamma)$ in terms of 3 rotations but with respect to axes of a *fixed* coordinate system. To do this consider the geometry (or the group algebra),

$$R_{y'}(\beta) = R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha)$$

Moreover,

$$\begin{aligned}
R_{z'}(\gamma) &= R_{y'}(\beta)R_z(\gamma)R_{y'}^{-1}(\beta) \\
&= \left(R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha)\right)R_z(\gamma)\left(R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha)\right)^{-1} \\
&= R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha)R_z(\gamma)R_z(\alpha)R_y^{-1}(\beta)R_z^{-1}(\alpha) \\
&= R_z(\alpha)R_y(\beta)R_z(\gamma+\alpha-\alpha)R_y^{-1}(\beta)R_z^{-1}(\alpha) \\
&= R_z(\alpha)R_y(\beta)R_z(\gamma)R_y^{-1}(\beta)R_z^{-1}(\alpha)
\end{aligned}$$

Therefore,

$$\begin{aligned}
R(\alpha,\beta,\gamma) &= R_{z'}(\gamma)R_{y'}(\beta)R_z(\alpha) \\
&= R_z(\alpha)R_y(\beta)R_z(\gamma)R_y^{-1}(\beta)R_z^{-1}(\alpha)R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha)R_z(\alpha) \\
&= R_z(\alpha)R_y(\beta)R_z(\gamma)R_y^{-1}(\beta)R_y(\beta) \\
&= R_z(\alpha)R_y(\beta)R_z(\gamma)
\end{aligned}$$

For spin-1/2 systems,

$$\begin{aligned}
D(\alpha,\beta,\gamma) &= D_z(\alpha)D_y(\beta)D_z(\gamma) \\
&= e^{-\frac{i}{2}\sigma_z\alpha}e^{-\frac{i}{2}\sigma_y\beta}e^{-\frac{i}{2}\sigma_z\gamma} \\
&= \left(\mathbb{1}\cos\frac{\alpha}{2} - i\sigma_z\sin\frac{\alpha}{2}\right)\left(\mathbb{1}\cos\frac{\beta}{2} - i\sigma_z\sin\frac{\beta}{2}\right)\left(\mathbb{1}\cos\frac{\gamma}{2} - i\sigma_z\sin\frac{\gamma}{2}\right)
\end{aligned}$$

$$
\begin{aligned}
&= \begin{pmatrix} e^{-i\frac{\alpha}{2}} & 0 \\ 0 & e^{i\frac{\alpha}{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} e^{-i\frac{\gamma}{2}} & 0 \\ 0 & e^{i\frac{\gamma}{2}} \end{pmatrix} \\
&= \begin{pmatrix} e^{-i\frac{\alpha}{2}} & 0 \\ 0 & e^{i\frac{\alpha}{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\beta}{2} e^{-i\frac{\gamma}{2}} & -\sin\frac{\beta}{2} e^{+i\frac{\gamma}{2}} \\ \sin\frac{\beta}{2} e^{-i\frac{\gamma}{2}} & \cos\frac{\beta}{2} e^{+i\frac{\gamma}{2}} \end{pmatrix} \\
&= \begin{pmatrix} \cos\frac{\beta}{2} e^{-i\frac{\gamma}{2}} e^{-i\frac{\alpha}{2}} & -\sin\frac{\beta}{2} e^{+i\frac{\gamma}{2}} e^{-i\frac{\alpha}{2}} \\ \sin\frac{\beta}{2} e^{-i\frac{\gamma}{2}} e^{+i\frac{\alpha}{2}} & \cos\frac{\beta}{2} e^{+i\frac{\gamma}{2}} e^{+i\frac{\alpha}{2}} \end{pmatrix} \\
&= \begin{pmatrix} \cos\frac{\beta}{2} e^{-i\frac{\gamma+\alpha}{2}} & -\sin\frac{\beta}{2} e^{+i\frac{\gamma-\alpha}{2}} \\ \sin\frac{\beta}{2} e^{-i\frac{\gamma-\alpha}{2}} & \cos\frac{\beta}{2} e^{+i\frac{\gamma+\alpha}{2}} \end{pmatrix}
\end{aligned}
$$

This is the operator of rotation by 3 Euler angles for a spin-1/2 system. This is a 2D representation of the algebra of rotations in 3D space. How can we generalize these results to different angular momentum?

2.6 Theory of Angular Momentum of Arbitrary Size

Consider the angular momentum operator $\vec{J}$ and its square,

$$\vec{J}^2 = J_x^2 + J_y^2 + J_z^2$$

Next consider the commutator with J_z,

$$
\begin{aligned}
\left[\vec{J}^2, J_z\right] &= \left[J_x^2 + J_y^2 + J_z^2, J_z\right] \\
&= \left[J_x^2 + J_y^2, J_z\right] \\
&= J_x^2 J_z - J_z J_x^2 + J_y^2 J_z - J_z J_y^2
\end{aligned}
$$

This can be written in terms of other commutators,

$$
\begin{aligned}
J_x[J_x, J_z] + [J_x, J_z]J_x &= J_x(J_xJ_z - J_zJ_x) + (J_xJ_z - J_zJ_x)J_x \\
&= (J_xJ_xJ_z - J_xJ_zJ_x) + (J_xJ_zJ_x - J_zJ_xJ_x) \\
&= J_xJ_xJ_z - J_zJ_xJ_x \\
&= J_x^2 J_z - J_z J_x^2
\end{aligned}
$$

Return to the above equation and making use of $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$,

$$
\begin{aligned}
\left[\vec{J}^2, J_z\right] &= J_x[J_x, J_z] + [J_x, J_z]J_x + J_y[J_y, J_z] + [J_y, J_z]J_y \\
&= i\hbar(-J_xJ_y - J_yJ_x + J_yJ_x + J_xJ_y) \\
&= 0
\end{aligned}
$$

Therefore the J_z commutes with $\vec{J}^2$. This also holds for all other components,

$$\left[\vec{J}^2, J_x\right] = \left[\vec{J}^2, J_y\right] = \left[\vec{J}^2, J_z\right] = 0$$

Compactly we may write,

$$\left[\vec{J}^2, \vec{J}\right] = \vec{0}$$

This result means we can choose angular momentum eigenstates to be simultaneous eigenstates of $\vec{J}^2$ and J_z. Let us explicitly calculate those eigenstates. Let $|a, b\rangle$ be this eigenstate where a is the eigenvalue of $\vec{J}^2$ and b is the eigenvalue of J_z,

$$
\begin{aligned}
\vec{J}^2|a, b\rangle &= a|a, b\rangle \\
J_z|a, b\rangle &= b|a, b\rangle
\end{aligned}
\tag{2.11}
$$

In order to solve for $|a,b\rangle$, define the following operators,

$$J_\pm = J_x \pm iJ_y \tag{2.12}$$

Note that $J_\pm$ are *not* Hermitian operators,

$$J_\pm^\dagger = J_\mp$$

We have the following properties,

$$\begin{aligned}[J_+, J_-] &= [J_x + iJ_y, J_x - iJ_y] \\ &= -i[J_x, J_y] + i[J_y, J_x] \\ &= -2i[J_x, J_y] \\ &= -2i(i\hbar J_z) \\ &= 2\hbar J_z \end{aligned} \tag{2.13}$$

Also,

$$\begin{aligned}[J_z, J_\pm] &= [J_z, J_x \pm iJ_y] \\ &= [J_z, J_x] \pm i[J_z, J_y] \\ &= i\hbar\epsilon_{zxy} J_y \pm i^2\hbar\epsilon_{zyx} J_x \\ &= i\hbar J_y - \mp\hbar J_x \\ &= i\hbar J_y \pm \hbar J_x \\ &= \pm\hbar J_\pm \end{aligned} \tag{2.14}$$

Finally,

$$\left[\vec{J}^2, J_\pm\right] = 0$$

We now solve eq. (2.11),

$$\begin{aligned} J_z J_+ |a,b\rangle &= ([J_z, J_+] + J_+ J_z)|a,b\rangle \\ &= (\hbar J_+ + J_+ J_z)|a,b\rangle \quad \text{Using eq. (2.14)} \\ &= (\hbar J_+ + bJ_+)|a,b\rangle \quad \text{Using eq. (2.11)} \\ &= (\hbar + b)J_+|a,b\rangle \end{aligned}$$

Thus $J_+|a,b\rangle$ is still an eigenket of J_z but with eigenvalue of $b + \hbar$. Analogously,

$$J_z J_- |a,b\rangle = (b - \hbar)J_-|a,b\rangle$$

In conclusion, J_+ increases the eigenvalue of J_z by $\hbar$ while J_- decreases it by $\hbar$. $J_\pm$ are called **ladder operators** (raising and lowering operators) because of this property. What about the eigenvalues of $\vec{J}^2$?

$$\vec{J}^2 J_+|a,b\rangle = J_+\vec{J}^2|a,b\rangle = aJ_+|a,b\rangle$$

No, J_+ doesn't affect the eigenvalues of $\vec{J}^2$.

Is there an upper limit to the eigenvalues of J_z? Notice that,

$$\begin{aligned}\vec{J}^2 - J_z^2 &= J_x^2 + J_y^2 \\ &= \left\{\frac{1}{2}(J_+ + J_-)\right\}^2 + \left\{\frac{1}{2i}(J_+ - J_-)\right\}^2 \\ &= \frac{1}{4}\Big\{(J_+ + J_-)^2 - (J_+ - J_-)^2\Big\} \\ &= \frac{1}{4}\big(J_+^2 + J_-^2 + J_+J_- + J_-J_+ - J_+^2 - J_-^2 + J_+J_- + J_-J_+\big)\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}(J_+J_- + J_-J_+) \\
&= \frac{1}{2}\left(J_+J_+^\dagger + J_+^\dagger J_+\right)
\end{aligned}
$$

Looking at matrix elements,

$$
\begin{aligned}
\langle a,b|\vec{J}^2 - J_z^2|a,b\rangle &= \left(a - b^2\right) \\
&= \frac{1}{2}\langle a,b|\left(J_+J_+^\dagger + J_+^\dagger J_+\right)|a,b\rangle \\
&= \frac{1}{2}\langle a,b|J_+J_+^\dagger|a,b\rangle + \frac{1}{2}\langle a,b|J_+^\dagger J_+|a,b\rangle
\end{aligned}
$$

Notice that $\langle a,b|J_+J_+^\dagger|a,b\rangle$ can be written,

$$
\langle a,b|J_+J_+^\dagger|a,b\rangle = \{\langle a,b|J_+\}\left\{J_+^\dagger|a,b\rangle\right\} = \left|J_+^\dagger|a,b\rangle\right|^2 \geq 0
$$

Therefore,

$$
\begin{gathered}
\left(a - b^2\right) = \frac{1}{2}\left(\left|J_+^\dagger|a,b\rangle\right|^2 + |J_+|a,b\rangle|^2\right) \geq 0 \\
b^2 \leq a \\
-\sqrt{a} \leq b \leq \sqrt{a}
\end{gathered}
$$

This is nothing more than a consequence of $\left\langle \vec{J}^2 \right\rangle \geq \left\langle J_z^2 \right\rangle$. We can conclude that there must be some eigenvalue b_{max} that is the maximum eigenvalue of J_z such that,

$$
J_+|a,b_{\text{max}}\rangle = 0
$$

We also obtain,

$$
J_-J_+|a,b_{\text{max}}\rangle = J_- \cdot 0 = 0
$$

On the other hand,

$$
\begin{aligned}
J_-J_+|a,b_{\text{max}}\rangle &= (J_x - iJ_y)(J_x + iJ_y)|a,b_{\text{max}}\rangle \\
&= \left(J_x^2 + J_y^2 + iJ_xJ_y - iJ_yJ_x\right)|a,b_{\text{max}}\rangle \\
&= \left(J_x^2 + J_y^2 + i[J_x,J_y]\right)|a,b_{\text{max}}\rangle \\
&= \left(\vec{J}^2 - J_z^2 - \hbar J_z\right)|a,b_{\text{max}}\rangle \\
&= \left(a - b_{\text{max}}^2 - \hbar b_{\text{max}}\right)|a,b_{\text{max}}\rangle
\end{aligned}
$$

Therefore,

$$
\left(a - b_{\text{max}}^2 - \hbar b_{\text{max}}\right) = 0 \implies a = b_{\text{max}}(b_{\text{max}} + \hbar) \tag{2.15}
$$

Analogously we must have b_{min} such that,

$$
J_-|a,b_{\text{min}}\rangle = 0
$$

Skipping details we have the following property,

$$
a = b_{\text{min}}(b_{\text{min}} - \hbar) \tag{2.16}
$$

Combining eqs. (2.16) and (2.15),

$$
a = b_{\text{min}}(b_{\text{min}} - \hbar) = b_{\text{max}}(b_{\text{max}} + \hbar)
$$

This is only possible if $b_{\text{min}} = -b_{\text{max}}$. Imagine that one starts from $|a, b_{\text{min}}\rangle$. After a certain number of repeated applications of J_+, one must arise at $|a, b_{\text{max}}\rangle$.

$$J_+^n|a, b_{\text{min}}\rangle = (b_{\text{min}} + n\hbar)|a, b_{\text{min}} + n\hbar\rangle = b_{\text{max}}|a, b_{\text{max}}\rangle$$

Therefore,

$$2b_{\text{max}} = n\hbar \implies b_{\text{max}} = \frac{n\hbar}{2}$$

Defining $j = b_{\text{max}}/\hbar$ we have that,

$$j = \frac{n}{2}$$

Which is either an integer or a half-integer. Making use of eq. (2.15),

$$a = b_{\text{max}}(b_{\text{max}} + \hbar) = \hbar j(\hbar j + \hbar) = \hbar^2 j(j + 1)$$

Similarly we can say that $b = m\hbar$ where m ranges from $-j$ to j.

$$m = -j, -j + 1, \ldots, j - 1, j$$

Thus there are $2j + 1$ potential values for m. Moving forward, we replace eq. (2.11) we the more familiar,

$$\begin{aligned}\vec{J}^2|j, m\rangle &= \hbar^2 j(j + 1)|j, m\rangle \\ J_z^2|j, m\rangle &= \hbar m|j, m\rangle \\ -j \leq m &\leq j\end{aligned}$$

Where $j = n/2$ is the magnitude of the angular momentum. As an example, $j = 1/2$ is the spin of the electron. The matrix elements for $\vec{J}^2$ and J_z can be computed easily,

$$\begin{aligned}\langle j', m'|\vec{J}^2|j, m\rangle &= \hbar^2 j(j + 1)\langle j', m'|j, m\rangle \\ &= \hbar^2 j(j + 1)\delta_{jj'}\delta_{mm'}\end{aligned}$$

$$\begin{aligned}\langle j', m'|J_z|j, m\rangle &= \hbar m\langle j', m'|j, m\rangle \\ &= \hbar m\delta_{jj'}\delta_{mm'}\end{aligned}$$

Moreover we can compute expectations for J_-J_+,

$$\begin{aligned}\langle j, m|J_-J_+|j, m\rangle &= \langle j, m|J_+^\dagger J_+|j, m\rangle \\ &= \langle j, m|\vec{J}^2 - J_z^2 - \hbar J_z|j, m\rangle \\ &= \hbar^2 j(j + 1) - \hbar^2 m^2 - \hbar^2 m \\ &= \hbar^2 j(j + 1) - \hbar^2 m(m + 1)\end{aligned} \tag{2.17}$$

For completeness, we should also calculate the expectations for J_+ and J_-. We know that the raising and lower operators satisfy,

$$\begin{aligned}J_+|j, m\rangle &= C_{jm}^+|j, m + 1\rangle \\ J_-|j, m\rangle &= C_{jm}^-|j, m - 1\rangle\end{aligned}$$

Being clever, recognize that eq. (2.17) is related to $J_+|j, m\rangle$,

$$|J_+|j, m\rangle|^2 = \left|C_{jm}^+\right|^2 = \hbar^2 j(j + 1) - \hbar^2 m(m + 1)$$

Choose C_{jm}^+ to be real and positive,

$$C_{jm}^+ = \hbar\sqrt{j(j + 1) - m(m + 1)}$$

Which allows us to write,

$$J_+|j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j,m+1\rangle$$

A similar analysis of J_- gives the relation,

$$J_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle$$

This result is sufficient for determining the matrix elements of J_+, J_-,

$$\langle j',m'|J_+|j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}\delta_{jj'}\delta_{m',m+1}$$
$$\langle j',m'|J_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}\delta_{jj'}\delta_{m',m-1}$$

Recalling the definition of J_+, J_- (eq. (2.12)),

$$J_x = \frac{1}{2}(J_+ + J_-) \qquad J_y = \frac{1}{2i}(J_+ - J_-)$$

Therefore we now know explicitly what the matrix elements of J_x, J_y are. J_z has matrix elements,

$$J_z|\psi\rangle = \sum_{i,m,j',m'} |j',m'\rangle\langle j',m'|J_z|j,m\rangle\langle j_m|\psi\rangle$$

Returning to the rotation representations,

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

Since $\vec{J}^2$ commutes with any component of $\vec{J}$,

$$\left[\vec{J}^2, D(R)\right] = 0$$

Therefore we can determine $D(R)|j,m\rangle$ by first examining,

$$\vec{J}^2 D(R)|j,m\rangle = D(R)\vec{J}^2|j,m\rangle = \hbar^2 j(j+1)D(R)|j,m\rangle$$

This rotated eigenket of $\vec{J}^2$ is still an eigenket of $\vec{J}^2$ with the same eigenvalue $\hbar^2 j(j+1)$. However, $D(R)$ is general does not commute with J_z,

$$[J_z, D(R)] \neq 0$$

$$\begin{aligned}
D(R)|j,m\rangle &= \sum_{j',m'} |j',m'\rangle\langle j',m'|D(R)|j,m\rangle \\
&= \sum_{j,m'} |j,m'\rangle\langle j,m'|D(R)|j,m\rangle \quad \text{Orthogonal} \\
&= \sum_{j,m'} |j,m'\rangle D^{(j)}_{m'm}(R) \quad \text{Notation}
\end{aligned}$$

We refer to this as a $2j+1$ dimensional representation of the group of rotations. $D^{(j)}_{m'm}(R)$ is a $(2j+1) \times (2j+1)$ matrix of probability amplitudes to find the system in a state $|j,m'\rangle$ after a rotation. Recalling Euler angles,

$$D(\alpha,\beta,\gamma) = e^{-\frac{i}{\hbar}J_z\alpha}e^{-\frac{i}{\hbar}J_y\beta}e^{-\frac{i}{\hbar}J_z\gamma}$$

We can write $D^{(j)}_{m'm}(R)$ in terms of α, β, γ,

$$D^{(j)}_{m'm}(\alpha,\beta,\gamma) = \langle j,m'|e^{-\frac{i}{\hbar}J_z\alpha}e^{-\frac{i}{\hbar}J_y\beta}e^{-\frac{i}{\hbar}J_z\gamma}|j,m\rangle$$

This is very useful because J_z has $|j,m\rangle$ as an eigenket. The only non-trivial operator is $e^{-\frac{i}{\hbar}J_y\beta}$. Replacing J_z with relevant eigenvalues,

$$D^{(j)}_{m'm}(\alpha,\beta,\gamma) = \langle j,m'|e^{-\frac{i}{\hbar}(\hbar m')\alpha}e^{-\frac{i}{\hbar}J_y\beta}e^{-\frac{i}{\hbar}(\hbar m)\gamma}|j,m\rangle$$

Extracting out constants,

$$\begin{aligned} D^{(j)}_{m'm}(\alpha,\beta,\gamma) &= e^{-\frac{i}{\hbar}\left(\hbar m'\right)\alpha} e^{-\frac{i}{\hbar}(\hbar m)\gamma} \langle j,m'|e^{-\frac{i}{\hbar}J_y\beta}|j,m\rangle \\ &= e^{-i\left(m'\alpha+m\gamma\right)} \underbrace{\langle j,m'|e^{-\frac{i}{\hbar}J_y\beta}|j,m\rangle}_{d^{(j)}_{m'm}(\beta)} \end{aligned}$$

Compactly we write $d^{(j)}_{m'm}$ as the matrix elements for $e^{-\frac{i}{\hbar}J_y\beta}$,

$$D^{(j)}_{m'm}(\alpha,\beta,\gamma) = e^{-i\left(m'\alpha+m\gamma\right)} d^{(j)}_{m'm}(\beta)$$

Compare this with the $j = 1/2$ result,

$$D^{(1/2)}(\alpha,\beta,\gamma) = \begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}$$

Where we used the basis of the eigenstates of S_z ($\{|\uparrow\rangle, |\downarrow\rangle\}$). In this case $j = 1/2$ and $m = \pm 1/2$.

$$|\uparrow\rangle = |m = 1/2\rangle \qquad |\downarrow\rangle = |m = -1/2\rangle$$

$$d^{1/2}_{m'm}(\beta) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}$$

2.7 Orbital and Spin Angular Momentum

Up until now we have only discuss the total angular momentum $\vec{J}$ and the spin angular momentum $\vec{S}$. They are related to the **orbital angular momentum** $\vec{L}$,

$$\vec{J} = \vec{L} + \vec{S}$$

The orbital angular momentum is defined in terms of its classic definition,

$$\vec{L} = \vec{r} \times \vec{p}$$

Where $\vec{r}$ and $\vec{p}$ are both operators. We must have the canonical commutation relation,

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$$

We can check this relation by examining $[L_x, L_y]$ directly,

$$\begin{aligned} [L_x, L_y] &= [yp_z - zp_y, zp_x - xp_z] \\ &= [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z] \\ &= [yp_z, zp_x] - \cancelto{0}{[y,x]} p_z - z\cancelto{0}{[p_y,p_x]} + [zp_y, xp_z] \\ &= [yp_z, zp_x] + [zp_y, xp_z] \\ &= yp_x[p_z, z] + p_y x[z, p_z] \\ &= -i\hbar(yp_x - xp_y) \\ &= i\hbar L_z \end{aligned}$$

Next consider spin-less infinitesimal rotations about the z-axis. In such spin-less cases $\vec{J} = \vec{L}$.

$$D_z(\delta\varphi) = e^{-\frac{i}{\hbar}L_z\delta\varphi} = \mathbb{1} - \frac{i}{\hbar}L_z\delta\varphi + \mathcal{O}\left(\delta\varphi^2\right)$$

In terms of the linear momentum operators, Acting on a position eigenket $|\vec{x}\,'\rangle$ is,

$$D_z(\delta\varphi)|\vec{x}\,'\rangle = D_z(\delta\varphi)|x', y', z'\rangle$$

$$= \left[\mathbb{1} - \frac{i}{\hbar}(xp_y - yp_x)\delta\varphi\right]|x', y', z'\rangle$$

Recalling that,

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

We have that,

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

Returning to the rotation operator,

$$D_z(\delta\varphi)|\vec{x}\,'\rangle = |x' - \delta\varphi y', y' + \delta\varphi x', z'\rangle$$

This is exactly the classical action of rotating a vector $\vec{x}\,'$. Recall the infinitesimal rotation matrix,

$$R_z(\delta\varphi)\cdot\vec{x}\,' = \begin{pmatrix}\cos\delta\varphi & -\sin\delta\varphi & 0\\ \sin\delta\varphi & \cos\delta\varphi & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x'\\ y'\\ z'\end{pmatrix} = \begin{pmatrix}1 & -\delta\varphi & 0\\ \delta\varphi & 1 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x'\\ y'\\ z'\end{pmatrix} = \begin{pmatrix}x' - \delta\varphi y'\\ y' + \delta\varphi x'\\ z'\end{pmatrix}$$

What affect does rotation have on wave functions $\psi(\vec{x}\,') = \langle\vec{x}\,'|\psi\rangle$?

$$\begin{aligned}\langle\vec{x}\,'|\mathbb{1} - \frac{i}{\hbar}L_z\delta\varphi|\psi\rangle &= \left\{\langle\psi|\mathbb{1} + \frac{i}{\hbar}L_z\delta\varphi|\vec{x}\,'\rangle\right\}^* \\ &= \left\{\langle\psi|\mathbb{1} + \frac{i}{\hbar}(xp_y - yp_x)\delta\varphi|x', y', z'\rangle\right\}^* \\ &= \left\{\langle\psi|x' + \delta\varphi y', y' - \delta\varphi x', z'\rangle\right\}^* \\ &= \langle x' + \delta\varphi y', y' - \delta\varphi x', z'|\psi\rangle\end{aligned}$$

It will be helpful (as it is classically) to represent these types of rotations in spherical coordinates.

$$\vec{x}\,' = x'\hat{x} + y'\hat{y} + z'\hat{z} = r\hat{r}$$

Where,

$$\begin{aligned}x' &= r\sin\theta\cos\varphi \\ y' &= r\sin\theta\sin\varphi \\ z' &= r\cos\theta \\ r &= \sqrt{x'^2 + y'^2 + z'^2}\end{aligned}$$

The only effect of rotation about the z-axis is that $\varphi \mapsto \varphi - \delta\varphi$.

$$\langle r,\theta,\varphi|\mathbb{1} - \frac{i}{\hbar}L_z\delta\varphi|\psi\rangle = \langle r,\theta,\varphi - \delta\varphi|\psi\rangle$$

As a first order Taylor series,

$$\begin{aligned}\langle r,\theta,\varphi - \delta\varphi|\psi\rangle &= \langle r,\theta,\varphi|\psi\rangle - \delta\varphi\frac{\partial}{\partial\varphi}\langle r,\theta,\varphi|\psi\rangle \\ &= \langle r,\theta,\varphi|\psi\rangle - \frac{i}{\hbar}\delta\varphi\langle r,\theta,\varphi|L_z|\psi\rangle\end{aligned}$$

Therefore,

$$L_z = -i\hbar\frac{\partial}{\partial\varphi}$$

In spherical coordinates,

$$\hat{r} = \hat{x}\sin\theta\cos\varphi + \hat{y}\sin\theta\sin\varphi + \hat{z}\cos\theta$$

$$\hat{\varphi} = -\hat{x}\sin\varphi + \hat{y}\cos\varphi$$
$$\hat{\theta} = \hat{x}\cos\varphi\cos\theta + \hat{y}\sin\varphi\cos\theta - \hat{z}\sin\theta$$

These unit directions can be used to determine,

$$L_x = yp_z - zp_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$L_y = zp_x - xp_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

Or more compactly,

$$\begin{aligned}\vec{\nabla} &= \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} \\ &= \hat{r}\frac{\partial}{\partial r} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}\end{aligned}$$

Therefore derivatives in the x, y, z directions can be written in terms of θ, φ derivatives,

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}$$
$$\frac{\partial}{\partial y} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta}$$
$$\frac{\partial}{\partial x} = \sin\theta\cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta}$$

Therefore,

$$\vec{L}^{\,2} = L_x^2 + L_y^2 + L_z^2 = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]$$

Moreover in just the same way that $\left[\vec{J}^{\,2}, J_z\right] = 0$ we have that,

$$\left[\vec{L}^{\,2}, L_z\right] = 0$$

Just as we derived eigenstates common to both $\vec{J}^{\,2}$ and J_z, we derive eigenstates of $\vec{L}^{\,2}$ and L_z. This can also be derived by noticing that $\vec{L}^{\,2}$ is only a function of $\vec{\theta}$. The common eigenstates of $\vec{L}^{\,2}, L_z$ are,

$$\vec{L}^{\,2}|\ell, m\rangle = \hbar^2\ell(\ell+1)|\ell, m\rangle$$
$$L_z|\ell, m\rangle = \hbar m|\ell, m\rangle$$

Where $m = -\ell, -\ell+1, \cdots, \ell-1, \ell$. We can also define the wave function,

$$\langle\theta, \varphi|l, m\rangle = Y_\ell^m(\theta, \varphi)$$

Such that $|Y_\ell^m(\theta, \varphi)|^2$ is the probability of finding a particle in state $|\ell, m\rangle$ at $|\theta, \varphi\rangle$. We call Y_ℓ^m **spherical harmonics**. They have a number of useful properties,

$$\langle\theta, \varphi|L_z|\ell, m\rangle = -i\hbar\frac{\partial}{\partial\varphi}Y_\ell^m(\theta, \varphi) = \hbar m Y_\ell^m(\theta, \varphi)$$

This differential equation fixes the φ dependence of $Y_\ell^m(\theta, \varphi)$ to be,

$$Y_\ell^m(\theta, \varphi) \sim e^{im\varphi}$$

Now since $\vec{L}^{\,2}$ only depends on θ,

$$-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]Y_\ell^m(\theta, \varphi) = \hbar^2\ell(\ell+1)Y_\ell^m(\theta, \varphi)$$

Using separation of variables (for θ, φ) we get,

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{m^2}{\sin^2\theta} + \ell(\ell+1)\right]Y_\ell^m(\theta,\varphi) = 0$$

Whose solutions are the spherical harmonics. The solution has the following form,

$$Y_\ell^m(\theta,\varphi) = (-1)^m\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\varphi} \tag{2.18}$$

Where $P_\ell^m(x)$ are the **Legendre Polynomials**. Remember that for the total angular momentum $\vec{J}$ had magnitude j where j was either an integer or half-integer. A question is posed: *Does this also hold true for ℓ?* It turns out it is not true. Consider that there is a rotational symmetry $\varphi \mapsto \varphi + 2\pi$. Therefore,

$$Y_\ell^m(\theta,\varphi) = Y_\ell^m(\theta,\varphi+2\pi)$$

Inspecting eq. (2.18) and this rotational property, one should see that,

$$e^{im\varphi} = e^{im(\varphi+2\pi)} \implies e^{2\pi i m} = 1$$

This implies that m must be an integer which enforces that ℓ is also an integer. ℓ cannot be a half-integer.

3 Symmetries in Quantum Mechanics

Suppose S is a transformation operation, such as T or D. For an infinitesimal transformation,

$$S = \mathbb{1} - \frac{i\epsilon}{\hbar}G$$

Where G is a Hermitian operator (this is a consequence of S being assumed unitary) and $\epsilon \ll 1$. Suppose the Hamiltonian H is invariant with respect to S,

$$S^\dagger H S = H$$

As an example $H = \vec{p}^2/2m$ has $T^\dagger(\vec{a})HT(\vec{a}) = H$ symmetry. Also $H = \vec{p}^2/2m + V(r)$ has $D^\dagger H D = H$ rotational symmetry (provided V is spherically symmetric). In general,

$$\begin{aligned} S^\dagger H S &= \left(\mathbb{1} + \frac{i\epsilon}{\hbar}G\right)H\left(\mathbb{1} - \frac{i\epsilon}{\hbar}G\right) \\ &= H + \frac{i\epsilon}{\hbar}GH - \frac{i\epsilon}{\hbar}HG + \mathbb{1}\cdot\mathcal{O}(\epsilon^2) \\ &= H + \frac{i\epsilon}{\hbar}[G,H] \end{aligned}$$

If S is to be a symmetry, $[G,H] = 0$. The generator G of S must commute with H. The Heisenberg equation of motion for G then becomes,

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{i}{\hbar}[H,G] = 0$$

G represents a conserved physical quantity. If a system is invariant with respect to symmetry transformation S, the generator of S is a conserved quantity. Since S is unitary,

$$S^\dagger H S = S^{-1}HS = H \implies [H,S] = 0$$

This allows us to consider energy eigenkets $|n\rangle$ of H with eigenvalue E_n.

$$\begin{aligned} H|n\rangle &= E_n|n\rangle \\ HS|n\rangle &= SH|n\rangle = E_nS|n\rangle \end{aligned}$$

Therefore $S|n\rangle$ is also an eigenket of H with eigenvalue E_n. Therefore $|n\rangle$ and $S|n\rangle$ are degenerate eigenkets of H. Symmetries in quantum mechanics are always associated with degeneracies.

As a case study, consider a rotationally invariant system,

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

Such that $[H, D(R)] = 0$. This implies that $\vec{J}$ (the generator of D) is,

$$\left[H, \vec{J}\right] = 0$$

Therefore $|j, m\rangle$ are also eigenstates of H.

$$H|n, j, m\rangle = E_n|n, j, m\rangle$$

We have that $D(R)|n, j, m\rangle$ is also and eigenket of H. Multiplying by the closure relation,

$$D(R)|n, j, m\rangle = \sum_{m'} |n, j, m'\rangle \underbrace{\langle n, j, m'|D(R)|n, j, m\rangle}_{D^{(j)}_{m'm}(R)}$$

This can only be true for arbitrary rotations $D(R)$ if,

$$H|n, j, m\rangle = E_n|n, j, m\rangle \quad \forall m = -j, \ldots, j$$

All eigenstates of H are at least $2j + 1$-fold degenerate.

Rotations are an example of continuous symmetry. There are also discrete symmetries (example: parity).

3.1 Parity Symmetry

Consider the parity operator π,

$$|\psi\rangle \mapsto \pi|\psi\rangle$$

We define the parity operator to reverse the sign of position expectations,

$$\langle\psi|\pi^\dagger \vec{x}\pi|\psi\rangle = -\langle\psi|\vec{x}|\psi\rangle$$

Which is equivalent to $\pi^\dagger \vec{x}\pi = -\vec{x}$.

$$\langle\psi|\pi^\dagger\pi|\psi\rangle = \langle\psi|\psi\rangle = 1 \implies \pi^\dagger\pi = \mathbb{1}$$

Therefore $\pi^\dagger = \pi^{-1}$ is a unitary operator.

$$\pi^{-1}\vec{x}\pi = -\vec{x}$$
$$\vec{x}\pi = -\pi\vec{x}$$
$$\vec{x}\pi + \pi\vec{x} = \{\vec{x}, \pi\} = 0$$

We say that π and $\vec{x}$ anti-commute. When acting on position eigenkets,

$$\vec{x}\pi|\vec{x}\,'\rangle = -\pi\vec{x}|\vec{x}\,'\rangle = -\pi\vec{x}\,'|\vec{x}\,'\rangle = -\vec{x}\,'\pi|\vec{x}\,'\rangle$$

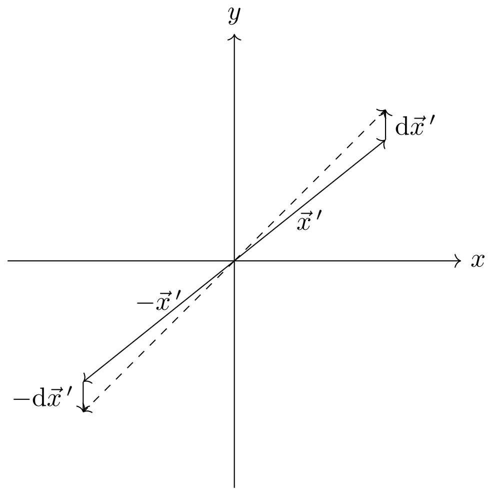
This result demonstrates that $\pi|\vec{x}\,'\rangle$ is an eigenket of $\vec{x}$ with eigenvalue $-\vec{x}\,'$. We may choose an arbitrary phase δ such that $\pi|\vec{x}\,'\rangle = e^{i\delta}$ so we choose $e^{i\delta} = 1$.

$$\pi|\vec{x}\,'\rangle = |-\vec{x}\,'\rangle$$

Thus π^2 has a determinined form,

$$\pi^2|\vec{x}\,'\rangle = \pi|-\vec{x}\,'\rangle = |\vec{x}\,'\rangle$$

Since $\pi^2 = \mathbb{1}$, $\pi^{-1} = \pi = \pi^\dagger$. The parity operator is not only unitary, but also Hermitian. The eigenvalues of π are ± 1. Notice that the order of party and translation operators matters.



Explicitly,

$$\pi T(\mathrm{d}\vec{x}\,') = T(-\mathrm{d}\vec{x}\,')\pi \implies \pi T(\mathrm{d}\vec{x}\,')\pi^\dagger = T(-\mathrm{d}\vec{x}\,')$$

As an infinitesimal translation,

$$\pi\left(\mathbb{1} - \frac{i}{\hbar}\vec{p}\cdot \mathrm{d}\vec{x}\,'\right)\pi^\dagger = \left(\mathbb{1} + \frac{i}{\hbar}\vec{p}\cdot \mathrm{d}\vec{x}\,'\right)$$

$$\pi\pi^\dagger - \frac{i}{\hbar}\pi\vec{p}\pi^\dagger \cdot \mathrm{d}\vec{x}\,' = \mathbb{1} + \frac{i}{\hbar}\vec{p}\cdot \mathrm{d}\vec{x}\,'$$

$$\pi\vec{p}\pi^\dagger = \pi^\dagger\vec{p}\pi = -\vec{p}$$

Both position $\vec{x}$ and momentum $\vec{p}$ operators have odd symmetry under parity. This leads us to see that $\vec{L} = \vec{x}\times\vec{p}$ is even under parity.

$$\pi^\dagger \vec{L}\pi = \vec{L}$$

As a matrix, we can represent the parity operator as,

$$R_\pi = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

R_π will commute with any rotation matrix R.

$$[R_\pi, R] = 0 \implies [\pi, D(R)] = 0$$

As an infinitesimal rotation,

$$D(R) = \mathbb{1} - \frac{i}{\hbar}\vec{J}\cdot\hat{n}\mathrm{d}\varphi$$

We have that,

$$\pi^\dagger\left(\mathbb{1} - \frac{i}{\hbar}\vec{J}\cdot\hat{n}\mathrm{d}\varphi\right)\pi = \mathbb{1} - \frac{i}{\hbar}\vec{J}\cdot\hat{n}\mathrm{d}\varphi$$

$$\pi^\dagger\vec{J}\pi = \vec{J}$$

$\vec{J}$ is even under parity. We say that $\vec{x}$ and $\vec{p}$ are polar vectors ad $\vec{J}$ is an axial vector. Scalar operators that change sign under parity are called **pseudoscalars**.

$$\text{Scalar:} \quad \pi^\dagger\vec{p}\cdot\vec{x}\pi = \vec{p}\cdot\vec{x}$$
$$\text{Pseudoscalar:} \quad \pi^\dagger\vec{J}\cdot\vec{x}\pi = -\vec{J}\cdot\vec{x}$$

How does parity affect the wave function $\psi(\vec{x}\,') = \langle \vec{x}\,'|\psi\rangle$?

$$\langle \vec{x}\,'|\pi|\psi\rangle = \langle \psi|\pi^\dagger|\vec{x}\,'\rangle^* = \langle \psi|\pi|\vec{x}\,'\rangle^* = \langle \psi|-\vec{x}\,'\rangle^* = \langle -\vec{x}\,'|\psi\rangle = \psi(-\vec{x}\,')$$

Now consider that $|\psi\rangle$ is a eigenket of π ($\pi|\psi\rangle = \pm|\psi\rangle$).

$$\langle \vec{x}\,'|\pi|\psi\rangle = \psi(-\vec{x}\,') = \pm\langle \vec{x}\,'|\psi = \pm\psi(\vec{x}\,')$$

Therefore the wavefunction of a parity eigenstate is either an even function or an odd function. For example, an eigenstate of $\vec{p}$ can never be a parity eigenstate because π and $\vec{p}$ do not commute,

$$\pi^\dagger\vec{p}\pi = -\vec{p} \implies [\pi, \vec{p}] \neq 0$$

In contrast, the angular momentum operator does commute with π,

$$\pi^\dagger\vec{L}\pi = \vec{L} \implies \left[\pi, \vec{L}\right] = 0$$

Therefore the eigenstates of $\vec{L}$ are simultaneously eigenstates of π and thus have definite parity.

How do the Spherical Harmonics transform under parity?

$$\begin{aligned} \vec{L}^2 Y_\ell^m(\theta,\varphi) &= \hbar^2\ell(\ell+1)Y_\ell^m(\theta,\varphi) \\ L_z Y_\ell^m(\theta,\varphi) &= \hbar m Y_\ell^m(\theta,\varphi) \end{aligned}$$

It should be clear that under parity, $\theta \mapsto \pi - \theta$ and $\varphi \mapsto \varphi + \pi$. A property of the Legendre Polynomials gives the following relationship,

$$Y_\ell^m(\pi-\theta, \varphi+\pi) = (-1)^\ell Y_\ell^m(\theta,\varphi)$$

Therefore,

$$\pi|\ell, m\rangle = (-1)^\ell|\ell, m\rangle$$

States with even integer angular momentum ℓ are parity even while states with odd integer ℓ are always parity odd.

Let us assume that H commutes with π ($[H, \pi] = 0$). For example,

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

If $\pi^\dagger V(\vec{x})\pi = V(\vec{x})$ then we have $\pi^\dagger H\pi = H$. Next consider an eigenket of this Hamiltonian,

$$H|n\rangle = E_n|n\rangle$$

Further condition $|n\rangle$ to be non-degenerate. We will now show that $|n\rangle$ is also a parity eigenstate (i.e. either parity even or parity odd). Consider the state $\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle$ and the action of π on it,

$$\pi\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle = \frac{1}{2}(\pi \pm \mathbb{1})|n\rangle = \pm\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle$$

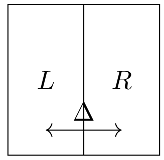
Therefore $\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle$ is an eigenstate of π. Now examine the action of H on this special state. Since H commutes with π,

$$H\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle = \frac{1}{2}(\mathbb{1} \pm \pi)H|n\rangle = E_n\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle$$

Therefore $\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle$ is an eigenstate of H with eigenvalue E_n. Since the eigenstates of H are assumed non-degenerate,

$$\frac{1}{2}(\mathbb{1} \pm \pi)|n\rangle = |n\rangle \implies \pi|n\rangle = \pm|n\rangle$$

As an example, suppose we have the following system.



Where $|L\rangle$ indicates that the particle is on the left half and $|R\rangle$ indicates that the particle is on the right half. The tunneling Hamiltonian becomes,

$$H = -\Delta(|L\rangle\langle R| + |R\rangle\langle L|)$$

The parity operator takes $|L\rangle$ to $|R\rangle$ and vice versa. As a matrix,

$$H = \begin{pmatrix} 0 & -\Delta \\ -\Delta & 0 \end{pmatrix} \qquad E_{\pm} = \pm\Delta$$

The energy eigenstates are,

$$\begin{aligned} E_- = -\Delta &\implies |S\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle) \\ E_+ = +\Delta &\implies |A\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle) \end{aligned}$$

As a demonstration of $H|S\rangle \propto |S\rangle$,

$$\begin{aligned} H|S\rangle &= -\Delta(|L\rangle\langle R| + |R\rangle\langle L|)\frac{1}{\sqrt{2}}(|L\rangle + |R\rangle) \\ &= -\frac{\Delta}{\sqrt{2}}\left(|L\rangle\cancelto{0}{\langle R|L\rangle} + |R\rangle\langle L|L\rangle + |R\rangle\cancelto{0}{\langle L|R\rangle} + |L\rangle\langle R|R\rangle\right) \\ &= -\frac{\Delta}{\sqrt{2}}(|R\rangle + |L\rangle) \\ &= -\Delta|S\rangle \end{aligned}$$

Since $\pi|L\rangle = |R\rangle$ and $\pi|R\rangle = |L\rangle$,

$$\begin{aligned} \pi|S\rangle &= |S\rangle \\ \pi|A\rangle &= -|A\rangle \end{aligned}$$

If we were to set $\Delta = 0$, (i.e. prevent the possibility of tunneling) then we have that E_+ and E_- become 0. Then eigenstates are $|L\rangle$ and $|R\rangle$ which are not parity eigenstates.

3.2 Parity Selection Rules

Suppose we have two parity eigenstates $|\alpha\rangle$ and $|\beta\rangle$.

$$\begin{aligned} \pi|\alpha\rangle &= \epsilon_\alpha|\alpha\rangle \\ \pi|\beta\rangle &= \epsilon_\beta|\beta\rangle \end{aligned}$$

Where $\epsilon_\alpha, \epsilon_\beta = \pm 1$. We can not look at the matrix elements of $\vec{x}$,

$$\langle\beta|\vec{x}|\alpha\rangle = \langle\beta|\pi^{-1}\pi\vec{x}\pi^{-1}\pi|\alpha\rangle$$

But we know that π is unitary and Hermitian,

$$\langle\beta|\vec{x}|\alpha\rangle = \langle\beta|\pi^\dagger\pi\vec{x}\pi^\dagger\pi|\alpha\rangle$$

Or we can also right,

$$\langle\beta|\vec{x}|\alpha\rangle = \langle\beta|\pi^\dagger\pi^\dagger\vec{x}\pi\pi|\alpha\rangle$$

But $|\alpha\rangle$ and $|\beta\rangle$ are eigenstates of π.

$$\langle\beta|\vec{x}|\alpha\rangle = \epsilon_\alpha\epsilon_\beta\langle\beta|\pi^\dagger\vec{x}\pi|\alpha\rangle$$

Moreover $\pi^\dagger\vec{x}\pi = -\vec{x}$ by definition,

$$\langle\beta|\vec{x}|\alpha\rangle = -\epsilon_\alpha\epsilon_\beta\langle\beta|\vec{x}|\alpha\rangle$$

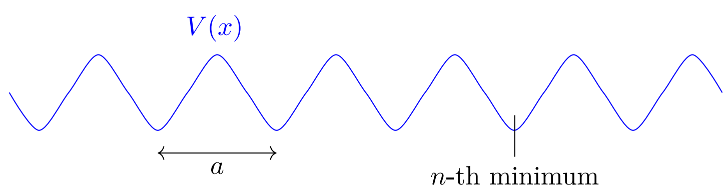
Therefore we have one of two cases:

1. $\epsilon_\alpha\epsilon_\beta = -1$: one of the states is parity-odd while the other one is parity-even
2. $\langle\beta|\vec{x}|\alpha\rangle = 0$: matrix elements of parity-odd operators can only be non-zero between states of different parity

3.3 Symmetries of Discrete Translations

Heretofore we have talked about continuous symmetries like the symmetries of translations. Alternatively we can have symmetries associated with discrete translations. These symmetries arise all the time in condensed matter when considering the translations of a crystal lattice.

As a foundational example, consider a 1D periodic potential.



Where $V(x+a) = V(x)$. We have symmetry of translations by a or any integer multiple of a. Therefore,

$$T^\dagger(a)V(x)T(a) = V(x+a) = V(x)$$

We also have that $T^\dagger(a)\frac{\vec{p}^2}{2m}T(a) = \frac{\vec{p}^2}{2m}$ so that $T(a)H = HT(a)$.

$$[H, T(a)] = 0$$

We can find eigenstates of H which are also eigenstate of $T(a)$. We will look at the limit of infinite barrier height; the particle has to be stuck in any of the minimal of the potential. Let $|n\rangle$ be the state in which the particle is in the n-th minimum.

$$H|n\rangle = E_0|n\rangle$$

And $T(a)|n\rangle = |n+1\rangle$ which implies that $|n\rangle$ is not an eigenstate of $T(a)$. Instead consider the state $|\theta\rangle$ that is a sum over eigenstates of H,

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle$$

Since $\theta \mapsto \theta + 2\pi m$, where m is an integer does not change $e^{in\theta}$ (for all $-\pi \leq \theta \leq \pi$). The transition operator acting on $|\theta\rangle$ is,

$$\begin{aligned} T(a)|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta}T(a)|n\rangle \\ &= \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle \end{aligned}$$

$$
\begin{aligned}
&= \sum_{n'-1=-\infty}^{\infty} e^{i\left(n'-1\right)\theta}|n'\rangle \\
&= e^{-i\theta} \sum_{n'=-\infty}^{\infty} e^{in'\theta}|n'\rangle \\
&= e^{-i\theta}|\theta\rangle
\end{aligned}
$$

Therefore have that $T(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$ is an eigenstate of $T(a)$ with eigenstate $e^{i\theta}$. But since $[T(a), H] = 0$ so that $|\theta\rangle$ is *also* and eigenstate of H.

$$H|\theta\rangle = E_0|\theta\rangle$$

To generalize this analysis assume that the barrier height is finite but large enough so that particles may only tunnel between nearest neighbor minimum. This is called the **tight binding approximation**. In this case our Hamiltonian will be very similar to the "left/right" tunneling amplitude discussed earlier. The matrix elements of H for this system are $\langle +1|H|n\rangle$. We assign to them the probability $-\Delta$ to be the probability amplitude for tunneling between nearest neighbor minima. We also assume define that $|n\rangle$ be an eigenstate $\langle n|H|n\rangle = E_0$. Therefore,

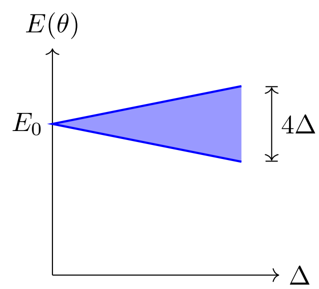
$$H|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle$$

Which means that H acting on the translation eigenstate $|\theta\rangle = \sum_n = e^{in\theta}|n\rangle$ becomes,

$$
\begin{aligned}
H|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta} H|n\rangle \\
&= \sum_{n=-\infty}^{\infty} e^{in\theta}(E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle) \\
&= \sum_{n=-\infty}^{\infty} e^{in\theta}E_0|n\rangle - \sum_{n=-\infty}^{\infty} e^{in\theta}\Delta|n+1\rangle - \sum_{n=-\infty}^{\infty} e^{in\theta}\Delta|n-1\rangle \\
&= E_0 \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle - \Delta \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle - \Delta \sum_{n=-\infty}^{\infty} e^{in\theta}|n-1\rangle \\
&= E_0 \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle - \Delta \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle - \Delta \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle \\
&= E_0 \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle - \Delta e^{-i\theta} \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle - e^{i\theta}\Delta \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle \\
&= \left(E_0 - \Delta e^{-i\theta} - e^{i\theta}\Delta\right) \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle \\
&= \left(E_0 - \Delta e^{-i\theta} - e^{i\theta}\Delta\right)|\theta\rangle \\
&= (E_0 - 2\Delta\cos\theta)|\theta\rangle
\end{aligned}
$$

Therefore $|\theta\rangle$ is an eigenvalue of H with eigenvalue $E(\theta)$,

$$E(\theta) = E_0 - 2\Delta\cos\theta$$



Notice that when there is no tunneling, $\Delta = 0$, we recover a single eigen-energy E_0. However when tunneling is introduced, the parameter θ allows for a range of eigen-energies between $E_0 \pm 2\Delta$. Next consider the wave function $\langle x'|\theta\rangle$,

$$\langle x'|T(a)|\theta\rangle = \langle\theta|T^\dagger(a)|x'\rangle^* = \langle\theta|x'-a\rangle^* = \langle x'-a|\theta\rangle$$

But we also know that $T(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$. Therefore,

$$\langle x'-a|\theta\rangle = e^{-i\theta}\langle x'|\theta\rangle$$

The most general solution to this equation is,

$$\langle x'|\theta\rangle = e^{ikx'}u_k(x')$$

Where $u_k(x')$ is a **Bloch wavefunction** with $\theta = ka$. Bloch wavefunctions have the property that,

$$u_k(x'+a) = u_k(x')$$

When means that,

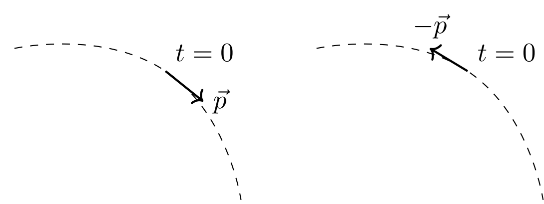
$$e^{ik(x'-a)}u_k(x'-a) = e^{-ika}u_k(x')e^{ikx'}$$

If $\theta \in [-\pi, \pi]$ then $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$. This interval is called the **first Brillouin zone**. We call $\hbar k$ the crystal momentum and its conservation is a consequence of discrete symmetry with respect to translations by a, which still remains in the crystal. The energy of a particle in a crystal with wavenumber k is given by,

$$E(k) = E_0 - 2\Delta\cos(ka)$$

3.4 Time-reversal Symmetry

The formalism of quantum time-reversal symmetries is more subtle and complicated than the other symmetries considered thus-far. To introduce time-reversal symmetries, we initially consider the classical case.



We consider a particle moving on a trajectory. Suppose that we have the ability to stop the particle and run time backward. In the absence of friction the particle will simply retrace its trajectory backward.

$$m\frac{\mathrm{d}^2\vec{x}}{\mathrm{d}t^2} = -\vec{\nabla}V(\vec{x})$$

Under the time-reversal map $t \mapsto -t$, the equations of motion do not change. Both $\vec{x}(t)$ and $\vec{x}(-t)$ are solutions to the equations of motion.

$$\vec{p} = m\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} \overset{t\mapsto -t}{\Longrightarrow} \vec{p} \mapsto -\vec{p}$$

An example of the lack of time-reversal symmetry is a charged particle in a magnetic field. Let $\vec{B}$ face into the board. The Lorentz force is $\vec{F} = \frac{e}{c}\vec{v}\times\vec{B}$. When the force in question is $-\vec{\nabla}V(\vec{x})$ then $\vec{F} \mapsto \vec{F}$. However since $\vec{v} \mapsto -\vec{v}$ and $\vec{B} \mapsto \vec{B}$, we have that $\vec{F} \mapsto -\vec{F}$.

In the quantum mechanic case, equations of motion are determined by the Schrödinger equation,

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + V(\vec{x})\right]\psi(\vec{x},t) \tag{3.1}$$

If $\psi(\vec{x},t)$ is a solution of the Schrödinger equation, will $\psi(\vec{x},-t)$ also be a solution? Reversing time,

$$-i\hbar\frac{\partial\psi(\vec{x},-t)}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + V(\vec{x})\right]\psi(\vec{x},-t) \tag{3.2}$$

Equation (3.2) is an *identical* equation to eq. (3.1) except that the sign of the LHS. Therefore it does not follow that $\psi(\vec{x},-t)$ is a solution of the time-reversed SE. Instead take the complex conjugate of eq. (3.2),

$$i\hbar\frac{\partial\psi^*(\vec{x},-t)}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + V(\vec{x})\right]\psi^*(\vec{x},-t)$$

This is identical to eq. (3.1). Therefore we can then say that if $\psi(\vec{x},t)$ is a solution to eq. (3.1) then $\psi^*(\vec{x},t)$ is solution to eq. (3.1) as well.

Motivated by this we introduce the **time-reversal** operator Θ taking kets $|\psi\rangle$ to $\Theta|\psi\rangle$. Let's look at some desired properties: If a ket starts at $t=0$, we can apply the infinitesimal time translation operator,

$$|\psi, t=\delta t\rangle = \left(\mathbb{1} - \frac{i}{\hbar}H\delta t\right)|\psi\rangle$$

Now suppose at time $t=0$ we perform a time-reversal operation such that,

$$\begin{aligned}\left(\mathbb{1} - \frac{i}{\hbar}H\delta t\right)\Theta|\psi\rangle &= \Theta|\psi, t=-\delta t\rangle \\ &= \Theta\left(\mathbb{1} - \frac{i}{\hbar}H{-\delta t}\right)|\psi\rangle \\ &= \Theta\left(\mathbb{1} + \frac{i}{\hbar}H\delta t\right)|\psi\rangle\end{aligned}$$

This fixes a relationship between H and Θ, namely,

$$-\frac{i}{\hbar}H\delta t\Theta|\psi\rangle = +\Theta\frac{i}{\hbar}H\delta t|\psi\rangle$$

Since $|\psi\rangle$ is arbitrary and $\hbar$ and δt are real constants,

$$-iH\Theta = +\Theta iH \tag{3.3}$$

You might wonder why we can't also cancel i. Suppose we also canceled i such that $-H\Theta = \Theta H$. Then if we consider energy eigenstates $|n\rangle$,

$$H\Theta|n\rangle = -\Theta H|n\rangle = -E_n\Theta|n\rangle$$

This means that $\Theta|n\rangle$ is an eigenket of H with negative energy E_n. However for a free particle, the energy is always positive! Therefore we *cannot* cancel the i's in eq. (3.3).[5] This is resolved by recognizing that Θ is not a unitary operator and is instead an anti-unitary operator. Recall that unitary operators U act on kets such that,

$$\langle\tilde{\varphi}|\tilde{\psi}\rangle = \langle\varphi|U^\dagger U|\psi\rangle = \langle\varphi|\psi\rangle$$

Since $U^\dagger U = \mathbb{1}$ defines unitary operators, unitary operators preserve inner products. However anti-unitary operators θ have the dual characterization,

$$\langle\tilde{\varphi}|\tilde{\psi}\rangle = \langle\varphi|\psi\rangle^* = \langle\psi|\varphi\rangle$$

Which conjugates inner products. This means that,

$$\theta(c_1|\psi\rangle + c_2|\varphi\rangle) = c_1^*\theta|\psi\rangle + c_2^*\theta|\varphi\rangle$$

[5] Alternatively we could resolve this conundrum by asserting that $\Theta|n\rangle = 0$ for all eigenstates. But this is only possible if $\Theta = 0$ is the null operator.

Anti-unitary operators conjugate coefficients. We define the **complex conjugation operator** K such that if $|\psi\rangle = \sum_a |a\rangle\langle a|\psi\rangle$, then,

$$K|\psi\rangle = \sum_a |a\rangle\langle a|\psi\rangle^*$$

In this way we can define the time-reversal operator as $\Theta = UK$. Returning to eq. (3.3),

$$\Theta i = UKi = U(-i)K = -iUK = -i\Theta$$

Which means that the time reversal operator commutes with the Hamiltonian,

$$[\Theta, H] = 0$$

How does Θ act on Hermitian operators? Well, consider two kets,

$$|\tilde{\varphi}\rangle = \Theta|\varphi\rangle \quad |\tilde{\psi}\rangle = \Theta|\psi\rangle$$

And a generic Hermitian operator A such that,

$$\begin{aligned} |\xi\rangle &= A^\dagger|\varphi\rangle = A|\varphi\rangle \\ \langle\xi| &= \langle\varphi|A = \langle\varphi|A^\dagger \end{aligned}$$

Therefore,

$$\begin{aligned} \langle\varphi|A|\psi\rangle &= \langle\xi|\psi\rangle \\ &= \langle\tilde{\xi}|\tilde{\psi}\rangle^* \\ &= \langle\tilde{\psi}|\tilde{\xi}\rangle \\ &= \langle\tilde{\psi}|\Theta|\xi\rangle \\ &= \langle\tilde{\psi}|\Theta A|\varphi\rangle \\ &= \langle\tilde{\psi}|\Theta A\Theta^{-1}\Theta|\varphi\rangle \\ &= \langle\tilde{\psi}|\Theta A\Theta^{-1}|\tilde{\varphi}\rangle \end{aligned}$$

Such that the time reversed operator of A is denoted $\Theta A\Theta^{-1}$. In fact there are two possibilities for $\Theta A\Theta^{-1}$. If $\Theta A\Theta^{-1} = A$ then we say that A is *time reversal even* and if $\Theta A\Theta^{-1} = -A$ we say that A is *time reversal odd*. As examples,

$$\begin{aligned} \Theta\vec{p}\Theta^{-1} &= -\vec{p} && \text{Time Reversal Odd} \\ \Theta\vec{x}\Theta^{-1} &= \vec{x} && \text{Time Reversal Even} \end{aligned}$$

What about the operator $[x_i, p_j]$? We know that,

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

Under time-reversal,

$$\Theta[x_i, p_j]|\psi\rangle = \Theta i\hbar\delta_{ij}|\psi\rangle$$

Since Θ conjugates,

$$\Theta[x_i, p_j]|\psi\rangle = -i\hbar\delta_{ij}\Theta|\psi\rangle$$

Therefore $\Theta[x_i, p_j]\Theta^{-1} = -[x_i, x_j]$. What about $[J_i, J_k] = i\hbar\epsilon_{ijk}J_k$? Since both J_i and J_k are time reversal odd,

$$\Theta[J_i, J_j]\Theta^{-1} = [J_i, J_j]$$

While,

$$\Theta\vec{J}\Theta^{-1} = -\vec{J}$$

In confirmation with all of these results, lets check $|\psi\rangle$ written in the position basis,

$$|\psi\rangle = \int \mathrm{d}\vec{x}\,'|\vec{x}\,'\rangle\langle\vec{x}\,'|\psi\rangle$$

Under the action of Θ,

$$\Theta|\psi\rangle = \int \mathrm{d}\vec{x}\,'\Theta|\vec{x}\,'\rangle\langle\vec{x}\,'|\psi\rangle = \int \mathrm{d}\vec{x}\,'|\vec{x}\,'\rangle\langle\vec{x}\,'|\psi\rangle^*$$

Which makes,

$$\langle\vec{x}\,''|\Theta|\psi\rangle = \langle\vec{x}\,''|\psi\rangle^*$$

However for $\vec{p}$ we have that,

$$\langle\vec{p}\,''|\Theta|\psi\rangle = \langle-\vec{p}\,''|\psi\rangle^*$$

3.5 Time-Reversal of Spin-1/2 System

Consider an eigenket of the spin operator in some arbitrary direction $\hat{n}$,

$$\hat{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$$

We can find an eigenket of $\vec{S}\cdot\hat{n}$ by finding an eigenket of S_z and rotating it to the direction $\hat{n}$. This result was previously obtained as eq. (2.10). We define the eigenket as,

$$|\hat{n};\uparrow\rangle = e^{-\frac{i}{\hbar}S_z\varphi}e^{-\frac{i}{\hbar}S_y\theta}|\uparrow\rangle$$

How does Θ act on $|\hat{n};\uparrow\rangle$?

$$\Theta|\hat{n};\uparrow\rangle = \Theta e^{-\frac{i}{\hbar}S_z\varphi}e^{-\frac{i}{\hbar}S_y\theta}|\uparrow\rangle$$

Note that $\Theta\vec{S} = -\vec{S}\Theta$ is time reversal odd (but $\Theta i = -i\Theta$ so the factors cancel out). Therefore,

$$\Theta|\hat{n};\uparrow\rangle = e^{-\frac{i}{\hbar}S_z\varphi}e^{-\frac{i}{\hbar}S_y\theta}\Theta|\uparrow\rangle$$

What then is $\Theta|\uparrow\rangle$?

$$S_z\Theta|\uparrow\rangle = -\Theta S_z|\uparrow\rangle = -\frac{\hbar}{2}\Theta|\uparrow\rangle$$

There $\Theta|\uparrow\rangle$ is the eigenket of S_z with eigenvalue $-\hbar/2$. This is nothing more that $|\downarrow\rangle$. More specifically,

$$\Theta|\uparrow\rangle = e^{i\eta}|\downarrow\rangle$$

Where η is just an arbitrary phase factor. Therefore,

$$\Theta|\hat{n};\uparrow\rangle = e^{-\frac{i}{\hbar}S_z\varphi}e^{-\frac{i}{\hbar}S_y\theta}e^{i\eta}|\downarrow\rangle$$

Recognize that $e^{-\frac{i}{\hbar}S_z\varphi}e^{-\frac{i}{\hbar}S_y\theta}|\downarrow\rangle = |\hat{n},\downarrow\rangle$ where,

$$|\hat{n},\downarrow\rangle = \begin{pmatrix} -e^{i\frac{\varphi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\varphi}{2}}\cos\frac{\theta}{2} \end{pmatrix}$$

Therefore,

$$|\hat{n}(\theta,\varphi);\downarrow\rangle = |\hat{n}(\theta+\pi,\varphi);\uparrow\rangle$$

Explicitly this means that Θ can be written as,

$$\Theta|\hat{n};\uparrow\rangle = \Theta e^{-\frac{i}{\hbar}S_z\varphi}e^{-\frac{i}{\hbar}S_y\theta}|\uparrow\rangle = e^{i\eta}e^{-\frac{i}{\hbar}S_z\varphi}e^{-\frac{i}{\hbar}S_y(\theta+\pi)}|\uparrow\rangle$$

Which means that,

$$\Theta = UK$$

$$
\begin{aligned}
&= e^{i\eta} e^{-\frac{i}{\hbar} S_y \pi} K \\
&= e^{i\eta} e^{-\frac{i}{2} \sigma_y \pi} K \\
&= e^{i\eta} \left(\cos \frac{\pi}{2} - i\sigma_y \sin \frac{\pi}{2} \right) K \\
&= -ie^{i\eta} \sigma_y K
\end{aligned}
$$

This allows use to determine how Θ affects $|\uparrow\rangle$ and $|\downarrow\rangle$ directly,[6]

$$
\begin{aligned}
\Theta|\uparrow\rangle &= -ie^{i\eta}\sigma_y \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= -ie^{i\eta} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= -ie^{i\eta} \begin{pmatrix} 0 \\ i \end{pmatrix} \\
&= e^{i\eta} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= e^{i\eta} |\uparrow\rangle
\end{aligned}
$$

This is a result we have seen previously. Next consider how Θ affects $|\downarrow\rangle$.

$$
\begin{aligned}
\Theta|\downarrow\rangle &= -ie^{i\eta}\sigma_y \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= -ie^{i\eta} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= -ie^{i\eta} \begin{pmatrix} -i \\ 0 \end{pmatrix} \\
&= -e^{i\eta} |\downarrow\rangle
\end{aligned}
$$

For an arbitrary spinor $|z\rangle = z_\uparrow|\uparrow\rangle + z_\downarrow|\downarrow\rangle$.

$$\Theta|z\rangle = z_\uparrow^* e^{i\eta}|\downarrow\rangle - z_\downarrow^* e^{i\eta}|\uparrow\rangle$$

Applying Θ twice gives,

$$\Theta^2|z\rangle = -|z\rangle$$

Therefore for spin-1/2 particles,

$$\Theta^2 = -1$$

In general for a spin j particles,

$$\Theta^2 = (-1)^{2j} \tag{3.4}$$

3.6 Time-Reversal Invariant System With Half-integer Spin

A time reversal invariant system is one whereby $[\Theta, H] = 0$. In this case we can also say that H is time reversal even,

$$\Theta H \Theta^{-1} = H$$

For this case consider the eigen-system $H|n\rangle = E_n|n\rangle$. Therefore,

$$H\Theta|n\rangle = \Theta H|n\rangle = E_n \Theta|n\rangle$$

Assuming that $|n\rangle$ is non-degenerate,

$$\Theta|n\rangle = e^{i\delta}|n\rangle$$

[6] Since $|\uparrow\rangle$ is a real spinor, the charge conjugation operator doesn't affect it: $K|\uparrow\rangle = |\uparrow\rangle$.

$$\Theta^2|n\rangle = e^{-i\delta}\Theta|n\rangle = e^{-i\delta}e^{i\delta}|n\rangle = |n\rangle$$

Therefore $\Theta^2 = 1$. But eq. (3.4) contradicts this. If j is a half integer, then $\Theta^2 = -1$. Therefore the assumption that $|n\rangle$ was non-degenerate is wrong.

Kramer's Theorem: In a time-reversal invariant system with half integer spin j, all energy eigenstates are degenerate.

For $j = 1/2$, $|\uparrow\rangle$ and $|\downarrow\rangle$ always have the same energy (degeneracy 2).

4 Time-Dependent Hamiltonian

So far we have assumed that H is time-independent (i.e. $\frac{\partial H}{\partial t} = 0$).

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

However in generality, H can be time-dependent through $V(\vec{x}, t)$. To facilitate the discussions, we isolate the time-dependent component of the Hamiltonian,

$$H = H_0 + V(t)$$

This type of perturbation is typical when attempting to experimentally probe a given system. Recall that in the Schrödinger picture,

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

This only holds if H is independent of time. In the Heisenberg picture,

$$|\psi\rangle_H = |\psi\rangle = e^{-\frac{i}{\hbar}Ht}|\psi, t\rangle_S$$

With $A^{(H)}(t) = e^{\frac{i}{\hbar}Ht}A^{(S)}e^{-\frac{i}{\hbar}Ht}$ and,

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

We now introduce the **interaction picture** which is an intermediate between the Schrödinger and Heisenberg pictures.

$$|\psi, t\rangle_I = e^{\frac{i}{\hbar}H_0 t}|\psi, t\rangle_S$$

Which reduces to the Heisenberg representation is $V(t) = 0$. Notice that $|\psi, t\rangle_S$ is only time-evolved by the time-independent components of the Hamiltonian. What happens to operators in the interaction picture?

$${}_S\langle\psi, t|A^{(S)}|\psi, t\rangle_S = {}_I\langle\psi, t|e^{\frac{i}{\hbar}H_0 t}A^{(S)}e^{-\frac{i}{\hbar}H_0 t}|\psi, t\rangle_I$$

This leads us to define,

$$A^{(I)} = e^{\frac{i}{\hbar}H_0 t}A^{(S)}e^{-\frac{i}{\hbar}H_0 t}$$

Which would coincide with $A^{(H)}(t)$ if $H = H_0$. The Schrödinger equation is modified as well,

$$i\hbar\frac{\partial}{\partial t}|\psi, t\rangle_I = i\hbar\frac{\partial}{\partial t}e^{\frac{i}{\hbar}H_0 t}|\psi, t\rangle_S$$

Using product rule,

$$i\hbar\frac{\partial}{\partial t}|\psi, t\rangle_I = -H_0 e^{\frac{i}{\hbar}H_0 t}|\psi, t\rangle_S + e^{\frac{i}{\hbar}H_0 t}i\hbar\frac{\partial}{\partial t}|\psi, t\rangle_S$$

We now make use of the Schrödinger equation for $|\psi, t\rangle_S$,

$$i\hbar\frac{\partial}{\partial t}|\psi, t\rangle_I = -H_0 e^{\frac{i}{\hbar}H_0 t}|\psi, t\rangle_S + e^{\frac{i}{\hbar}H_0 t}(H_0 + V(t))|\psi, t\rangle_S$$

Canceling terms in H_0 gives,

$$i\hbar\frac{\partial}{\partial t}|\psi,t\rangle_I = e^{\frac{i}{\hbar}H_0 t}V(t)|\psi,t\rangle_S$$

We insert $\mathbb{1} = e^{-\frac{i}{\hbar}H_0 t}e^{\frac{i}{\hbar}H_0 t}$ to the right of $V(t)$,

$$i\hbar\frac{\partial}{\partial t}|\psi,t\rangle_I = \underbrace{e^{\frac{i}{\hbar}H_0 t}V(t)e^{-\frac{i}{\hbar}H_0 t}}_{V^{(I)}(t)}e^{\frac{i}{\hbar}H_0 t}|\psi,t\rangle_S$$

Which gives the Schrödinger equation for $|\psi,t\rangle_I$,

$$i\hbar\frac{\partial}{\partial t}|\psi,t\rangle_I = V^{(I)}(t)|\psi,t\rangle_I \tag{4.1}$$

The time-dependence of $|\psi,t\rangle$ is entirely governed by the potential $V^{(I)}(t)$. Analogously to the Heisenberg equations of motion for operators, we have the interaction equations of motion,

$$\frac{\partial A^{(I)}}{\partial t} = \frac{i}{\hbar}\left[H_0, A^{(I)}\right]$$

To solve the equations of motion, consider the eigen-system for H_0. Namely,

$$H_0|n\rangle = E_n|n\rangle$$

From this complete orthonormal basis, we write $|\psi,t\rangle_I$ as,

$$|\psi,t\rangle_I = \sum_n c_n(t)|n\rangle$$

We can now arrive at a version of eq. (4.1) for the coefficients $c_n(t)$.

$$i\hbar\frac{\partial}{\partial t}|\psi,t\rangle_I = V^{(I)}(t)\left\{\sum_m c_m(t)|m\rangle\right\}$$

Applying the bra $|n\rangle$,

$$\langle n|i\hbar\frac{\partial}{\partial t}|\psi,t\rangle_I = \langle n|V^{(I)}(t)\left\{\sum_m c_m(t)|m\rangle\right\}$$

Since $|n\rangle$ is time independent,

$$i\hbar\frac{\partial}{\partial t}\langle n|\psi,t\rangle_I = i\hbar\frac{\partial c_n(t)}{\partial t} = \sum_m c_m(t)\langle n|V^{(I)}(t)|m\rangle$$

The matrix elements $\langle n|V^{(I)}(t)|m\rangle$ can be expressed in a more expressive manner,

$$\begin{aligned}\langle n|V^{(I)}(t)|m\rangle &= \langle n|e^{\frac{i}{\hbar}H_0 t}V(t)e^{-\frac{i}{\hbar}H_0 t}|m\rangle \\ &= e^{\frac{i}{\hbar}E_n t}\langle n|V(t)|m\rangle e^{-\frac{i}{\hbar}E_m t} \\ &= e^{i\omega_{nm}t}\langle n|V(t)|m\rangle \\ &= e^{i\omega_{nm}t}V_{nm}(t)\end{aligned}$$

Where the transition frequency is,

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}$$

To conclude we have,

$$i\hbar\frac{\mathrm{d}c_n}{\mathrm{d}t} = \sum_m e^{i\omega_{nm}t}V_{nm}(t)c_m(t) \tag{4.2}$$

There are very few systems that omit analytic solutions to eq. (4.2). These systems will be the immediate focus.

4.1 Two-State Harmonic Potential

Consider a two-state problem on a harmonic potential. We call these states $|1\rangle, |2\rangle$ together with energies E_1, E_2,

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$$

The time dependent potential is constructed in such a way to induce transitions between $|1\rangle$ and $|2\rangle$,

$$V(t) = \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1|$$

This means that $\langle 1|V(t)|2\rangle = \gamma e^{-i\omega t}$ is the probability amplitude for $V(t)$ to produce a transition from $|2\rangle$ to $|1\rangle$. The equations of motion can be worked out explicitly,

$$\begin{aligned} i\hbar\frac{\mathrm{d}c_1}{\mathrm{d}t} &= V_{12}(t)e^{i\omega_{12}t}c_2 = \gamma e^{i(\omega-\omega_{21}t)}c_2 \\ i\hbar\frac{\mathrm{d}c_2}{\mathrm{d}t} &= V_{21}(t)e^{i\omega_{21}t}c_1 = \gamma e^{-i(\omega-\omega_{21}t)}c_1 \end{aligned}$$

Without loss of generality we let $E_2 > E_1$ so that $\omega_{21} = (E_2 - E_1)/\hbar > 0$. We also have the symmetry,

$$\omega_{12} = \frac{E_1 - E_2}{\hbar} = -\omega_{21}$$

By inspection we can expect the solution to have the ansatz form,

$$\begin{aligned} c_1(t) &= c_1 e^{i\lambda t + \frac{i}{2}(\omega-\omega_{21})t} \\ c_2(t) &= c_2 e^{i\lambda t - \frac{i}{2}(\omega-\omega_{21})t} \end{aligned} \tag{4.3}$$

Substitute to check if this solution is permissible,

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left(c_1 e^{i\lambda t + \frac{i}{2}(\omega-\omega_{21})t}\right) &= \gamma e^{i(\omega-w_{21})t}c_2 e^{i\lambda t - \frac{i}{2}(\omega-\omega_{21})t} \\ -\hbar c_1\left(\lambda + \frac{\omega-\omega_{21}}{2}\right)e^{i\lambda t + \frac{i}{2}(\omega-\omega_{21})t} &= \gamma c_2 e^{i\lambda t + \frac{i}{2}(\omega-\omega_{21})t} \\ -\hbar c_1\left(\lambda + \frac{\omega-\omega_{21}}{2}\right) &= \gamma c_2 \end{aligned}$$

Similarly we arrive at an equation for $\frac{\mathrm{d}c_2}{\mathrm{d}t}$,

$$-\hbar c_2\left(\lambda - \frac{\omega-\omega_{21}}{2}\right) = \gamma c_1$$

We now have a linear system over c_1, c_2 and λ. Rearranged, our system is,

$$\begin{aligned} \left(\lambda + \frac{\omega-\omega_{21}}{2}\right)c_1 + \frac{\gamma}{\hbar}c_2 &= 0 \\ \left(\lambda - \frac{\omega-\omega_{21}}{2}\right)c_2 + \frac{\gamma}{\hbar}c_1 &= 0 \end{aligned} \tag{4.4}$$

This is a homogeneous system over c_1 and c_2. The only want to have a non-trivial solution is if the determinant is zero. This singularity condition fixes λ.

$$0 = \det\begin{pmatrix} (\lambda + \frac{\omega-\omega_{21}}{2}) & \frac{\gamma}{\hbar} \\ \frac{\gamma}{\hbar} & (\lambda - \frac{\omega-\omega_{21}}{2}) \end{pmatrix} = \lambda^2 - \left(\frac{\omega-\omega_{21}}{2}\right)^2 - \left(\frac{\gamma}{\hbar}\right)^2$$

Therefore,

$$\lambda = \pm\sqrt{\left(\frac{\omega-\omega_{21}}{2}\right)^2 + \left(\frac{\gamma}{\hbar}\right)^2} = \pm\Omega$$

Where Ω is the **Rabi-frequency**. Each λ induces a solution for $c_1(t)$ and $c_2(t)$. Plugging $\lambda = +\Omega$ back into eq. (4.4) we can solve for coefficients $c_{1,+}$ and $c_{2,+}$,

$$c_{1,+} = -c_{2,+}\frac{\gamma/\hbar}{\Omega + \frac{\omega-\omega_{21}}{2}}$$

This equation fixes $c_{1,+}$ given $c_{2,+}$ but their relationship enforces normalization as well,

$$|c_{1,+}|^2 + |c_{2,+}|^2 = 1$$

Therefore,

$$\begin{aligned}
1 &= |c_{2,+}|^2 + |c_{2,+}|^2\frac{(\gamma/\hbar)^2}{\left(\Omega + \frac{\omega-\omega_{21}}{2}\right)^2} \\
&= |c_{2,+}|^2\frac{\Omega^2 + 2\frac{\omega-\omega_{21}}{2}\Omega + \left(\frac{\omega-\omega_{21}}{2}\right)^2\Omega^2 + \left(\frac{\gamma}{\hbar}\right)^2}{\left(\Omega + \frac{\omega-\omega_{21}}{2}\right)^2} \\
&= |c_{2,+}|^2\frac{2\Omega^2 + 2\frac{\omega-\omega_{21}}{2}\Omega}{\left(\Omega + \frac{\omega-\omega_{21}}{2}\right)^2} \\
&= |c_{2,+}|^2\frac{2\Omega}{\Omega + \frac{\omega-\omega_{21}}{2}}
\end{aligned}$$

Therefore,

$$|c_{2,+}|^2 = \frac{1}{2}\left(1 + \frac{\omega-\omega_{21}}{2\Omega}\right)$$

We choice $c_{2,+}$ to be real and positive,

$$c_{2,+} = \sqrt{\frac{1}{2}\left(1 + \frac{\omega-\omega_{21}}{2\Omega}\right)}$$

Similarly,

$$c_{1,+} = -\sqrt{\frac{1}{2}\left(1 - \frac{\omega-\omega_{21}}{2\Omega}\right)}$$

The solution corresponding to $\lambda = -\Omega$ is,

$$\begin{aligned}
c_{1,-} &= \sqrt{\frac{1}{2}\left(1 + \frac{\omega-\omega_{21}}{2\Omega}\right)} \\
c_{2,-} &= \sqrt{\frac{1}{2}\left(1 - \frac{\omega-\omega_{21}}{2\Omega}\right)}
\end{aligned}$$

Plugging λ back into eq. (4.3). The general solution is,

$$\begin{aligned}
c_1(t) &= Ac_{1,+}e^{i\left(\Omega+\frac{\omega-\omega_{21}}{2}\right)t} + Bc_{1,-}e^{-i\left(\Omega-\frac{\omega-\omega_{21}}{2}\right)t} \\
c_2(t) &= Ac_{2,+}e^{i\left(\Omega-\frac{\omega-\omega_{21}}{2}\right)t} + Bc_{2,-}e^{-i\left(\Omega+\frac{\omega-\omega_{21}}{2}\right)t}
\end{aligned}$$

Where A, B are determined by initial conditions. As an example suppose that the state of the particle is initially $|1\rangle$. This means that,

$$c_1(t=0) = 1 \quad c_2(t=0) = 0$$

Therefore,

$$Ac_{1,+} + Bc_{1,-} = 1$$

$$Ac_{2,+} + Bc_{2,-} = 0$$

Therefore,

$$B = -A\frac{c_{2,+}}{c_{2,-}}$$

And A is fully determined,

$$A = \frac{c_{2,-}}{c_{1,+}c_{2,-} - c_{1,-}c_{2,+}}$$

Where the denominator can be greatly simplified,

$$\begin{aligned} c_{1,+}c_{2,-} - c_{1,-}c_{2,+} &= -c_{1,+}c_{1,+} - c_{2,+}c_{2,+} \\ &= -\left(c_{1,+}^2 + c_{2,+}^2\right) \\ &= -1 \end{aligned}$$

Therefore,

$$\begin{aligned} A &= -\sqrt{\frac{1}{2}\left(1 - \frac{\omega - \omega_{21}}{2\Omega}\right)} \\ B &= \sqrt{\frac{1}{2}\left(1 + \frac{\omega - \omega_{21}}{2\Omega}\right)} \end{aligned}$$

Altogether,

$$c_2(t) = i\frac{\gamma}{\hbar\Omega}e^{-i\frac{\omega-\omega_{21}}{2}t}\sin(\Omega t)$$

Which means that,

$$|c_2(t)|^2 = \frac{\left(\frac{\gamma}{\hbar}\right)^2}{\left(\frac{\omega-\omega_{21}}{2}\right)^2 + \left(\frac{\gamma}{\hbar}\right)^2}\sin^2(\Omega t)$$

Where $|c_1(t)|^2 = 1 - |c_2(t)|^2$. Physically this means that the probability of finding the particle in state i ($|c_i(t)|^2$) oscillates with frequency Ω. Recall that ω is the frequency of the driving potential. When $\omega = \omega_{21}$ we have two phenomena occurring:

1. The amplitude of Rabi oscillations is maximal and equal to 1,

$$\frac{\left(\frac{\gamma}{\hbar}\right)^2}{\left(\frac{\omega-\omega_{21}}{2}\right)^2 + \left(\frac{\gamma}{\hbar}\right)^2} \to \frac{\left(\frac{\gamma}{\hbar}\right)^2}{\left(\frac{\gamma}{\hbar}\right)^2} = 1$$

2. The Rabi frequency can be set by the strength of the applied potential γ; Ω becomes equal to $\gamma/\hbar$,

$$\sqrt{\left(\frac{\omega - \omega_{21}}{2}\right)^2 + \left(\frac{\gamma}{\hbar}\right)^2} \to \frac{\gamma}{\hbar}$$

4.1.1 Magnetic Resonance Imaging

The most well-known application of this model is to Magnetic Resonance Imaging (MNR). In the cause of medical MNR, we image the nuclei of the hydrogen atoms in water in one's body. In this case the frequency associated with the unperturbed system is the spin of the hydrogen atom. Our Hamiltonian in this case is,

$$H_0 = -\vec{\mu}\cdot\vec{B}_0$$

Where $\vec{B}_0$ is a time-independent magnetic field where $\vec{B}_0 = B_0\hat{z}$. The magnetic dipole of a proton is,

$$\vec{\mu} = \frac{e}{mc}\vec{S}$$

Therefore,

$$H_0 = -\frac{e}{mc}B_0 S_z = -\frac{eB_0\hbar}{2mc}(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)$$

Which has two eigenvalues,

$$E_\uparrow = -\frac{e\hbar B_0}{2mc} = E_1$$
$$E_\downarrow = \frac{e\hbar B_0}{2mc} = E_2$$

With frequency element,

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{eB_0}{mc}$$

Where eB_0/mc is the **Larmor frequency** and corresponds to the frequency of precession of a dipole μ in a magnetic field. We can now apply a time dependent magnetic field that is perpendicular to $\vec{B}_0$.

$$\vec{B}_1(t) = B_1(\hat{x}\cos\omega t + \hat{y}\sin\omega t)$$

Which rotates in the xy-plane with frequency ω. Then we have,

$$\begin{aligned}
V(t) &= -\vec{\mu}\cdot\vec{B}_1 \\
&= -\frac{eB_1}{mc}(S_x\cos\omega t + S_y\sin\omega t) \\
&= -\frac{eB_1}{mc}\frac{\hbar}{2}[(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)\cos\omega t + (-i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow|)\sin\omega t] \\
&= -\frac{eB_1}{mc}\frac{\hbar}{2}\left[e^{-i\omega t}|\uparrow\rangle\langle\downarrow| + e^{i\omega t}|\downarrow\rangle\langle\uparrow|\right] \\
&= -\gamma\left[e^{-i\omega t}|1\rangle\langle 2| + e^{i\omega t}|2\rangle\langle 1|\right]
\end{aligned}$$

Where,

$$\gamma = \frac{eB_1}{mc}\frac{\hbar}{2}$$

4.2 Adiatbatic Time-Dependence and Berry Phase

In some time-dependent systems where the time-dependence varies slowly compared to the natural time scales of the system, we make use of the **adiabatic approximation**. The principle feature is to write down the eigen-system for the time-dependent Hamiltonian and assume that the eigenkets at time $t = 0$ evolve in parallel,

$$H(t)|n;t\rangle = E_n(t)|n;t\rangle \tag{4.5}$$

Then an arbitrary state evolves with time in the $|n;t\rangle$ basis,

$$|\alpha;t\rangle = \sum_n c_n(t)e^{i\theta_n(t)}|n;t\rangle \tag{4.6}$$

Where $\theta_n(t)$ is the time-dependent phase associated with the evolution of $|\alpha;t\rangle$'s n-th energy coefficient.

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\mathrm{d}t' \tag{4.7}$$

These coefficients are also governed by the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}|\alpha;t\rangle = H(t)|\alpha;t\rangle$$

Expanding this out in terms of eq. (4.6),

$$i\hbar\frac{\partial}{\partial t}\sum_n c_n(t)e^{i\theta_n(t)}|n;t\rangle = H(t)\sum_n c_n(t)e^{i\theta_n(t)}|n;t\rangle$$

$$i\hbar\sum_n \frac{\partial}{\partial t}\Big(c_n(t)e^{i\theta_n(t)}|n;t\rangle\Big) = \sum_n c_n(t)e^{i\theta_n(t)}H(t)|n;t\rangle$$

$$i\hbar\sum_n \left[\frac{\partial}{\partial t}\Big(c_n(t)e^{i\theta_n(t)}|n;t\rangle\Big) + \frac{i}{\hbar}c_n(t)e^{i\theta_n(t)}E_n(t)|n;t\rangle\right] = 0$$

Applying product rule,

$$\sum_n \left[\frac{\partial c_n}{\partial t}e^{i\theta_n(t)} + i\frac{\partial \theta_n}{\partial t}c_n(t)e^{i\theta_n(t)} + c_n(t)e^{i\theta_n(t)}\frac{\partial}{\partial t} + \frac{i}{\hbar}c_n(t)e^{i\theta_n(t)}E_n(t)\right]|n;t\rangle = 0$$

But $\frac{\partial \theta_n}{\partial t} = -\frac{1}{\hbar}E_n(t)$ by eq. (4.7),

$$\sum_n e^{i\theta_n(t)}\left[\frac{\partial c_n}{\partial t} + c_n(t)\frac{\partial}{\partial t}\right]|n;t\rangle = 0$$

Using orthonormal properties one can calculate,

$$\langle m;t|\sum_n e^{i\theta_n(t)}\left[\frac{\partial c_n}{\partial t} + c_n(t)\frac{\partial}{\partial t}\right]|n;t\rangle = 0$$

$$\sum_n e^{i\theta_n(t)}\left[\frac{\partial c_n}{\partial t}\delta_{m,n}(t) + c_n(t)\langle m;t|\left[\frac{\partial}{\partial t}|n;t\rangle\right]\right] = 0$$

$$e^{i\theta_m(t)}\frac{\partial c_m}{\partial t} + \sum_n e^{i\theta_n(t)}c_n(t)\langle m;t|\left(\frac{\partial}{\partial t}|n;t\rangle\right) = 0$$

$$\frac{\partial c_m}{\partial t} = -\sum_n c_n(t)e^{i[\theta_n(t)-\theta_m(t)]}\langle m;t|\left(\frac{\partial}{\partial t}|n;t\rangle\right)$$

The θ phase contribution vanishes when $m = n$,

$$\frac{\partial c_m}{\partial t} = -c_m(t)\langle m;t|\left(\frac{\partial}{\partial t}|m;t\rangle\right) - \sum_{n\neq m} c_n(t)e^{i[\theta_n(t)-\theta_m(t)]}\langle m;t|\left(\frac{\partial}{\partial t}|n;t\rangle\right) \tag{4.8}$$

The second term indicates that as time evolves, $c_m(t)$ changes due to the difference $\theta_n(t) - \theta_m(t)$. Recall the familiar term $\langle m;t|\big(\frac{\partial}{\partial t}|n;t\rangle\big)$ which can be calculated directly from $H(t)$ using eq. (4.5).

$$\frac{\partial}{\partial t}[H(t)|n;t\rangle] = \frac{\partial}{\partial t}[E_n(t)|n;t\rangle]$$

Product rule again,

$$\dot{H}(t)|n;t\rangle + H(t)\frac{\partial}{\partial t}|n;t\rangle = \dot{E}_n(t)|n;t\rangle + E_n(t)\frac{\partial}{\partial t}|n;t\rangle$$

Therefore the matrix elements of $\dot{H}(t)$ are,

$$\dot{H}_{mn}(t) = \langle m;t|\dot{H}(t)|n;t\rangle = \dot{E}_n(t)\langle m;t|n;t\rangle - \langle m;t|H(t)\frac{\partial}{\partial t}|n;t\rangle + E_n(t)\langle m;t|\frac{\partial}{\partial t}|n;t\rangle$$

$$\dot{H}_{mn}(t) = \dot{E}_n(t)\delta_{nm}(t) + [E_n(t) - E_m(t)]\langle m;t|\frac{\partial}{\partial t}|n;t\rangle$$

Which has two cases,

$$m = n : \dot{H}_{mm}(t) = \dot{E}_m(t)$$

$$m \neq n : \dot{H}_{mn}(t) = [E_n(t) - E_m(t)]\langle m; t|\frac{\partial}{\partial t}|n; t\rangle$$

Applying this result to eq. (4.8) gives,

$$\frac{\partial c_m}{\partial t} = -c_m(t)\langle m; t|\left(\frac{\partial}{\partial t}|m; t\rangle\right) - \sum_{n\neq m} c_n(t)e^{i[\theta_n(t)-\theta_m(t)]}\frac{\dot{H}_{mn}(t)}{E_n(t) - E_m(t)}$$

We may now make the Adiabatic approximation by saying that the leading frequency dominates,

$$\frac{\partial c_m}{\partial t} \simeq -c_m(t)\langle m; t|\left(\frac{\partial}{\partial t}|m; t\rangle\right) \tag{4.9}$$

Fantastic! Equation (4.9) is a differential equation for $c_m(t)$ with no dependence on n. This is the essence of the Adiabatic approximation. If $c_m(0) = \delta_{nm}$ then $c_m(t) = \delta_{nm}(t)$. This suggests the ansatz,

$$c_m(t) = e^{i\gamma_m(t)}c_m(0) \tag{4.10}$$

With solution given by construction,

$$\gamma_m(t) = i\int_0^t \langle m; t'|\left[\frac{\partial}{\partial t'}|m; t'\rangle\right]\mathrm{d}t'$$

For convenience of notation, remove the primes on t by letting $t, t' = T, t$,

$$\gamma_m(T) = i\int_0^T \langle m; t|\left[\frac{\partial}{\partial t}|m; t\rangle\right]\mathrm{d}t \tag{4.11}$$

This is called the **Berry Phase**. Altogether we have,

$$|\alpha; t\rangle = \sum_n c_n(0)e^{i\gamma_n(t)}e^{i\theta_n(t)}|n; t\rangle$$

It is instructive to show that $\gamma_m(t)$ is real by demonstrating that $\langle m; t|\left[\frac{\partial}{\partial t}|m; t\rangle\right]$ is imaginary. Using product rule, note that,

$$\langle m; t|\left[\frac{\partial}{\partial t}|m; t\rangle\right] + \left[\frac{\partial}{\partial t}\langle m; t|\right]|m; t\rangle = \frac{\partial}{\partial t}\langle m; t|m; t\rangle = 0$$

Therefore,

$$\langle m; t|\left[\frac{\partial}{\partial t}|m; t\rangle\right] = -\left[\frac{\partial}{\partial t}\langle m; t|\right]|m; t\rangle = -\left(\langle m; t|\left[\frac{\partial}{\partial t}|m; t\rangle\right]\right)^*$$

As a demonstration, assume that we start in an eigenstate $|n, t\rangle$ and evolve under an adiabatic evolution. Then the state but will pick up an extra phase,

$$|\psi, t\rangle = e^{i\gamma_n(t)}e^{-\frac{i}{\hbar}\int_0^t \mathrm{d}t' E_n(t')}|n, t\rangle$$

Typically, the time dependence isn't directly parameterized by time but through a time-dependent coordinate $\vec{R}$[7] We can represent this auxiliary parameter dependence by the vector $\vec{R}$ in parameter space. Using $\vec{R}$ we can change the integral in eq. (4.11) from time to these parameters $\vec{R}$,

$$\langle m; t|\left[\frac{\partial}{\partial t}|m; t\rangle\right] = \langle m; t|\left[\vec{\nabla}_{\vec{R}}|m; t\rangle\right]\cdot\frac{\mathrm{d}\vec{R}}{\mathrm{d}t}$$

[7] For example $H(t) = -\vec{\mu}\cdot\vec{B}(t)$ is parameterized by $\vec{B}(t)$: $H\big(\vec{B}(t)\big)$.

Therefore,

$$\gamma_m(T) = i\int_{\vec{R}(0)}^{\vec{R}(T)} \langle m;t|\left[\vec{\nabla}_{\vec{R}}|m;t\rangle\right]\cdot \mathrm{d}\vec{R} \tag{4.12}$$

The integrand is the **Berry connection vector** for each eigenstate $|m;t\rangle$,

$$\vec{\mathcal{A}}_m = i\langle m;t|\left[\vec{\nabla}_{\vec{R}}|m;t\rangle\right]$$

This picture is particularly useful when considering complete cycles in parameter space where $\vec{R}(T) = \vec{R}(0)$. In such cases we can write the connection vector and the Berry phase as,

$$\vec{\mathcal{A}}_n\left(\vec{R}\right) = i\left\langle n(\vec{R})\right|\left[\vec{\nabla}_{\vec{R}}\left|n(\vec{R})\right\rangle\right]$$

$$\gamma_n(c) = \oint \vec{\mathcal{A}}_n\left(\vec{R}\right)\mathrm{d}\vec{R}$$

Which suggests the use of Stoke's theorem by defining the **Berry curvature**,

$$\vec{\Omega}_n\left(\vec{R}\right) = \vec{\nabla}_{\vec{R}} \times \vec{\mathcal{A}}_n\left(\vec{R}\right)$$

Which makes the Berry phase over a closed path c,

$$\gamma_n(c) = \oint \vec{\mathcal{A}}_n\left(\vec{R}\right)\mathrm{d}\vec{R} = \int \vec{\Omega}_n\left(\vec{R}\right)\mathrm{d}\vec{a}$$

4.3 Time-Dependent Perturbation Theory

So far we have looked at Rabi oscillations and adiabatic time dependence; two examples of a time-dependent Hamiltonian in which the wave equations can be solved analytically. Most problems unfortunately cannot be solved analytically. To solve this problems, we introduce time-dependent perturbation theory for small perturbations.

For a time-dependent potential $V(t)$, the complete solution to the time evolution of the system in the interaction picture is governed by,

$$|\psi,t\rangle_I = U^I(t)|\psi\rangle$$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U^{(I)}(t) = V^{(I)}(t)U^{(I)}(t) \tag{4.13}$$

Which can be solved using an iterative process. First notice that,

$$U^{(I)}(0) = \mathbb{1}$$

Which suggests (under the first order approximation) that,

$$U^{(I)}(t) \approx \mathbb{1} - \frac{i}{\hbar}\int_0^t \mathrm{d}t' V^{(I)}(t')U^{(I)}(t') \tag{4.14}$$

Further corrective terms can be computed by supplanting eq. (4.14) into eq. (4.13).

$$U^{(I)}(t) \approx \mathbb{1} - \frac{i}{\hbar}\int_0^t \mathrm{d}t' V^{(I)}(t')\left[\mathbb{1} - \frac{i}{\hbar}\int_0^{t'} \mathrm{d}t'' V^{(I)}(t'')\right]$$

This process can be continued to find the n-th order correction to $U(t)$. The resultant series is terms the **Dyson series**,

$$U^{(I)}(t) = \mathbb{1} - \frac{i}{\hbar}\int_0^t \mathrm{d}t' V(t') + \cdots + \left(\frac{i}{\hbar}\right)^n \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \cdots \int_0^{t^{(n-1)}} \mathrm{d}t^{(n)} V(t') \cdots V\left(t^{(n)}\right) + \cdots$$

Solving this series is frequently impossible/intractable. However for the purposes of perturbation theory we are only interested in calculating the lower-order corrections in order to get an approximation. Write $|\psi, t\rangle_I$ in turns of the unperturbed energy eigen-system $H_0|n\rangle = E_n|n\rangle$

$$|\psi, t\rangle_I = \sum_n c_n(t)|n\rangle = \sum_n |n\rangle \underbrace{\langle n|U(t)|\psi\rangle}_{c_n(t)}$$

Then we have that $c_n(t) = \langle n|U(t)|\psi\rangle$ and,

$$c_n(t) = c_n^{(0)}(t) + c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots$$

Where $c_n^{(0)} \sim V^0(t)$ and $c_n^{(1)} \sim V(t)$. Suppose that our initial state was in state $|i\rangle$,

$$|\psi\rangle = |i\rangle \qquad H_0|i\rangle = E_i|i\rangle$$

In this case $c_n^{(0)} = \delta_{ni}$: the initial state is $|i\rangle$ with certainty. In order to calculate $|\psi, t\rangle_I$ we simply need to calculate,

$$\begin{aligned}
c_n^{(1)}(t) &= -\frac{i}{\hbar}\int_0^t \mathrm{d}t' \langle n|V^{(I)}(t')|i\rangle \\
&= -\frac{i}{\hbar}\int_0^t \mathrm{d}t' \langle n|e^{\frac{i}{\hbar}H_0 t'} V(t') e^{-\frac{i}{\hbar}H_0 t'}|i\rangle \\
&= -\frac{i}{\hbar}\int_0^t \mathrm{d}t' e^{i\omega_{ni}t'} \langle n|V(t')|i\rangle \qquad \omega_{ni} = \frac{E_n - E_i}{\hbar} \\
&= -\frac{i}{\hbar}\int_0^t \mathrm{d}t' e^{i\omega_{ni}t'} V_{ni}(t')
\end{aligned}$$

Moreover we can calculate $c_n^{(2)}$ but inserting a resolution of identity,

$$\begin{aligned}
c_n^{(2)}(t) &= \left(-\frac{i}{\hbar}\right)^2 \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \langle n|V^{(I)}(t')V^{(I)}(t'')|i\rangle \\
&= \left(-\frac{i}{\hbar}\right)^2 \sum_m \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \langle n|V^{(I)}(t')|m\rangle\langle m|V^{(I)}(t'')|i\rangle \\
&= \left(-\frac{i}{\hbar}\right)^2 \sum_m \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' e^{i\omega_{nm}t'} e^{i\omega_{mi}t''} \langle n|V(t')|m\rangle\langle m|V(t'')|i\rangle \\
&= \left(-\frac{i}{\hbar}\right)^2 \sum_m \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' e^{i\omega_{nm}t'} e^{i\omega_{mi}t''} V_{nm}(t')V_{mi}(t'')
\end{aligned}$$

These two example illuminate how it is possible to write down the correct terms for any order. As an exercise, let us find the probability of transition from $|i\rangle$ to $|n\rangle$ at time t,

$$P(i \to n) = \left|c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots\right|^2$$

We will calculate this in a first-order perturbation theory by only considering the first term,

$$P(i \to n) = \left|c_n^{(1)}(t)\right|^2$$

$$= \left| -\frac{i}{\hbar} \int_0^t \mathrm{d}t' e^{i\omega_{ni}t'} V_{ni}(t') \right|^2$$
$$= \frac{1}{\hbar^2} \left| \int_0^t \mathrm{d}t' e^{i\omega_{ni}t'} V_{ni}(t') \right|^2$$

Let us choose a specific example for $V(t')$; the harmonic perturbation:

$$V(t) = Ve^{i\omega t} + V^\dagger e^{-i\omega t}$$

Where V is just come operator with the same dimension as H_0.

$$\begin{aligned}
c_n^{(1)}(t) &= -\frac{i}{\hbar} \int_0^t \mathrm{d}t' e^{i\omega_{ni}t'} V_{ni}(t') \\
&= -\frac{i}{\hbar} \int_0^t \mathrm{d}t' e^{i\omega_{ni}t'} \left[V_{ni} e^{i\omega t'} + V_{ni}^\dagger e^{-i\omega t'} \right] \\
&= -\frac{i}{\hbar} \left[V_{ni} \frac{e^{i(\omega_{ni}+\omega)t} - 1}{i(\omega_{ni}+\omega)} + V_{ni}^\dagger \frac{e^{i(\omega_{ni}-\omega)t} - 1}{i(\omega_{ni}-\omega)} \right] \\
&= -\frac{i}{\hbar} \left[V_{ni} \frac{e^{i(\omega_{ni}+\omega)t} - 1}{i(\omega_{ni}+\omega)} + V_{in}^* \frac{e^{i(\omega_{ni}-\omega)t} - 1}{i(\omega_{ni}-\omega)} \right]
\end{aligned}$$

This coefficient has two resonances; $c_n^{(1)}(t)$ is large only when $\omega \simeq \omega_{ni}$ or when $\omega \simeq -\omega_{ni}$. Let us restrict ourselves to the former condition ($\omega \simeq \omega_{ni}$). Here,

$$c_n^{(1)}(t) \simeq -\frac{V_{in}^*}{\hbar} \frac{e^{i(\omega_{ni}-\omega)t} - 1}{\omega_{ni} - \omega}$$

Which determined the transition probability,

$$\begin{aligned}
P(i \to n) &= \left| c_n^{(1)}(t) \right|^2 \\
&= \frac{|V_{in}^*|^2}{\hbar^2} \left| \frac{e^{i(\omega_{ni}-\omega)t} - 1}{\omega_{ni} - \omega} \right|^2 \\
&= \frac{|V_{in}|^2}{\hbar^2 (\omega_{ni} - \omega)^2} \left[(\cos(\omega_{ni} - \omega)t - 1)^2 + \sin^2(\omega_{ni} - \omega)t \right]^2 \\
&= \frac{|V_{in}|^2}{\hbar^2 (\omega_{ni} - \omega)^2} [2 - 2\cos(\omega_{ni} - \omega)t] \\
&= \frac{4|V_{in}|^2}{\hbar^2 (\omega_{ni} - \omega)^2} \sin^2\left(\frac{\omega_{ni} - \omega}{2} t \right) \\
&= \frac{|V_{in}|^2}{\hbar^2} \frac{\sin^2\left(\frac{\omega_{ni}-\omega}{2} t \right)}{\left(\frac{\omega_{ni}-\omega}{2} t \right)^2} t^2
\end{aligned}$$

An important feature of this transition probability is its long term behaviour. We should be carful moving forward however; the time-dependent perturbation becomes less and less valid at later times. Therefore we qualify our analysis by saying that we are looking at large times, but not too large that the perturbation breaks down. We define $\alpha = \frac{\omega_{ni}-\omega}{2}$ and examine the transition probability at large times,

$$f(\alpha) = \lim_{t \to \infty} \frac{\sin^2(\alpha t)}{\pi(\alpha)^2 t} = 0 \qquad \alpha \neq 0$$

$$f(0) = \lim_{t\to\infty}\lim_{\alpha\to 0}\frac{\sin^2(\alpha t)}{\pi(\alpha)^2 t} = \lim_{t\to\infty}\lim_{\alpha\to 0}\frac{(\alpha t)^2}{\pi(\alpha)^2 t} = \infty$$

Clearly $f(\alpha) \propto \delta(\alpha)$ is related to the Dirac delta function.

$$\int_{-\infty}^{\infty} \mathrm{d}\alpha f(\alpha) = \lim_{t\to\infty}\int_{-\infty}^{\infty} \mathrm{d}\alpha \frac{\sin^2(\alpha t)}{\pi\alpha^2 t} = 1$$

As it turns out, the factor of π present in the denominator makes $f(\alpha) = \delta(\alpha)$ precisely. Therefore the transition probability can be written,

$$P(i\to n) = \frac{|V_{in}|^2}{\hbar^2}\frac{\sin^2(\alpha t)}{(\alpha t)^2}t^2$$

We define the transition rate (probability of transition per unit time),

$$W_{i\to n} = \frac{\mathrm{d}P(i\to n)}{\mathrm{d}t}$$

In this way, the long term behaviour of $W_{i\to n}$ is set by $f(\alpha)$,

$$W_{i\to n} = \frac{|V_{in}|^2}{\hbar^2}\delta(\alpha)\pi$$

Recall that $\delta(ax) = \frac{1}{a}\delta(x)$,

$$\int_{-\infty}^{\infty} f(x)\delta(ax)\mathrm{d}x = \int_{-\infty}^{\infty} f\left(\frac{y}{a}\right)\delta(y)\frac{\mathrm{d}y}{a} = \frac{1}{a}\int_{-\infty}^{\infty} f\left(\frac{y}{a}\right)\delta(y)\mathrm{d}y = \frac{1}{a}f(0)$$

Applying this to $W_{i\to n}$,

$$W_{i\to n} = \frac{2\pi|V_{in}|^2}{\hbar^2}\delta(\omega_{ni}-\omega)$$

Or in terms of energies,

$$W_{i\to n} = \frac{2\pi|V_{in}|^2}{\hbar^2}\delta\left(\frac{1}{\hbar}(E_n - E_i - \hbar\omega)\right)$$

Pull out the factor of $\hbar^{-1}$,

$$W_{i\to n} = \frac{2\pi|V_{in}|^2}{\hbar}\delta(E_n - E_i - \hbar\omega)$$

This result is so important is in known as **Fermi's golden rule**. Physically, the δ-function expresses energy conservation in the sense that it is only non-zero if $E_n - E_i = \hbar\omega$. For example, if the energy of the final state is larger than the energy of the initial state, $E_n > E_i$ then the only way to transition from i to n is to absorb a quanta of energy with the amount $\hbar\omega$. This phenomena is called **absorbtion**. Similarly when $E_i > E_n$ we have **stimulated emissions**.

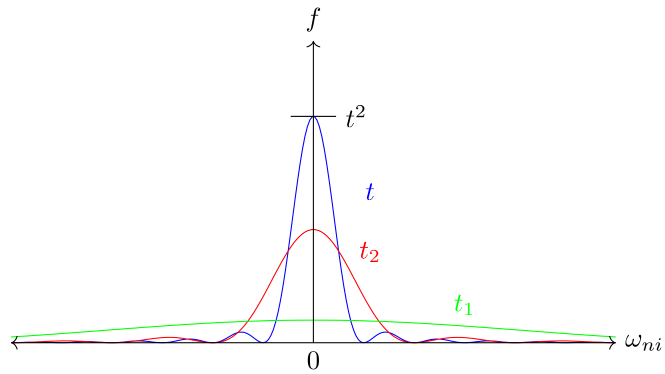
The probability under a time independent perturbation can be computed by seting $\omega = 0$. The transition frequency in this case becomes,

$$P(i\to n) = \frac{|V_{in}|^2}{\hbar^2}\frac{\sin^2\left(\frac{\omega_{ni}}{2}t\right)}{\left(\frac{\omega_{ni}}{2}\right)^2}$$

Where the function,

$$f(\omega_{ni}) = \frac{\sin^2\left(\frac{\omega_{ni}}{2}t\right)}{\left(\frac{\omega_{ni}}{2}\right)^2}$$

Can be plotted for different times $t_1 < t_2 < t$,



At $\omega_{ni} = 0$,

$$f(0) = \lim_{\omega_{ni} \to 0} \frac{\sin^2\left(\frac{\omega_{ni}}{2}t\right)}{\left(\frac{\omega_{ni}}{2}\right)^2} = t^2$$

As time increases, the height of the central peak increases as t^2 while its width decreases as $\frac{2\pi}{t}$. At long times $P(i \to n)$ is significant only when,

$$|w_{ni}| < \frac{2\pi}{t} \quad \left|\frac{E_n - E_i}{\hbar}\right| \sim \frac{2\pi}{t}$$

Which means that,

$$|E_n - E_i| t \sim 2\pi\hbar$$

This is similar to the energy-uncertainty relation $\Delta E \Delta t \sim \hbar$.

What happens to the state $|i\rangle$ itself? Consider a gradual turn-on of the perturbation,

$$V(t) = e^{\eta t} V \quad \eta > 0, \eta \to 0^+$$

For any finite η, $V(t \to -\infty) = 0$. The perturbation is absent at $t \to -\infty$ and is slowly turned on. In this case,

$$\begin{aligned}
c_n^{(1)}(t) &= -\frac{i}{\hbar} V_{ni} \int_{-\infty}^{t} \mathrm{d}t' e^{\eta t'} e^{i\omega_{ni} t'} \\
&= -\frac{i}{\hbar} V_{ni} \left(\frac{e^{(\eta + i\omega_{ni})t'}}{\eta + i\omega_{ni}} \right|_{-\infty}^{t} \\
&= -\frac{i}{\hbar} V_{ni} \frac{e^{(\eta + i\omega_{ni})t}}{\eta + i\omega_{ni}} \\
\left| c_n^{(1)}(t) \right|^2 &= \frac{|V_{ni}|^2}{\hbar^2} \frac{e^{2\eta t}}{\eta^2 + \omega_{ni}^2} = P(i \to n)
\end{aligned}$$

Therefore the transition rate is,

$$W_{i \to n} = \frac{\mathrm{d}P(i \to n)}{\mathrm{d}t} = \frac{2|V_{ni}|^2}{\hbar^2} \frac{\eta e^{2\eta t}}{\eta^2 + \omega_{ni}^2}$$

Which in the limit of $\eta \to 0$ is,

$$\lim_{\eta \to 0} \frac{\eta}{\eta^2 + \omega_{ni}^2} = \begin{cases} 0 & \omega_{ni} \neq 0 \\ \infty & \omega_{ni} = 0 \end{cases}$$

Also note that,

$$\int_{-\infty}^{\infty} \mathrm{d}\omega_{ni} \frac{\eta}{\eta^2 + \omega_{ni}^2} = \pi$$

Therefore,

$$W_{i\to n} = \frac{2\pi}{\hbar^2}|V_{ni}|^2 \delta(\omega_{ni}) = \frac{2\pi}{\hbar}|V_{ni}|^2 \delta(E_n - E_i)$$

This is another instance of Fermi's golden rule. We can then calculate,

$$c_i^{(0)}(t) = 1$$

$$c_i^{(1)}(t) = -\frac{i}{\hbar}V_{ii}\int_0^t \mathrm{d}t' e^{\eta t'} = -\frac{i}{\hbar\eta}V_{ii}e^{\eta t}$$

And the second order coefficient,

$$\begin{aligned}
c_i^{(2)}(t) &= \left(-\frac{i}{\hbar}\right)^2 \sum_m \int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}t'' e^{i\omega_{in}t'} e^{i\omega_{im}t''} V_{im}V_{mi} e^{\eta t'} e^{\eta t''} \\
&= \left(-\frac{i}{\hbar}\right)^2 \sum_m |V_{im}|^2 \int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}t'' e^{(\eta + i\omega_{im})t'} e^{(\eta + i\omega_{im})t''} \\
&= \left(-\frac{i}{\hbar}\right)^2 \sum_m |V_{im}|^2 \int_{-\infty}^{t} \mathrm{d}t' \frac{1}{(\eta + i\omega_{im})} e^{(\eta + i\omega_{im})t'} e^{(\eta + i\omega_{im})t'} \\
&= \left(-\frac{i}{\hbar}\right)^2 \sum_m |V_{im}|^2 \int_{-\infty}^{t} \mathrm{d}t' \frac{1}{(\eta + i\omega_{im})} e^{2\eta t'} \qquad \omega_{im} = -\omega_{mi} \\
&= \left(-\frac{i}{\hbar}\right)^2 \sum_m |V_{im}|^2 \frac{1}{2\eta(\eta + i\omega_{im})} e^{2\eta t}
\end{aligned}$$

Since $\omega_{ii} = 0$ for $V(t) = e^{\eta t}V$ we can break up the sum,

$$c_i^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 |V_{ii}|^2 \frac{1}{2\eta^2} e^{2\eta t} + \left(-\frac{i}{\hbar}\right)^2 \sum_{m\neq i} |V_{im}|^2 \frac{1}{2\eta(\eta + i\omega_{im})} e^{2\eta t}$$

Recombining contributions from all orders up to 2,

$$\begin{aligned}
c_i(t) &\simeq c_i^{(0)} + c_i^{(1)} + c_i^{(2)} \\
&\simeq 1 - \frac{i}{\hbar\eta}V_{ii}e^{\eta t} + \left(-\frac{i}{\hbar}\right)^2 |V_{ii}|^2 \frac{1}{2\eta^2} e^{2\eta t} + \left(-\frac{i}{\hbar}\right)^2 \sum_{m\neq i} |V_{im}|^2 \frac{1}{2\eta(\eta + i\omega_{im})} e^{2\eta t}
\end{aligned}$$

If we compute the derivative of $c_i(t)$ is arrive at,

$$\frac{1}{c_i(t)}\frac{\mathrm{d}c_i(t)}{\mathrm{d}t} = \frac{-\frac{i}{\hbar}V_{ii}e^{\eta t} + \left(-\frac{i}{\hbar}\right)^2 |V_{ii}|^2 \frac{1}{\eta} e^{2\eta t} + \left(-\frac{i}{\hbar}\right)^2 \sum_{m\neq i} |V_{im}|^2 \frac{1}{\eta + i\omega_{im}} e^{2\eta t}}{1 - \frac{i}{\hbar}V_{ii}\frac{e^{\eta t}}{\eta}}$$

Since $V_{ii}/\hbar\eta \ll 1$, we can Taylor series the denominator,

$$\left[1 - \frac{i}{\hbar}V_{ii}\frac{e^{\eta t}}{\eta}\right]^{-1} \simeq 1 + \frac{i}{\hbar}V_{ii}\frac{e^{\eta t}}{\eta}$$

And keep only second order terms in V,

$$\frac{1}{c_i(t)}\frac{\mathrm{d}c_i(t)}{\mathrm{d}t} = -\frac{i}{\hbar}V_{ii}e^{\eta t} + \left(-\frac{i}{\hbar}\right)^2\sum_{m\neq i}|V_{im}|^2\frac{1}{\eta + i\omega_{im}}e^{2\eta t}$$

Which is the essential result of second order perturbation theory for $V(t) = e^{\eta t}V$.

$$\frac{1}{c_i(t)}\frac{\mathrm{d}c_i(t)}{\mathrm{d}t} = -\frac{i}{\hbar}V_{ii}e^{\eta t} - \frac{i}{\hbar}\sum_{m\neq i}|V_{im}|^2\frac{e^{2\eta t}}{E_i - E_m + i\hbar\eta}$$

If we take the limit of long times or small $\eta \to 0$, we obtain the result for constant potentials. We retain the η contribution in the denominator.

$$\frac{1}{c_i(t)}\frac{\mathrm{d}c_i(t)}{\mathrm{d}t} = -\frac{i}{\hbar}V_{ii} - \frac{i}{\hbar}\sum_{m\neq i}|V_{im}|^2\frac{1}{E_i - E_m + i\hbar\eta}$$

If we define Δ_i to be,

$$\Delta_i = V_{ii} + \sum_{m\neq i}|V_{mi}|^2\frac{1}{E_i - E_m + i\hbar\eta}$$

Then we arrive at,

$$\frac{\mathrm{d}c_i(t)}{\mathrm{d}t} = -\frac{i}{\hbar}\Delta_i c_i(t) \implies c_i(t) = c_i e^{-\frac{i}{\hbar}\Delta_i t}$$

Or in the Schrödinger picture,

$$c_i(t) = c_i e^{-\frac{i}{\hbar}\Delta_i t}e^{-\frac{i}{\hbar}E_i t}$$

What is the physical meaning of this result? Recall that $c_i(t)$ are the coefficients of the wavefunction in the interaction picture.

$$|\psi, t\rangle_I = \sum_n c_n(t)|n\rangle$$

Therefore the real part of Δ_i has the meaning of the shift of the energy of $|i\rangle$ under the action of the perturbation. We can decompose the contributions into the two orders,

$$\Delta_i = \Delta_i^{(1)} + \Delta_i^{(2)}$$

Where $\Delta_i^{(1)} = V_{ii}$ agrees with time-independent perturbation theories. However the second order contribution is,

$$\Delta_i^{(2)} = \sum_{m\neq i}|V_{mi}|^2\frac{1}{E_i - E_m + i\hbar\eta}$$

Notice that the fractional term can the following structure,

$$\frac{1}{x + i\epsilon} = \frac{x - i\epsilon}{x^2 + \epsilon^2} = \frac{x}{x^2 + \epsilon^2} + i\frac{-\epsilon}{x^2 + \epsilon^2}$$

Where $\lim_{\epsilon\to 0}\epsilon/\left(\epsilon^2 + x^2\right) = \pi\delta(x)$. Therefore the imaginary part is sifting,

$$\Im\left(\Delta_i^{(2)}\right) = -\pi\sum_{m\neq i}|V_{im}|^2\delta(E_i - E_m)$$

If you recall Fermi's golden rule,

$$W_{i\to m} = \frac{2\pi}{\hbar}|V_{im}|^2\delta(E_i - E_m)$$

You can suggestively write,

$$\Im\left(\Delta_i^{(2)}\right) = -\frac{\hbar}{2}\sum_{m\neq i}W_{i\to m}$$

Therefore,

$$c_i(t) \sim e^{-\frac{i}{\hbar}\Re(\Delta_i)t} e^{-\frac{1}{2\hbar}\Gamma_i t}$$

Where $\Gamma_i = -2\Im\left(\Delta_i^{(2)}\right)$ acts as a decay constant,

$$\left|c_i(t)\right|^2 \sim e^{-\frac{\Gamma_i}{\hbar}t}$$

Which suggests that $\tau_i = \hbar/\Gamma_i$ is the lifetime of state $|i\rangle$. Therefore for $t > \tau_i$ the probability to still find the system in the initial state is exponentially small.

5 Relativistic Quantum Mechanics

Todo (TC Fraser): Missed 2 lectures