

Single Particle Systems

First Quantization

The Schrödinger Equation governs non-relativistic quantum particles wave functions $\Psi(\vec{r}, t)$

The single particle Hamiltonian of a non-relativistic particle under a scalar potential $V(\vec{r})$ and a vector potential \vec{A} ($\nabla \times \vec{A} = \vec{B}$)

$$\hat{H} = \frac{(\vec{p} - q\vec{A})^2}{2m^*} + V(\vec{r}) \quad \begin{matrix} (q: \text{charge of the particle}) \\ (m^*: \text{effective mass}) \end{matrix}$$

The Schrödinger equation in the Dirac notation

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

Time Evolution Operator $\xleftarrow{\partial t}$ Hamiltonian Operator $\xrightarrow{\hat{H}}$

$|\Psi(t)\rangle$: "Ket"

$(|\Psi(t)\rangle)^\dagger = \langle \Psi(t)|$: "bra"

$\langle \vec{r} | \Psi(t) \rangle = \Psi(\vec{r}, t)$: wave-function in real space

$\langle \phi | \Psi \rangle = \int \phi^*(\vec{r}) \Psi(\vec{r}) d^3\vec{r}$: Inner product (notice that we can omit the space dependence)

Basis and the Hilbert Space

The set of all square integrable functions over an interval constitutes a vector space. Mathematically it is called $L^2(a, b)$ but in physics we call it the Hilbert space. Single-particle wavefunctions live in Hilbert space.
Hilbert space : Inner-product space of square integrable function in an interval.

Since we have a vector space (Hilbert space) we can define its basis

$\{\lvert \Phi_\alpha \rangle\}$: Orthonormal basis (complete set) of the Hilbert space

$$\langle \Phi_\alpha | \Phi_\beta \rangle = \delta_{\alpha,\beta} \quad (\text{Orthogonality and normalization})$$

$$\sum_{\alpha} |\Phi_{\alpha}\rangle \langle \Phi_{\alpha}| = \mathbb{I} \quad (\text{Completeness})$$

We can express wavefunctions in the Hilbert space as a linear combination of the basis set

$$|\Psi(t)\rangle = \sum_{\alpha} C_{\alpha}(t) |\Phi_{\alpha}\rangle \quad \text{with} \quad C_{\alpha}(t) = \langle \Phi_{\alpha} | \Psi(t) \rangle$$

Operators

$$\hat{O}|\Psi\rangle = |\Phi\rangle \quad \text{and} \quad \langle \Psi | \hat{O} = \langle \Phi |$$

The representation of the operator \hat{O} in the set of basis $\{\lvert \Phi_\alpha \rangle\}$

$$\hat{O}_{\alpha\beta} = \langle \Phi_\alpha | \hat{O} | \Phi_\beta \rangle$$

$$\hat{O}_{\beta\alpha}^* = \langle \Phi_\beta | \hat{O}^\dagger | \Phi_\alpha \rangle$$

Now, consider the 1D Schrödinger equation (with $\vec{r}=0$, for simplicity)

$$i\partial_t |\Psi(t)\rangle = \frac{\hat{p}^2}{2m} |\Psi(t)\rangle + \hat{V} |\Psi(t)\rangle$$

act with $\langle \vec{r} |$

$$\langle \vec{r} | i\partial_t |\Psi(t)\rangle = \langle \vec{r} | \frac{\hat{p}^2}{2m} |\Psi(t)\rangle + \langle \vec{r} | \hat{V} |\Psi(t)\rangle$$

$$\langle \vec{r} | \hat{p} |\Psi(t)\rangle = \frac{\hbar}{i} \frac{d}{dx} \Psi(x,t)$$

$$\langle \vec{r} | \hat{p}^2 | \Psi(x,t) \rangle = -\hbar^2 \frac{\partial^2 \Psi(x,t)}{\partial x^2}$$

$$\langle \vec{r} | \hat{V} | \Psi(x,t) \rangle = V(x) \Psi(x,t)$$

Then the real space representation of the 1D Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) + V(x) \Psi(x,t)$$

Position and Momentum Basis Vectors (Non-denumerable basis)

$$\langle \vec{r} | \Psi \rangle = \Psi(\vec{r}), \quad \langle \vec{p} | \Psi \rangle = \Psi(\vec{p}) \text{ or } \langle \vec{x} | \Psi \rangle = \Psi(\vec{x})$$

Position basis : $\hat{r} | \vec{r} \rangle = \vec{r} | \vec{r} \rangle$ ($\hat{x} | \vec{x} \rangle = \vec{x} | \vec{x} \rangle$)

Momentum basis : $\hat{p} | \vec{p} \rangle = \vec{p} | \vec{p} \rangle$ or $\hat{p} | \vec{k} \rangle = \hbar \vec{k} | \vec{k} \rangle$

$$\begin{aligned} \text{They are orthogonal : } & \langle \vec{r} | \vec{r}' \rangle = \delta(\vec{r} - \vec{r}') \\ & \langle \vec{k} | \vec{k}' \rangle = \delta(\vec{k} - \vec{k}') \end{aligned}$$

They are also complete basis

$|\alpha\rangle = \int d^3 \vec{r} C(\vec{r}) |\vec{r}\rangle$ if we act with $\langle \vec{r}' |$ we get

$$\langle \vec{r}' | \alpha \rangle = \int d^3 \vec{r} C(\vec{r}) \langle \vec{r}' | \vec{r} \rangle = C(\vec{r}') \text{ since } \langle \vec{r}' | \vec{r}' \rangle = \delta(\vec{r}' - \vec{r}')$$

Then

$$|\alpha\rangle = \int d^3 \vec{r} \langle \vec{r} | \alpha \rangle |\vec{r}\rangle = \int d^3 \vec{r} |\vec{r}\rangle \langle \vec{r} | \alpha \rangle = \mathbb{1} |\alpha\rangle, \text{ hence}$$

$$\int d^3 \vec{r} |\vec{r}\rangle \langle \vec{r}| = \mathbb{1}$$

This also works for momentum basis

$$\int d^3\vec{r} |\vec{r}\rangle \langle \vec{r}| = \int d^3\vec{p} |\vec{p}\rangle \langle \vec{p}| = \int \hbar^3 d^3\vec{k} |\vec{k}\rangle \langle \vec{k}|, \text{ then}$$

$$|\vec{P}\rangle = \frac{1}{\hbar^{3/2}} |\vec{k}\rangle$$

If we start with a state vector $|\psi\rangle$

$$|\psi\rangle = \underbrace{\int d^3\vec{r} |\vec{r}\rangle \langle \vec{r}|}_{\int d^3\vec{k} |\vec{k}\rangle \langle \vec{k}|} \psi(\vec{r}) |\vec{r}\rangle = \int d^3\vec{k} \psi(\vec{k}) |\vec{k}\rangle$$

$$\int d^3\vec{p} |\vec{p}\rangle \langle \vec{p}| \psi(\vec{p}) = \int d^3\vec{p} \psi(\vec{p}) |\vec{p}\rangle$$

Observables (Hermitian Operators)

The expectation value of an operator \hat{O} in the state $|\psi\rangle$

$$\langle \hat{O} \rangle_\psi = \langle \psi | \hat{O} | \psi \rangle = \int \psi^\dagger \hat{O} \psi d^3x$$

If \hat{O} is an observable operator

$$\langle \hat{O} \rangle_\psi = \langle \hat{O} \rangle_\psi^* \rightarrow \langle \psi | \hat{O} \psi \rangle = (\langle \psi | \hat{O} \psi \rangle)^* = \langle \hat{O} \psi | \psi \rangle$$

$$\rightarrow \int \psi^\dagger \hat{O} \psi d^3x = \int (\hat{O} \psi)^\dagger \psi d^3x = \int \psi^\dagger \hat{O}^\dagger \psi d^3x$$

Observables are represented by Hermitian operators

Hermitian Operators Satisfy

$$\rightarrow \langle \phi | \hat{O} \psi \rangle = \langle \hat{O} \phi | \psi \rangle \text{ for any } |\phi\rangle \text{ and } |\psi\rangle,$$

\rightarrow this condition is equivalent to $\hat{O} = \hat{O}^\dagger$

The momentum operator

$$\langle \hat{O} | \hat{P}_x | \Psi \rangle = \int_{-\infty}^{\infty} \hat{O}^\dagger (-i\hbar \frac{d}{dx}) \Psi dx = -i\hbar \hat{O}^\dagger \Psi \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \left(-i\hbar \frac{d}{dx} \hat{O} \right)^\dagger \Psi dx$$

$$= \langle P_x \hat{O} | \Psi \rangle$$

→ The eigenvalues of a Hermitian operator are real

$$\hat{O} |\hat{O}_\alpha \rangle = \alpha |\hat{O}_\alpha \rangle \text{ with } \alpha \in \mathbb{R}$$

→ Let $\{\hat{O}_n\}$ be a complete set of eigenvectors of \hat{O} with eigenvalues α_n

$$|\Psi\rangle = \sum_{n=0}^{\infty} C_n |\hat{O}_n\rangle \text{ with } C_n = \langle \hat{O}_n | \Psi \rangle$$

$$\text{Then } \langle \hat{O} \rangle_\Psi = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} C_n^* C_m \langle \hat{O}_n | \hat{O}_m | \Psi \rangle = \sum_{n=0}^{\infty} \alpha_n |C_n|^2$$

So, the probability of measuring the eigenvalue α_n of the observable \hat{O} if the particle is in the state $|\Psi\rangle$

$$P_\Psi(\alpha_n) = |C_n|^2 = |\langle \hat{O}_n | \Psi \rangle|^2$$

for a continuous representation, for example $|\vec{r}\rangle$

$$|\Psi\rangle = \int d^3\vec{r} C(\vec{r}) |\vec{r}\rangle \text{ with } C(\vec{r}) = \langle \vec{r} | \Psi \rangle$$

$$\langle \vec{r} \rangle_\Psi = \iint d^3\vec{r}' d^3\vec{r} C(\vec{r}') C(\vec{r}) \langle \vec{r}' | \vec{r} | \Psi \rangle$$

$$\langle \vec{r} \rangle_\Psi = \int d^3\vec{r} \vec{r} |C(\vec{r})|^2$$

$$dP_\Psi(\vec{r}) = d^3\vec{r} |\langle \vec{r} | \Psi \rangle|^2 = d^3\vec{r} |\Psi(\vec{r})|^2 \quad (\text{Probability density})$$

Probability of the particle in state $|\Psi\rangle$ being in a volume $d^3\vec{r}$ around the

position \vec{r} at time t (t was implicit in $|\Psi\rangle$).

Time Independent Schrödinger Equation

Consider the Schrödinger Equation in real space (1D)

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} \Psi(x,t) + V(x) \Psi(x,t)$$

Since V is independent of t we can use separation of variables

$$\Psi(x,t) = \Psi(x) \Phi(t)$$

$$\frac{\Psi(x)}{\Psi(x,t)} i\hbar \frac{\partial}{\partial t} \Phi(t) = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} \Psi(x) + V(x) \Psi(x) \Phi(t)$$

$$i\hbar \frac{1}{\Phi(t)} \frac{\partial}{\partial t} \Phi(t) = -\frac{\hbar^2}{2m^*} \frac{1}{\Psi(x)} \frac{\partial^2}{\partial x^2} \Psi(x) + V(x)$$

Since the left side is a function of t alone and the right side is a function of x alone, the only way the equation can be satisfied is if both sides are a constant

$$i\hbar \frac{1}{\Phi(t)} \frac{\partial}{\partial t} \Phi(t) = E \rightarrow \frac{\partial \Phi(t)}{\partial t} = -\frac{iE}{\hbar} \Phi(t) \rightarrow \Phi(t) = C e^{-iEt/\hbar}$$

absorbing C in $\Psi(x)$ we have $\Phi(t) = e^{-iEt/\hbar}$, and for the time independent part we get

$$\left[-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x) = E \Psi(x)$$

then the time independent Schrödinger equation is

$$\hat{H} \Psi(x) = E \Psi(x)$$

The solution to this equation are stationary states

$$\Psi(x,t) = \Psi(x) e^{iEt/\hbar}$$

the probability density is independent of time $|\Psi(x,t)|^2 = |\Psi(x)|^2$

The operator $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$ is the Hamiltonian.

The expectation value of \hat{H}

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \hat{H} \Psi(x,t) dx = E \int_{-\infty}^{\infty} |\Psi(x)|^2 dx = E$$

and

$$\hat{H} \Psi(x) = E \Psi(x) \rightarrow \hat{H}^2 \Psi(x) = E^2 \Psi(x)$$

$$\langle \hat{H}^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \hat{H}^2 \Psi(x,t) dx = E^2$$

Then the variance $\sigma_H = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = 0$

The time independent Schrödinger equation leads to an infinite collection of solutions $\{\Psi_n(x)\}$ corresponding to the energies $\{E_n\}$, then for each allowed energy we have

$$\langle \vec{r} | \Psi_n(t) \rangle = \Psi_n(x) e^{-iE_n t / \hbar}$$

and a general eigen state can be written as

$$|\Psi(t)\rangle = \sum_{n=0}^{\infty} C_n |\Psi_n(t)\rangle$$

$$\langle \vec{r} | \Psi(t) \rangle = \Psi(x,t) = \sum_{n=0}^{\infty} C_n \Psi_n(x) e^{-iE_n t / \hbar}$$

Using the time independent Schrödinger equation we can solve several problems, such as

Particle in a box, Square well, Step potential, S-potential, hydrogen atom, etc.

In all these problems the solution to the Schrödinger equation is supplemented by boundary conditions:

- 1) Ψ is continuous
- 2) $\partial_x \Psi$ is also continuous (The S-potential requires special treatment).

Now we will focus on the Quantum Harmonic oscillator problem as it introduces us to 2nd quantization

Second Quantization:

The 1D Quantum Harmonic Oscillator

The Hamiltonian of a particle in a harmonic oscillator is

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

in quantum mechanics $[\hat{x}, \hat{p}] = i\hbar$.

In position representation $\langle \vec{r} | \hat{p} | \Psi(t) \rangle = -i\hbar \partial_x \Psi(x, t)$, we can solve the differential equations but there is a different and more compact way to solve this problem

define :
$$\begin{cases} \hat{X} = \sqrt{m\omega/\hbar} \hat{x} \\ \hat{P} = \hat{p}/\sqrt{m\omega\hbar} \end{cases}$$

notice that $\hat{x} = \sqrt{\frac{\hbar}{m\omega}} \hat{X}$ and $\hat{p} = \sqrt{m\omega\hbar} \hat{P}$

$$\text{also } \hat{x}^2 = \frac{\hbar}{m\omega} \hat{X}^2 \text{ and } \hat{p} = m\hbar\omega \hat{P}^2$$

The Hamiltonian becomes

$$\hat{H} = \frac{1}{2m} m\hbar\omega \hat{P}^2 + \frac{1}{2} m\omega^2 \frac{\hbar}{m\omega} \hat{X}^2, \text{ then}$$

$$\hat{H} = \frac{\hbar\omega}{2} (\hat{P}^2 + \hat{X}^2)$$

$$\begin{cases} \hat{a} = (\hat{X} + i\hat{P})/\sqrt{2} \\ \hat{a}^\dagger = (\hat{X} - i\hat{P})/\sqrt{2} \end{cases}$$

$$\text{Then, } \hat{X} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}} \text{ and } \hat{P} = \frac{i(\hat{a}^\dagger - \hat{a})}{\sqrt{2}}$$

Now we need to determine the commutation relations of, i.e.,

$$[\hat{X}, \hat{P}] = i \quad \text{and} \quad [\hat{a}, \hat{a}^\dagger] = 1.$$

Proof

$$[\hat{X}, \hat{P}] = \sqrt{\frac{m\omega}{\hbar}} \frac{1}{\sqrt{m\hbar\omega}} [\hat{X}, \hat{P}] = \frac{1}{\hbar} i\hbar = i$$

$$[\hat{a}, \hat{a}^\dagger] = \frac{1}{2} [\hat{X} + i\hat{P}, \hat{X} - i\hat{P}] = \frac{1}{2} (-i[\hat{X}, \hat{P}] + i[\hat{P}, \hat{X}])$$

$$[\hat{a}, \hat{a}^\dagger] = \frac{1}{2} [-i\hbar + i(-\hbar)] = 1.$$

So, we can show that

$$\hat{H} = \hbar\omega (\hat{a}^\dagger \hat{a} + \frac{1}{2})$$

Proof

$$\hat{H} = \frac{\hbar\omega}{2} (\hat{P}^2 + \hat{X}^2) = \frac{\hbar\omega}{2} \left[-\frac{(\hat{a}^\dagger - \hat{a})(\hat{a}^\dagger - \hat{a})}{2} + \frac{(\hat{a}^\dagger + \hat{a})(\hat{a}^\dagger + \hat{a})}{2} \right]$$

$$\hat{H} = \frac{\hbar\omega}{4} \left[-\cancel{\hat{a}^\dagger \hat{a}^\dagger} + \hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger - \cancel{\hat{a} \hat{a}} + \cancel{\hat{a}^\dagger \hat{a}^\dagger} + \cancel{\hat{a}^\dagger \hat{a}} + \cancel{\hat{a} \hat{a}^\dagger} + \cancel{\hat{a} \hat{a}} \right]$$

$$\hat{H} = \frac{\hbar\omega}{2} [\hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger], \text{ but } [\hat{a}, \hat{a}^\dagger] = 1 = \hat{a} \hat{a}^\dagger - \hat{a}^\dagger \hat{a}$$

$$\hat{H} = \frac{\hbar\omega}{2} [\hat{a}^\dagger \hat{a} + 1 + \hat{a}^\dagger \hat{a}] = \hbar\omega \left[\hat{a}^\dagger \hat{a} + \frac{1}{2} \right]$$

We can show that

1) The number operator $\hat{N} \equiv \hat{a}^\dagger \hat{a}$ is Hermitian and commutes with \hat{H} (they have simultaneous eigen states).

2) $\hat{N}|n\rangle = n|n\rangle$ where $n=0, 1, 2, \dots$

3) $\hat{H}|n\rangle = E_n|n\rangle$ with $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, $n=0, 1, 2, \dots$

4) $\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$, $\hat{a}|n\rangle = \sqrt{n} |n-1\rangle$, and $|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle$

Proof of show that if $\hat{N}|n\rangle = n|\hat{N}\rangle$, then $n=0, 1, 2, \dots$

Let $\hat{N}|n\rangle = n|n\rangle$

act with \hat{a} $\rightarrow \hat{a}\hat{N}|n\rangle = n\hat{a}|n\rangle$, but $\hat{N} = \hat{a}^\dagger \hat{a}$
 $\hat{a} \hat{a}^\dagger \hat{a}|n\rangle = n\hat{a}|n\rangle$, and $\hat{a} \hat{a}^\dagger - \hat{a}^\dagger \hat{a} = 1$
 $(1 + \hat{a}^\dagger \hat{a})\hat{a}|n\rangle = n\hat{a}|n\rangle$
 $\hat{N}(\hat{a}|n\rangle) = (n-1)(\hat{a}|n\rangle)$

then $\hat{a}|n\rangle$ is an eigenstate of \hat{N} with the eigenvalue $(n-1)$. Moreover $\hat{a}|n\rangle \sim |n-1\rangle$

$$\text{Apply } \hat{a} \text{ again, } \hat{a}\hat{a}^\dagger\hat{a}(\hat{a}|n\rangle) = (n-1)(\hat{a})^2|n\rangle$$

$$(\hat{I} + \hat{a}\hat{a}^\dagger)(\hat{a})^2|n\rangle = (n-1)(\hat{a})^2|n\rangle$$

$$\hat{N}(\hat{a}^2|n\rangle) = (n-2)(\hat{a}^2|n\rangle)$$

which means that $\hat{a}^2|n\rangle$ is an eigen state of \hat{N} with the eigenvalue $(n-2)$ and $\hat{a}^2|n\rangle \sim |n-2\rangle$

Hence, the application of \hat{a} S times leads

$$\hat{N}(\hat{a}^S|n\rangle) = (n-S)(\hat{a}^S|n\rangle).$$

Therefore, the sequence $\hat{a}|n\rangle, \hat{a}^2|n\rangle, \dots, \hat{a}^S|n\rangle, \dots$ are eigenstates of \hat{N} with the eigenvalues $n-1, n-2, \dots, n-S, \dots$.

What if we apply \hat{a}^\dagger to $\hat{N}|n\rangle = n|n\rangle$

$$\hat{a}^\dagger\hat{a}^\dagger\hat{a}^\dagger\hat{N}|n\rangle = n\hat{a}^\dagger|n\rangle$$

$$\hat{a}^\dagger(\hat{a}\hat{a}^\dagger - 1)|n\rangle = n\hat{a}^\dagger|n\rangle$$

$$\hat{N}(\hat{a}^\dagger|n\rangle) = (n+1)(\hat{a}^\dagger|n\rangle)$$

then $\hat{a}^\dagger|n\rangle$ is an eigenstate of \hat{N} with the eigenvalue $(n+1)$.

Similar to the procedure for \hat{a} , we find that the application of \hat{a}^\dagger S times leads to

$$\hat{N}[(\hat{a}^\dagger)^S|n\rangle] = (n+S)[(\hat{a}^\dagger)^S|n\rangle]$$

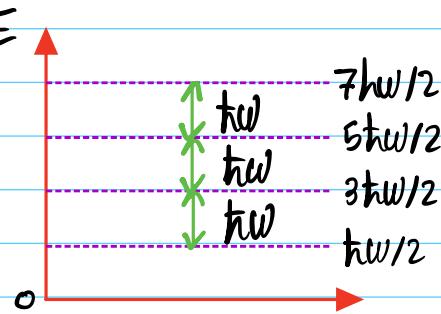
which means that the sequence $\hat{a}^\dagger|n\rangle, (\hat{a}^\dagger)^2|n\rangle, \dots, (\hat{a}^\dagger)^S|n\rangle, \dots$ are eigen states of \hat{N} with the eigen values $(n+1), (n+2), \dots, (n+S), \dots$

By successive applications of \hat{a}^\dagger and \hat{a} we found that the eigen values of $|n\rangle$ belong to the sequence $\dots, n+2, n+1, n, n-1, n-2, \dots$.

If we let n_0 be the smallest of the eigenvalues of \hat{N} . Then it is clear that

$\hat{a}|n_0\rangle = 0$ and $\hat{N}|n_0\rangle = \hat{a}^\dagger \hat{a}|n_0\rangle = 0$. Hence $n_0 = 0$. Moreover, by successive application of $\hat{a}^\dagger|0\rangle$ we see that the eigenvalues of \hat{N} are $0, 1, 2, \dots$

Single-particle spectrum



$$\hat{H}|n\rangle = E_n |n\rangle$$

$$E_n = \hbar\omega \left(n + \frac{1}{2}\right), n=0,1,2,\dots$$

$\{|n\rangle\} \rightarrow$ Orthonormal basis
 $\langle n|n'\rangle = \delta_{n,n'}$ and

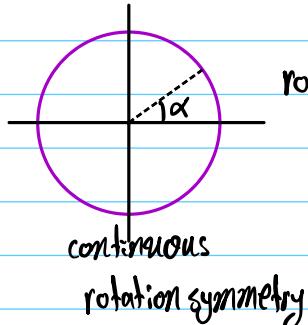
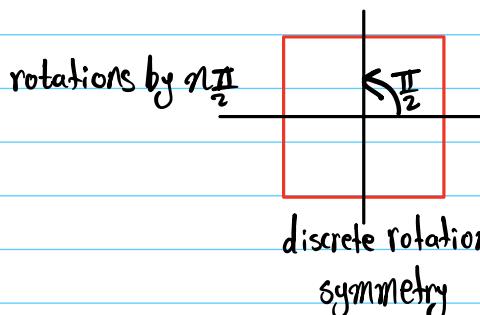
$$\sum_n |n\rangle \langle n| = \mathbb{I}$$

$$|\Psi(t)\rangle = \sum_n c_n(t) |n\rangle \text{ with } c_n(t) = \langle n | \Psi(t) \rangle$$

$P_{\Psi}(n) = |\langle n | \Psi \rangle|^2$ The probability of measuring E_n for the energy of a particle in the state $|\Psi\rangle$.

Symmetries

What is a symmetry: It is a transformation that leaves a system unchanged



In quantum mechanics we say that a system has a symmetry if the Hamiltonian is unchanged by some transformation

Space Translation

Assume that a state is localized around \vec{x}^i . Consider an operation that changes this state into another localized state around $\vec{x}^i + d\vec{x}^i$ with everything else unchanged. Such operation is called an infinitesimal translation by $d\vec{x}^i$, and the operator that does the job is $\hat{T}(d\vec{x}^i)$:

$$\hat{T}(d\vec{x}^i)|\vec{x}^i\rangle = |\vec{x}^i + d\vec{x}^i\rangle \quad (\text{we have set the arbitrary phase factors to 1 by convention})$$

Consider an arbitrary ket $|\alpha\rangle$. Then expand $|\alpha\rangle$ in terms of the position eigenkets

$$|\alpha\rangle = \int d^3\vec{x}^i |\vec{x}^i\rangle \langle \vec{x}^i | \alpha \rangle, \text{ and we examine the effect of } T(d\vec{x}^i)$$

$$T(d\vec{x}^i)|\alpha\rangle = \int d^3\vec{x}^i T(d\vec{x}^i) |\vec{x}^i\rangle \langle \vec{x}^i | \alpha \rangle = \int d^3\vec{x}^i |\vec{x}^i + d\vec{x}^i\rangle \langle \vec{x}^i | \alpha \rangle$$

$$\text{Notice that } \int d^3\vec{x}^i |\vec{x}^i + d\vec{x}^i\rangle \langle \vec{x}^i | \alpha \rangle = \int d^3\vec{x}^i |\vec{x}^i\rangle \langle \vec{x}^i - d\vec{x}^i | \alpha \rangle$$

The translation operator should satisfy some properties:

1) It should be unitary for probability conservation

2) Two successive infinitesimal translations, by $d\vec{x}^i$ and $d\vec{x}^{ii}$ second, are the net result of a single translation operation by $d\vec{x}^i + d\vec{x}^{ii}$

3) Translations in opposite directions are inverse operations

4) If $d\vec{x}^i \rightarrow 0$ the translation operator must be the identity.

Mathematically

$$1) \hat{T}^+(d\vec{x}') = \hat{T}^{-1}(d\vec{x}') \longrightarrow \hat{T}^+(d\vec{x}') \hat{T}(d\vec{x}') = 1$$

$$2) \hat{T}(d\vec{x}'') \hat{T}(d\vec{x}') = \hat{T}(d\vec{x}'' + d\vec{x}')$$

$$3) \hat{T}(-d\vec{x}') = \hat{T}^{-1}(d\vec{x}')$$

$$4) \lim_{d\vec{x}' \rightarrow 0} \hat{T}(d\vec{x}') = 1$$

Assume that $\hat{T}(d\vec{x}') = 1 - i \vec{\partial} \cdot d\vec{x}'$, where $\vec{\partial} = \partial_x \hat{x} + \partial_y \hat{y} + \partial_z \hat{z}$

∂_j is the translations generator in the j -direction, and ∂_j is Hermitian.

Then

$$1) \hat{T}^+(d\vec{x}') \hat{T}(d\vec{x}') = (1 + i \vec{\partial}^\dagger \cdot d\vec{x}') (1 - i \vec{\partial} \cdot d\vec{x}') \\ = 1 + O[(d\vec{x}')^2] \approx 1$$

$$2) \hat{T}(d\vec{x}'') \hat{T}(d\vec{x}') = (1 - i \vec{\partial} \cdot d\vec{x}'') (1 - i \vec{\partial} \cdot d\vec{x}') \\ = 1 - i \vec{\partial} \cdot (d\vec{x}'' + d\vec{x}') + O[d\vec{x}'' d\vec{x}'] \\ = \hat{T}(d\vec{x}'' + d\vec{x}')$$

3) and 4) are obviously satisfied

Now we can deduce the relation between $\hat{T}(d\vec{x}')$ and \hat{x}

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

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

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

$$[\hat{x}, \hat{T}(d\vec{x}')] = d\vec{x}'$$

$$\hat{x}(1 - i\hat{P} \cdot d\vec{x}') - (1 - i\hat{P} \cdot d\vec{x}')\hat{x} = d\vec{x}'$$

$$-i\hat{x}\hat{P} \cdot d\vec{x}' + i\hat{P} \cdot d\vec{x}'\hat{x} = d\vec{x}'$$

Choosing $d\vec{x}'$ in the direction of \hat{x}_j

$$-i\hat{x}_j \hat{P}_K d\vec{x}_j \delta_{jk} + i\hat{P}_K d\vec{x}_j \delta_{jk} \hat{x}_j = d\vec{x}_j$$

$$\hat{x}_j \hat{P}_K - \hat{P}_K \hat{x}_j = i\delta_{jk}$$

$$[\hat{x}_j, \hat{P}_K] = i\delta_{jk}$$

But if we recall that

$$[\hat{x}_j, \hat{P}_K] = i\hbar \delta_{jk}, \text{ then we can conclude that}$$

$\hat{P} = \frac{\hat{p}}{\hbar}$, and the translation operator becomes

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

Now consider a finite translation $\Delta x'$ generated by infinitely many infinitesimal translations $\Delta x/n$

$$\hat{T}(\Delta x') = \lim_{n \rightarrow \infty} (\hat{T}(\Delta x/n))^n = \lim_{n \rightarrow \infty} \left(1 - i\frac{\hat{P}_K}{\hbar} \frac{\Delta x}{n}\right)^n$$

$$\hat{T}(\Delta x') = \exp\left(-i\frac{\hat{P}_K}{\hbar} \Delta x\right)$$

In Quantum mechanics we call unitary operators like the translat-

tion operator a symmetry operator. For infinitesimal symmetry operators, in general, we can write

$$\hat{J} = I - \frac{i}{\hbar} \epsilon \hat{G}$$

where \hat{G} is the Hermitian generator of the symmetry operator. If the Hamiltonian is invariant under \hat{J} then

$$\hat{J}^\dagger \hat{H} \hat{J} = \hat{H} \text{ which is equivalent to } [\hat{G}, \hat{H}] = 0.$$

Shared Eigenbasis

If operator \hat{A} and operator \hat{B} commute $[\hat{A}, \hat{B}] = 0$, then there is a set of basis states $\{\lvert \Psi_n \rangle\}$ such that $\hat{A} \lvert \Psi_n \rangle = a_n \lvert \Psi_n \rangle$ and $\hat{B} \lvert \Psi_n \rangle = b_n \lvert \Psi_n \rangle$

Proof: Assume $\hat{A} \lvert \Psi_n \rangle = a_n \lvert \Psi_n \rangle$, define $\lvert \Phi_n \rangle = \hat{B} \lvert \Psi_n \rangle$

$\hat{A} \lvert \Phi_n \rangle = \hat{A} \hat{B} \lvert \Psi_n \rangle = \hat{B} \hat{A} \lvert \Psi_n \rangle = \hat{B} a_n \lvert \Psi_n \rangle = a_n \lvert \Phi_n \rangle$, then $\lvert \Phi_n \rangle$ is an eigenvector of \hat{A} .

Now, consider 2-cases

(i) \hat{A} is non-degenerate ($a_m \neq a_n$ if $m \neq n$). Since $\lvert \Phi_n \rangle$ and $\lvert \Psi_n \rangle$ have the same eigenvalue $a_n \rightarrow$ they should be proportional $\lvert \Phi_n \rangle = \lambda \lvert \Psi_n \rangle$, but $\hat{B} \lvert \Psi_n \rangle = \lvert \Phi_n \rangle \rightarrow \hat{B} \lvert \Psi_n \rangle = \lambda \lvert \Psi_n \rangle \rightarrow$ The functions $\lvert \Psi_n \rangle$ are eigenfunctions of \hat{B} .

(ii) \hat{A} has a degenerate spectrum ($\exists a_m = a_n$ for $m \neq n$)

Assume $\hat{A} \lvert \Psi_m \rangle = a_m \lvert \Psi_m \rangle$ and $\hat{A} \lvert \Psi_n \rangle = a_m \lvert \Psi_n \rangle$

Now $\lvert \Phi_m \rangle$ and $\lvert \Phi_n \rangle$ become a general linear combination of $\lvert \Psi_m \rangle$ and $\lvert \Psi_n \rangle$ such that

$$\lvert \Phi_m \rangle = \hat{B} \lvert \Psi_m \rangle = C_1 \lvert \Psi_m \rangle + C_2 \lvert \Psi_n \rangle$$

$$|\Phi_n\rangle = \hat{B}|\Phi_n\rangle = C_3|\Psi_m\rangle + C_4|\Psi_n\rangle$$

depending on $C_{1,2,3,4}$ we can combine them to form $|\tilde{\Psi}_m\rangle$ and $|\tilde{\Psi}_n\rangle$ such that

$$\hat{B}|\tilde{\Psi}_m\rangle = d_1|\tilde{\Psi}_m\rangle \text{ and } \hat{B}|\tilde{\Psi}_n\rangle = d_2|\tilde{\Psi}_n\rangle$$

for example $|\tilde{\Psi}_m\rangle = \frac{1}{\sqrt{2}}(|\Psi_m\rangle - |\Psi_n\rangle)$

but $|\tilde{\Psi}_m\rangle$ and $|\tilde{\Psi}_n\rangle$ are also eigenfunctions of \hat{A} with eigenvalue a_m . Then \hat{A} and \hat{B} have shared eigenfunctions.

Note that we considered the case of 2-degenerate eigenvalues for simplicity but the proof works the same way for higher degeneracy.

Relation to Symmetry: If a quantum mechanical system is invariant under the symmetry \mathcal{J} , then the Hamiltonian and the hermitian generator of the symmetry operator have shared eigenkets.

For example : If H is translational invariant then $|\vec{p}\rangle$ are eigenkets of Hamiltonian since $\hat{p}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle$

Non-degenerate Perturbation Theory (Time-independent).

Assume that we know the solution to the Hamiltonian H_0 , such that

$$H_0|\Psi_n^{(0)}\rangle = E_n^{(0)}|\Psi_n^{(0)}\rangle, \text{ where } \langle \Psi_m^{(0)} | \Psi_n^{(0)} \rangle = S_{m,n}.$$

Now, we would like to find the eigenfunctions of H , where

$H = H_0 + \lambda H'$, where H' is the perturbation and λ is a small #.

Consider that Ψ_n and E_n can be written in a power series of λ , such that

$$|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + \lambda |\Psi_n^{(1)}\rangle + \lambda^2 |\Psi_n^{(2)}\rangle + \dots, \text{ and}$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots.$$

Here $E_n^{(1)}$ is the 1st order correction to the n th eigenvalue, and $|\Psi_n^{(1)}\rangle$ is the 1st correction to the n th eigenfunction. $E_n^{(2)}$ and $|\Psi_n^{(2)}\rangle$ are the 2nd order corrections.

Then,

$$(H^{(0)} + \lambda H^1) (|\Psi_n^{(0)}\rangle + \lambda |\Psi_n^{(1)}\rangle + \lambda^2 |\Psi_n^{(2)}\rangle + \dots)$$

$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots) (|\Psi_n^{(0)}\rangle + \lambda |\Psi_n^{(1)}\rangle + \lambda^2 |\Psi_n^{(2)}\rangle + \dots)$$

Collecting powers of λ

$$\lambda^0 : H^{(0)} |\Psi_n^{(0)}\rangle = E_n^{(0)} |\Psi_n^{(0)}\rangle \quad \text{--- (0)}$$

$$\lambda^1 : H^{(0)} |\Psi_n^{(1)}\rangle + H^1 |\Psi_n^{(0)}\rangle = E_n^{(0)} |\Psi_n^{(1)}\rangle + E_n^{(1)} |\Psi_n^{(0)}\rangle \quad \text{--- (1)}$$

$$\lambda^2 : H^{(0)} |\Psi_n^{(2)}\rangle + H^1 |\Psi_n^{(1)}\rangle = E_n^{(0)} |\Psi_n^{(2)}\rangle + E_n^{(1)} |\Psi_n^{(1)}\rangle + E_n^{(2)} |\Psi_n^{(0)}\rangle \quad \text{--- (2)}$$

1st Order Perturbation

Taking the inner product of Eq(1) with $|\Psi_n^{(0)}\rangle$

$$\langle \Psi_n^{(0)} | H^{(0)} | \Psi_n^{(1)} \rangle + \langle \Psi_n^{(0)} | H^1 | \Psi_n^{(0)} \rangle = E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle + E_n^{(1)} \langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle$$

$$\text{Since } H^{(0)} \text{ is Hermitian} \rightarrow \langle \Psi_n^{(0)} | H^{(0)} | \Psi_n^{(0)} \rangle = \langle H^{(0)} \Psi_n^{(0)} | \Psi_n^{(0)} \rangle = E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle$$

$$\langle \Psi_n^{(0)} | H^1 | \Psi_n^{(0)} \rangle = E_n^{(1)}$$

from Eq(1) we also notice that

$$(H^{(0)} - E_n^{(0)}) |\Psi_m^{(1)}\rangle = -(H^1 - E_n^{(1)}) |\Psi_m^{(0)}\rangle \quad (3)$$

and we know that $|\Psi_m^{(1)}\rangle$ can be written as a linear combination of the complete basis set $\{|\Psi_m^{(0)}\rangle\}$, such that

$$|\Psi_m^{(1)}\rangle = \sum_{m \neq n} C_m^{(n)} |\Psi_m^{(0)}\rangle \quad (4)$$

note that there is no need to exclude $m=n$ in the sum, as if $|\Psi_m^{(1)}\rangle$ satisfies Eq (3) so too does $(|\Psi_m^{(1)}\rangle + \alpha |\Psi_m^{(0)}\rangle)$ for any α , and we use this freedom to subtract off the $|\Psi_m^{(0)}\rangle$ term.

Substituting Eq. (4) in (5),

$$\sum_{m \neq n} (E_m^{(0)} - E_n^{(0)}) C_m^{(n)} |\Psi_m^{(0)}\rangle = -(H^1 - E_n^{(1)}) |\Psi_m^{(0)}\rangle,$$

taking the inner product with $|\Psi_l^{(0)}\rangle$

$$\sum_{m \neq n} (E_m^{(0)} - E_n^{(0)}) C_m^{(n)} \langle \Psi_l^{(0)} | \Psi_m^{(0)} \rangle = - \langle \Psi_l^{(0)} | H^1 - E_n^{(1)} | \Psi_m^{(0)} \rangle$$

if $l=n$ we have

$$\boxed{\langle \Psi_m^{(0)} | H^1 | \Psi_m^{(0)} \rangle = E_n^{(1)}}, \text{ which we have obtained before.}$$

if $l \neq n$ we have

$$(E_l^{(0)} - E_n^{(0)}) C_l^{(n)} = - \langle \Psi_l^{(0)} | H^1 | \Psi_m^{(0)} \rangle, \text{ which leads to}$$

$$C_l^{(n)} = \frac{\langle \Psi_l^{(0)} | H^1 | \Psi_m^{(0)} \rangle}{(E_n^{(0)} - E_l^{(0)})},$$

then we get

$$|\Psi_n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle \Psi_m^{(0)} | H | \Psi_n^{(0)} \rangle}{(E_n^{(0)} - E_m^{(0)})} |\Psi_m^{(0)}\rangle$$

2nd Order Perturbation

Taking the inner product of Eq (2) with $|\Psi_n^{(0)}\rangle$, we get

$$\cancel{\langle \Psi_m^{(0)} | H^{(0)} | \Psi_m^{(2)} \rangle} + \cancel{\langle \Psi_m^{(0)} | H^{(1)} | \Psi_n^{(1)} \rangle} = E_n^{(0)} \cancel{\langle \Psi_m^{(0)} | \Psi_m^{(2)} \rangle} + E_n^{(1)} \cancel{\langle \Psi_m^{(0)} | \Psi_n^{(1)} \rangle} + E_n^{(2)} \cancel{\langle \Psi_m^{(0)} | \Psi_n^{(0)} \rangle}$$

Also notice that $\langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle = \sum_{m \neq n} C_m^{(n)} \langle \Psi_n^{(0)} | \Psi_m^{(0)} \rangle = 0$

$$\langle \Psi_n^{(0)} | H^{(1)} | \Psi_n^{(1)} \rangle = E_n^{(2)}$$

$$E_n^{(2)} = \sum_{m \neq n} C_m^{(n)} \langle \Psi_n^{(0)} | H^{(1)} | \Psi_m^{(0)} \rangle = \sum_{m \neq n} \frac{\langle \Psi_m^{(0)} | H^{(1)} | \Psi_m^{(0)} \rangle \langle \Psi_n^{(0)} | H^{(1)} | \Psi_m^{(0)} \rangle}{(E_n^{(0)} - E_m^{(0)})}$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \Psi_m^{(0)} | H^{(1)} | \Psi_n^{(0)} \rangle|^2}{(E_n^{(0)} - E_m^{(0)})}$$

Degenerate Perturbation Theory

Two-fold Degeneracy

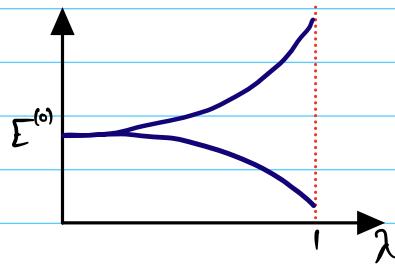
Assume that $H^{(0)} |\Psi_a^{(0)}\rangle = E^{(0)} |\Psi_a^{(0)}\rangle$ and $H^{(0)} |\Psi_b^{(0)}\rangle = E^{(0)} |\Psi_b^{(0)}\rangle$, where

$\langle \Psi_a^{(0)} | \Psi_b^{(0)} \rangle = 0$ and $|\Psi_a^{(0)}\rangle$ and $|\Psi_b^{(0)}\rangle$ are normalized.

Notice that any linear combination $|\Psi^{(0)}\rangle = \alpha |\Psi_a^{(0)}\rangle + \beta |\Psi_b^{(0)}\rangle$ is also an eigenstate of $H^{(0)}$ with an energy $E^{(0)}$, such that

$$H^{(0)} |\Psi^{(0)}\rangle = E^{(0)} |\Psi^{(0)}\rangle$$

If a perturbation H' lifts the degeneracy then the common unperturbed energy $E^{(0)}$ splits into two



Recall that

$$H^{(0)} |\Psi^{(0)}\rangle + H' |\Psi^{(0)}\rangle = E^{(0)} |\Psi^{(0)}\rangle + E^{(1)} |\Psi^{(0)}\rangle$$

Taking the inner product with $|\Psi_a^{(0)}\rangle$

$$\cancel{\langle \Psi_a^{(0)} | H^{(0)} | \Psi^{(1)} \rangle} + \cancel{\langle \Psi_a^{(0)} | H' | \Psi^{(0)} \rangle} = E^{(0)} \cancel{\langle \Psi_a^{(0)} | \Psi^{(1)} \rangle} + E^{(1)} \cancel{\langle \Psi_a^{(0)} | \Psi^{(0)} \rangle}$$

$$\alpha \cancel{\langle \Psi_a^{(0)} | H' | \Psi_a^{(0)} \rangle} + \beta \cancel{\langle \Psi_a^{(0)} | H' | \Psi_b^{(0)} \rangle} = \alpha E^{(1)}$$

$$\alpha W_{aa} + \beta W_{ab} = \alpha E^{(1)}, \text{ where } W_{ij} \equiv \langle \Psi_i^{(0)} | H' | \Psi_j^{(0)} \rangle \quad (i, j = a, b).$$

When we make the inner product with $|\Psi_b^{(0)}\rangle$ we get

$$\alpha W_{ba} + \beta W_{bb} = \beta E^{(1)}, \text{ hence}$$

$$\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^{(1)} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\begin{pmatrix} W_{aa} - E^{(1)} & W_{ab} \\ W_{ba} & W_{bb} - E^{(1)} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \text{ then we have a non-trivial solution}$$

for α and β if $|W| = 0$

$$(W_{aa} - E^{(1)}) (W_{bb} - E^{(1)}) - W_{ab} W_{ba} = 0, \text{ but } W_{ab} = W_{ba}^*$$

$$W_{aa} W_{bb} - E^{(1)} (W_{aa} + W_{bb}) + (E^{(1)})^2 - |W_{ab}|^2 = 0$$

Then

$$E_{\pm}^{(1)} = \frac{1}{2} \left(W_{aa} + W_{bb} \pm \sqrt{(W_{aa} + W_{bb})^2 + 4(W_{aa}W_{bb} - |W_{ab}|^2)} \right)$$

and this can be simplified to

$$E_{\pm}^{(1)} = \frac{1}{2} \left(W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right)$$

Many-particle Physics

First Quantization of Many-particle Systems

When we have a system of many identical particles, 3 more assumptions are added to the basic assumptions that define Quantum theory.

The natural extension of the single particle state wavefunction.

$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N)$, is an N -particle state wavefunction, which is a complex function in $3N$ -dimensional configuration space.

$|\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N)| \prod_{j=1}^N d\vec{r}_j$ = The probability for finding N particles in the $3N$ -dimensional volume $\prod_{j=1}^N d\vec{r}_j$ surrounding the point $(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$ in the $3N$ -D configuration space.

Permutation Symmetry and Indistinguishability

A fundamental difference between classical and quantum mechanics is the concept of indistinguishability. In CM each particle can be given an identity marker without influencing its behaviour. So in CM each particle in a group of identical particles can be identified.

This is not the case in QM, we cannot mark the particle without influencing its physical state, and if we bring a number of identical particles to the same region in space their wave functions will spread out and overlap with one

another, which makes it impossible to say which particle is where.

Then the second assumption for N -particle systems is that identical particles characterized by the same quantum #s are indistinguishable.

Now, due to indistinguishability

$$\Psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_k, \dots, \vec{r}_N) = \lambda \Psi(\vec{r}_1, \dots, \vec{r}_k, \dots, \vec{r}_j, \dots, \vec{r}_N) = \lambda^2 \Psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_k, \dots, \vec{r}_N)$$

Hence $\lambda = \pm 1$ since $\lambda^2 = 1$. Only two species of particles are possible within this condition, the so-called bosons and fermions.

$$\Psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_k, \dots, \vec{r}_N) = + \Psi(\vec{r}_1, \dots, \vec{r}_k, \dots, \vec{r}_j, \dots, \vec{r}_N) \quad (\text{Bosons})$$

$$\Psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_k, \dots, \vec{r}_N) = - \Psi(\vec{r}_1, \dots, \vec{r}_k, \dots, \vec{r}_j, \dots, \vec{r}_N) \quad (\text{Fermions}).$$

Indistinguishability is essential in QM:

for fermions it results into the Pauli exclusion principle.

for Bosons it is essential to understand Bose-Einstein condensates and superfluids.

Single-particle States as Basis:

Let us start by choosing a set of orthonormal single particle states $u_\alpha(\vec{r})$, then let us put n_α particles in the state $u_\alpha(\vec{r})$, then

$$n_\alpha = 0, 1, 2, \dots, \infty \quad (\text{Bosons})$$

$$n_\alpha = 0, 1 \quad (\text{Fermions})$$

The set of n_α s fully specifies the many particle wavefunction. This is called the fock space, which is the Hilbert space for an arbitrary # of particles.

What is the wavefunction for the many body state?

We need to consider the permutation symmetry for bosons and fermions

$$P_{ij} \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_i, \dots, \vec{r}_j, \dots) \equiv \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_j, \dots, \vec{r}_i, \dots)$$

P_{ij} is the exchange operator

$$P_{ij} \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_i, \dots, \vec{r}_j, \dots) = \begin{cases} +\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_j, \dots, \vec{r}_i, \dots) & (\text{Bosons}) \\ -\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_j, \dots, \vec{r}_i, \dots) & (\text{Fermions}) \end{cases}$$

Then we can express the manybody state as

$$\Psi(\vec{r}_1, \vec{r}_2, \dots) = \frac{1}{\sqrt{N!}} \sum_{\text{all } P} P \psi_{a_1}(\vec{r}_1) \psi_{a_2}(\vec{r}_2) \dots \psi_{a_N}(\vec{r}_N) \quad (\text{Bosons})$$

the sum is over all possible permutations.

$$\Psi(\vec{r}_1, \vec{r}_2, \dots) = \frac{1}{\sqrt{N!}} \sum_{\text{all } P} (-1)^P P \psi_{a_1}(\vec{r}_1) \psi_{a_2}(\vec{r}_2) \dots, \psi_{a_N}(\vec{r}_N) \quad (\text{Fermions}).$$

$(-1)^P = \pm 1$ for even/odd permutations.

These wavefunctions can be written as

$$\Psi(\vec{r}_1, \vec{r}_2, \dots) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{a_1}(\vec{r}_1) & \psi_{a_1}(\vec{r}_2) & \dots & \psi_{a_1}(\vec{r}_N) \\ \psi_{a_2}(\vec{r}_1) & \psi_{a_2}(\vec{r}_2) & \dots & \psi_{a_2}(\vec{r}_N) \\ \vdots & \vdots & & \vdots \\ \psi_{a_N}(\vec{r}_1) & \psi_{a_N}(\vec{r}_2) & \dots & \psi_{a_N}(\vec{r}_N) \end{vmatrix}^{\pm}$$

for fermions this is a determinant called the Slater determinant. for bosons we have a permanent.

Operators in first Quantization

The third assumption is that the single or few body operators remain unchanged

when acting on N -particle states.

Occupation # representation

$|\eta_1, \eta_2, \eta_3, \dots, \eta_N\rangle \equiv \overline{1}$ This is a shorthand for the Slater determinant.

$\eta_\alpha = 0, 1$ for fermions and $\eta_\alpha = 0, 1, 2, \dots, \alpha$ for bosons

$\sum_\alpha \eta_\alpha = N$ where N is the total # of particles.

→ One-body operator $\hat{V} = \sum_i V(\vec{r}_i)$ (the operator does not distinguish the particles).

the matrix elements of the operator

$$\langle \Psi_1 | \hat{V} | \Psi_2 \rangle, \text{ where } |\Psi_1\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(\vec{r}_1) & \dots \\ u_2(\vec{r}_1) & \dots \\ \vdots & \ddots \end{vmatrix} \text{ and}$$

$$|\Psi_2\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} w_1(\vec{r}_1) & \dots \\ w_2(\vec{r}_2) & \dots \\ \vdots & \ddots \end{vmatrix}$$

$$\langle \Psi_1 | \hat{V} | \Psi_2 \rangle = \frac{1}{N!} \int \Psi_1^*(\vec{r}_1, \vec{r}_2, \dots) \sum_i V(\vec{r}_i) \Psi_2(\vec{r}_1, \vec{r}_2, \dots) \prod_{i=1}^N d\vec{r}_i$$

This is a product of Slater determinants.

Looking at the expression above we can notice that when u_1 through u_N coincide with w_1 through w_N and they do not need to coincide for \vec{r}_i due to the presence of $V(\vec{r}_i)$.

Then we can see that the diagonal matrix element

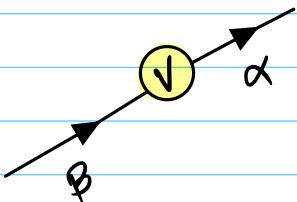
$$\langle \Psi_i | \hat{V} | \Psi_i \rangle = \sum_i \int d\vec{r} u_i(\vec{r}) V(\vec{r}) w_i(\vec{r}), \text{ here } i \text{-refers to the states that are}$$

occupied and \vec{r} is a dummy variable. Then

$$\langle n_1, n_2, \dots | \hat{W} | \dots, n_2, n_1 \rangle = \sum_{\alpha} n_{\alpha} \langle \alpha | \hat{W} | \alpha \rangle$$

The off diagonal elements

$$\langle n_1 \dots n_{\alpha+1} \dots n_{\beta-1} \dots | \hat{W} | n_1 \dots n_{\alpha} \dots n_{\beta} \rangle = e^{i\phi} \sqrt{(n_{\alpha+1}) n_{\beta}} \langle \alpha | \hat{W} | \beta \rangle$$



$e^{i\phi}$ is a phase factor for fermions.

$$e^{i\phi} = (-1)^{\sum_{\alpha < \beta} n_{\alpha} n_{\beta}}$$

→ The two body operator

$$\hat{W} = \frac{1}{2} \sum_{i \neq j} w(\vec{r}_i, \vec{r}_j)$$

This is non-zero when 2-particles change state

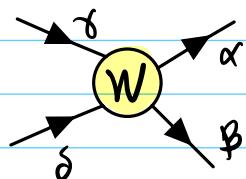
$$\langle \dots n_{\alpha+1} \dots n_{\beta+1} \dots n_{\gamma-1} \dots n_{\delta-1} | \hat{W} | \dots n_{\alpha} \dots n_{\beta} \dots n_{\gamma} \dots n_{\delta} \rangle =$$

$$\frac{1}{2} \sqrt{(n_{\alpha+1}) (n_{\beta+1}) n_{\gamma} n_{\delta}} \times \text{phase factor for fermions} \times (\langle \alpha, \beta | w | \gamma, \delta \rangle + f \langle \alpha, \beta | w | \delta, \gamma \rangle)$$

where

$$\langle \alpha, \beta | w | \gamma, \delta \rangle = \int d\vec{r}_1 d\vec{r}_2 u_{\alpha}^*(\vec{r}_1) u_{\beta}^*(\vec{r}_2) w(\vec{r}_1, \vec{r}_2) u_{\gamma}(\vec{r}_1) u_{\delta}(\vec{r}_2).$$

$f=+1$ for bosons and -1 for fermions



This was very tedious process. Is there a better way

The Method of 2nd Quantization

Creation and Annihilation Operators

for example, for one fermion the Fock space is $|0\rangle, |1\rangle$, and we can define

$$\hat{a}|1\rangle = |0\rangle ; \quad \hat{a}^+|1\rangle \equiv 0$$

$$\hat{a}^+|0\rangle = |1\rangle$$

then, we can think of \hat{a} and \hat{a}^+ as matrices

$$\hat{a} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \text{ and } \hat{a}^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

then if we have $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$

$$|\Psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \text{ and } \hat{a}|\Psi\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ 0 \end{pmatrix} = \beta|0\rangle$$

$$\hat{a}^+|\Psi\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ \alpha \end{pmatrix} = \alpha|1\rangle.$$

Now, we can also see that

$$\hat{a}\hat{a}^+ + \hat{a}^+\hat{a} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

→ for fermions $\{\hat{a}, \hat{a}^+\} = 1$

for bosons the space is $|0\rangle, |1\rangle, \dots, |N\rangle, \dots$ and it follows the algebra of the Harmonic oscillator, $[\hat{a}, \hat{a}^+] = 1$

Notice that these operators are useful in many body physics due to indistinguishability, which means that we only need to refer to the state.

These operators do not conserve the # of particles → But we know that the conservation of particles happens globally and locally the # of particles keeps changing. So we have a Fock space for each state.

Physical operators like \hat{N} and \hat{W} conserve total # of particles and they are

made of products of creation and annihilation operators.

Let us define the creation and annihilation operators of a many body state

$$\hat{a}_\alpha |n_1, \dots, n_\alpha, \dots \rangle = P_\alpha \sqrt{n_\alpha} |n_1, \dots, n_{\alpha-1}, \dots \rangle$$

$$\hat{a}_\alpha^\dagger |n_1, \dots, n_\alpha, \dots \rangle = P_\alpha \sqrt{1+f n_\alpha} |n_1, \dots, n_{\alpha+1}, \dots \rangle$$

$$f = \begin{cases} g+1 & \text{bosons} \\ -1 & \text{fermions} \end{cases} \quad \text{and} \quad P_\alpha = f \sum_{i=1}^{n_\alpha}$$

Now, we can verify the commutation relations

for bosons

$$\hat{a}_\beta \hat{a}_\alpha |n_1, \dots, n_\alpha, \dots, n_\beta, \dots \rangle = \sqrt{n_\alpha n_\beta} |n_1, \dots, n_{\alpha-1}, \dots, n_{\beta-1}, \dots \rangle$$

$$\hat{a}_\alpha \hat{a}_\beta |n_1, \dots, n_\alpha, \dots, n_\beta, \dots \rangle = \sqrt{n_\alpha n_\beta} |n_1, \dots, n_{\alpha-1}, \dots, n_{\beta-1}, \dots \rangle$$

$$\rightarrow \hat{a}_\alpha \hat{a}_\beta = \hat{a}_\beta \hat{a}_\alpha \rightarrow [\hat{a}_\alpha, \hat{a}_\beta] = 0.$$

Taking the Hermitian adjoint of $\hat{a}_\alpha \hat{a}_\beta$ $\hat{a}_\beta \hat{a}_\alpha$ we get $\hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger = \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger$ and we get

$$[\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger] = 0.$$

Notice that

$$\hat{a}_\alpha^\dagger \hat{a}_\alpha |n_1, \dots, n_\alpha, \dots \rangle = \hat{a}_\alpha^\dagger \sqrt{n_\alpha} |n_1, \dots, n_{\alpha-1}, \dots \rangle = n_\alpha |n_1, \dots, n_\alpha, \dots \rangle$$

$$\hat{a}_\alpha \hat{a}_\alpha^\dagger |n_1, \dots, n_\alpha, \dots \rangle = \hat{a}_\alpha \sqrt{n_\alpha + 1} |n_1, \dots, n_{\alpha+1}, \dots \rangle = n_{\alpha+1} |n_1, \dots, n_\alpha, \dots \rangle$$

$$\hat{a}_\alpha \hat{a}_\alpha^\dagger - 1 = \hat{a}_\alpha^\dagger \hat{a}_\alpha \rightarrow [\hat{a}_\alpha, \hat{a}_\alpha^\dagger] = 1$$

for $\alpha \neq \beta$

$$\hat{a}_\alpha \hat{a}_\beta^\dagger |n_1, \dots, n_\alpha, \dots, n_\beta, \dots \rangle = \sqrt{n_\beta + 1} |n_1, \dots, n_\alpha, \dots, n_\beta + 1, \dots \rangle = \sqrt{n_\alpha} \sqrt{n_\beta + 1} |n_1, \dots, n_{\alpha-1}, \dots, n_{\beta+1}, \dots \rangle$$

$$\hat{a}_\beta^\dagger \hat{a}_\alpha |n_1 \dots n_{\alpha} \dots n_\beta \dots \rangle = \sqrt{n_\alpha} |n_1 \dots n_{\alpha-1} \dots n_\beta \rangle = \sqrt{n_\beta+1} \sqrt{n_\alpha} |n_1 \dots n_{\alpha-1} \dots n_\beta \dots \rangle$$

$$\rightarrow \hat{a}_\alpha \hat{a}_\beta^\dagger = \hat{a}_\beta^\dagger \hat{a}_\alpha \rightarrow [\hat{a}_\alpha, \hat{a}_\beta^\dagger] = 0 \quad (\alpha \neq \beta)$$

Then in general, for bosons, $[\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha, \beta}$

for fermions we can show that

$$\hat{a}_\alpha \hat{a}_\beta = -\hat{a}_\beta \hat{a}_\alpha \rightarrow [\hat{a}_\alpha, \hat{a}_\beta] = 0,$$

$$\hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger = -\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \rightarrow [\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger] = 0, \text{ and}$$

$$[\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha, \beta}$$

Then we can combine the results for fermions and bosons

$$\hat{a}_\alpha \hat{a}_\beta - [\hat{a}_\beta \hat{a}_\alpha] = 0$$

$$\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger - [\hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger] = 0$$

$$\hat{a}_\alpha \hat{a}_\beta^\dagger - [\hat{a}_\beta^\dagger \hat{a}_\alpha] = \delta_{\alpha, \beta}, \text{ and}$$

$\hat{n}_\alpha = \hat{a}_\alpha^\dagger \hat{a}_\alpha$ is the number operator.

$|n_1 n_2 n_3 \dots \rangle \propto (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} (a_3^\dagger)^{n_3} \dots |0\rangle$, $|0\rangle$ is vacuum state.

These operators will help us build physical operators in a reasonable way.

Operators in 2nd Quantization

After some algebra (See any many-body or field theory book) we can show that

The one body operator is

$$\hat{V} = \sum_{\alpha, \beta} \hat{a}_\alpha^\dagger \langle \alpha | V | \beta \rangle a_\beta , \text{ we can understand it as initiating a particle from state } \beta, \text{ picking up the matrix element and creating a state in } \alpha.$$

field Operators

$$\hat{\Psi}(\vec{r}) = \sum_{\alpha} u_{\alpha}(\vec{r}) \hat{a}_{\alpha} , \text{ where } \langle \vec{r} | \Psi_{\alpha} \rangle = u_{\alpha}(\vec{r}) \text{ (wave function)}$$

$$\text{and } \hat{a}_{\alpha} = \int d\vec{r} u_{\alpha}^*(\vec{r}) \hat{\Psi}(\vec{r}).$$

$\hat{\Psi}(\vec{r})$ is an operator defined at every point in space \rightarrow field

$$\text{and } [\hat{\Psi}(\vec{r}), \hat{\Psi}^+(\vec{r}')]_- = \delta(\vec{r} - \vec{r}') \quad (\text{Here } [-]_- \text{ is commutator, and } [+]_+ \text{ is anticommutator}).$$

A general one body operator in 1st quantized form is

$$V = \sum_i V(\vec{r}_i) , \text{ then in its 2nd quantized form}$$

$$\hat{V} = \sum_{\alpha, \beta} \langle \alpha | V | \beta \rangle \hat{a}_{\alpha}^\dagger \hat{a}_{\beta} = \sum_{\alpha, \beta} \int d\vec{r}' u_{\alpha}^*(\vec{r}') V(\vec{r}') u_{\beta}(\vec{r}') \hat{a}_{\alpha}^\dagger \hat{a}_{\beta}$$

$$\hat{V} = \int d\vec{r}' \left(\sum_{\alpha} u_{\alpha}^*(\vec{r}') \hat{a}_{\alpha}^\dagger \right) V(\vec{r}') \left(\sum_{\beta} u_{\beta}(\vec{r}') \hat{a}_{\beta} \right)$$

$$\hat{V} = \int d\vec{r}' \hat{\Psi}_{\alpha}^+(\vec{r}') V(\vec{r}') \hat{\Psi}_{\beta}(\vec{r}')$$

Let us look at the density operator

$\rho(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i)$ (in 1st quantization), in 2nd quantization

$$\hat{\rho}(\vec{r}) = \int d\vec{r}' \hat{\Psi}^+(\vec{r}') \delta(\vec{r} - \vec{r}') \hat{\Psi}(\vec{r}') = \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r})$$

then the total # of particles is

$$\hat{N} = \int d\vec{r} \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r}).$$

The density operator is useful to get other operators in 2nd quantizat^o.

$$\hat{V} = \sum_i V(\vec{r}_i) = \int d\vec{r} V(\vec{r}) \sum_i \delta(\vec{r} - \vec{r}_i) = \int d\vec{r} V(\vec{r}) \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r})$$

$$\hat{V} = \sum_{\alpha, \beta} \langle \alpha | v | \beta \rangle \hat{a}_{\alpha}^+ \hat{a}_{\beta}$$

This also works for the 2-body operator

$$\hat{W} = \frac{1}{2} \sum_{i \neq j} w(\vec{r}_i, \vec{r}_j) = \frac{1}{2} \sum_{i, j} w(\vec{r}_i, \vec{r}_j) - \frac{1}{2} \sum_i w(\vec{r}_i, \vec{r}_i)$$

$$\hat{W} = \frac{1}{2} \int d\vec{r} d\vec{r}' w(\vec{r}, \vec{r}') \rho(\vec{r}) \rho(\vec{r}') - \frac{1}{2} \int d\vec{r} w(\vec{r}, \vec{r}) \rho(\vec{r})$$

$$\hat{W} = \frac{1}{2} \int d\vec{r} d\vec{r}' w(\vec{r}, \vec{r}') \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r}) \hat{\Psi}^+(\vec{r}') \hat{\Psi}(\vec{r}') - \frac{1}{2} \int d\vec{r} w(\vec{r}, \vec{r}) \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r})$$

$$\hat{W} = \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} \hat{a}_{\alpha}^+ \hat{a}_{\beta}^+ \langle \alpha, \beta | w | \gamma, \delta \rangle a_{\gamma} a_{\delta}$$

$$\text{where } \langle \alpha, \beta | w | \gamma, \delta \rangle = \int d\vec{r}' d\vec{r} U_{\alpha}^*(\vec{r}') U_{\beta}^*(\vec{r}) w(\vec{r}', \vec{r}) U_{\gamma}(\vec{r}) U_{\delta}(\vec{r})$$

Adiabatic Theorem

Consider a Slow Process, e.g., the process described by

$$\hat{H}(t) = \begin{cases} \hat{H}_0 & t < 0 \\ \hat{H}_0 + (t/T) \hat{V} & 0 \leq t \leq T \\ \hat{H}_0 + \hat{V} & t > T \end{cases}$$

for adiabatic $\Rightarrow T$ is large \rightarrow Change is slow

Define : Instantaneous Eigenstates of the Hamiltonian

$$\hat{H}(t) |\Psi_n(t)\rangle = E_n(t) |\Psi_n(t)\rangle$$

$$\langle \Psi_m(t) | \Psi_n(t) \rangle = \delta_{m,n}$$

These states are not solutions of the time dependent Schrödinger equation

The solutions to the time dependent Schrödinger Eqn are

$$i\hbar \partial_t |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

and we can write $|\Psi(t)\rangle$ in terms of the instantaneous eigenstates $|\Psi_n(t)\rangle$ as

$$|\Psi(t)\rangle = \sum_n c_n(t) e^{i\Theta_n} |\Psi_n(t)\rangle$$

$$\Theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(t') dt' \quad \text{Dynamical Phase factor}$$

(natural extension to the usual $e^{iEt/\hbar}$)

$$\text{Now } i\hbar \frac{\partial \Psi(t)}{\partial t} = i\hbar \sum_n (c_n |\Psi_n(t)\rangle + c_n |\dot{\Psi}_n(t)\rangle) + i\dot{\theta}(t) (c_n |\Psi_n(t)\rangle) e^{i\theta_n}$$

$$\hat{H}\Psi(t) = \hat{H} \sum_n c_n e^{i\theta_n} |\Psi_n(t)\rangle = \sum_n c_n e^{i\theta_n} E_n(t) |\Psi_n(t)\rangle$$

$$\dot{\Theta}_n = -\frac{1}{\hbar} \frac{d}{dt} \int_0^t E_n(t') dt' = -\frac{1}{\hbar} E_n(t)$$

$$\text{So } i\hbar \sum_n i\dot{\theta} \Psi_n e^{i\theta_n} = -\hbar \sum_n \left(-\frac{E_n}{\hbar} \right) c_n e^{i\theta_n} |\Psi_n(t)\rangle$$

$$= \sum_n (c_n(t) E_n(t) e^{i\theta_n} |\Psi_n(t)\rangle)$$

Now we go back to $i\hbar \frac{\partial \Psi(t)}{\partial t} = \hat{H}\Psi(t)$ and cancel the left and right hand sides to get

$$i\hbar \sum_n (c_n(t) |\dot{\Psi}_n(t)\rangle + c_n(t) |\dot{\Psi}_n(t)\rangle) e^{i\theta_n(t)} = 0$$

Multiply by $\langle \Psi_m(t) |$

$$i\hbar \sum_n (c_n(t) \delta_{m,n} + c_n(t) \langle \Psi_m | \frac{d}{dt} \Psi_n(t) \rangle) e^{i\theta_n(t)} = 0$$

$$c_m e^{i\theta_m(t)} = - \sum_n c_n(t) \langle \Psi_m | \frac{d}{dt} \Psi_n(t) \rangle e^{i\theta_n(t)}$$

$$\frac{d}{dt} c_m(t) = - \sum_n c_n(t) \langle \Psi_m | \frac{d}{dt} \Psi_n(t) \rangle e^{i(\theta_n(t) - \theta_m(t))}$$

$$\frac{d}{dt} c_m(t) = - c_m(t) \langle \Psi_m | \frac{d}{dt} \Psi_m(t) \rangle - \sum_{n \neq m} (c_n(t) \langle \Psi_m | \frac{d}{dt} \Psi_n(t) \rangle) e^{i(\theta_n - \theta_m)}$$

Recall that $\hat{H}(t) |\Psi_n(t)\rangle = E_n(t) |\Psi_n(t)\rangle$

taking the derivative ∂_t

$$(\partial_t \hat{H}(t)) |\Psi_n(t)\rangle + \hat{H}(t) |\partial_t \Psi_n(t)\rangle = (\partial_t E_n(t)) |\Psi_n(t)\rangle + E_n(t) |\partial_t \Psi_n(t)\rangle$$

multiply by $\langle \Psi_m(t) |$

$$\langle \Psi_m(t) | \partial_t \hat{H}(t) |\Psi_n(t)\rangle + \langle \Psi_m(t) | \hat{H}(t) |\partial_t \Psi_n(t)\rangle =$$

$$\partial_t E_m(t) \langle \Psi_m(t) | \Psi_n(t)\rangle + E_n(t) \langle \Psi_m(t) | \partial_t \Psi_n(t)\rangle$$

$$\langle \Psi_m(t) | (\partial_t \hat{H}(t)) |\Psi_n(t)\rangle = \partial_t E_n(t) \delta_{n,m} + (E_n(t) - E_m(t)) \langle \Psi_m(t) | \partial_t \Psi_n(t)\rangle$$

for $n \neq m$

$$\langle \Psi_m(t) | \partial_t \hat{H}(t) |\Psi_n(t)\rangle = (E_n(t) - E_m(t)) \langle \Psi_m(t) | \partial_t \Psi_n(t)\rangle$$

Substituting in the $\partial_t C_m(t)$ expression

$$\partial_t C_m(t) =$$

$$-C_m(t) \langle \Psi_m(t) | \partial_t \Psi_m(t)\rangle - \sum_{n \neq m} c_n(t) \frac{\langle \Psi_m(t) | \partial_t \hat{H}(t) | \Psi_n(t)\rangle}{(E_n(t) - E_m(t))} e^{i(E_n - E_m)t}$$

This is exact, and now we can make the adiabatic approximation

In the adiabatic approximation we will neglect $n \neq m$, i.e., the term

$$\sum_{n \neq m} c_n(t) \frac{\langle \Psi_m(t) | \partial_t \hat{H}(t) | \Psi_n(t)\rangle}{(E_n(t) - E_m(t))} e^{i(E_n - E_m)t}$$

for very slow variations of the Hamiltonian with time. Notice that

$|q_m\rangle$ and $|q_n\rangle$ are orthogonal and the transitions between them are mediated by $\partial_t \hat{H}(t) \rightarrow 0$. If $\partial_t \hat{H}(t) \rightarrow 0$ then these transitions also go to zero. (We can show this by perturbation theory)

Then, in the adiabatic approximation

$$\partial_t C_m(t) \simeq -C_m \langle q_m(t) | \partial_t q_m(t) \rangle$$

The solution of this equation is

$$C_m(t) = C_m(0) e^{i\theta_m(t)}, \text{ where}$$

$$\theta_m(t) = i \int_0^t \langle q_m(t') | \partial_t q_m(t') \rangle dt'$$

and $\theta_m(t)$ is the **Geometric phase (Berry's Phase)**

What is the difference between the phases?

$$\Theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(t') dt' \quad \text{and} \quad \gamma_n(t) = i \int_0^t \langle q_n(t') | \partial_t q_n(t') \rangle dt'.$$

We are going to show that Berry's phase is independent of the time it takes the process to happen.

Configuration Space

Consider $\hat{H}(\vec{R})$ where $\vec{R} = (R_1, R_2, R_3, \dots, R_N) \in \mathbb{R}^N$

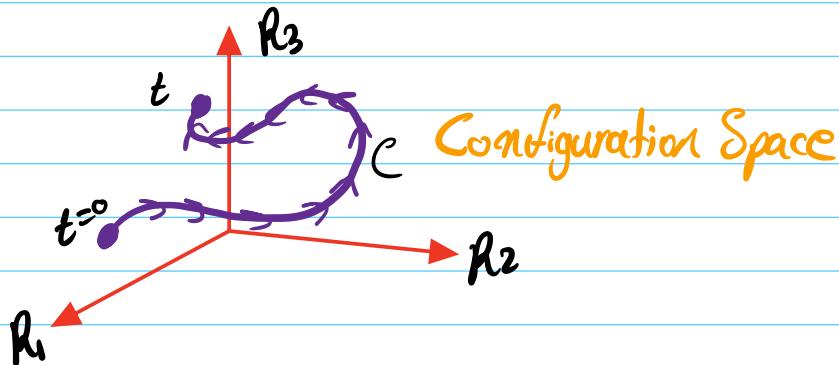
This means that the Hamiltonian has N parameters

Assume that we know how to solve the Hamiltonian for all set of parameters

$$\hat{H}(\vec{R}) |q_n(\vec{R})\rangle = E_n(\vec{R}) |q_n(\vec{R})\rangle; \quad n=1, 2, 3, \dots \text{ orthonormal states}$$

Now let us assume that the parameters of the Hamiltonian start to depend on time

$$\vec{R}(t) = (R_1(t), R_2(t), \dots, R_N(t))$$



The path C is parametrized by time

Since we assumed that we know how to solve the time-independent Hamiltonian \rightarrow we have the instantaneous eigenstates

$$\hat{H}(\vec{R}(t)) |\Psi_n(\vec{R}(t))\rangle = E_n(\vec{R}(t)) |\Psi_n(\vec{R}(t))\rangle$$

Now we need to evaluate the geometric (Berry's) Phase

Start with $\rightarrow i \langle \Psi_n(\vec{R}(t)) | \partial_t |\Psi_n(\vec{R}(t))\rangle$

Notice that

$$\partial_t f(\vec{R}(t)) = \partial_t f(R_1(t), R_2(t), R_3(t), \dots, R_N(t))$$

$$= \frac{\partial f}{\partial R_1} \frac{dR_1}{dt} + \frac{\partial f}{\partial R_2} \frac{dR_2}{dt} + \dots + \frac{\partial f}{\partial R_N} \frac{dR_N}{dt}$$

$$\frac{\partial f}{\partial t}(\vec{R}(t)) = \nabla_{\vec{R}} f \cdot \frac{d\vec{R}}{dt}$$

Important formula

Then $i \langle \psi_n(\vec{R}(t)) | \partial_t | \psi_n(\vec{R}(t)) \rangle$ can be written as

$$i \langle \psi_n(\vec{R}(t)) | \nabla_{\vec{R}} | \psi_n(\vec{R}(t)) \rangle \cdot \frac{d\vec{R}}{dt}$$

and

$$\gamma_{nl}(t) = i \int_0^t \langle \psi_n(\vec{R}(t')) | \nabla_{\vec{R}} | \psi_n(\vec{R}(t')) \rangle \cdot \frac{d\vec{R}}{dt'} dt'$$

We can think of the integral as just happening in configuration space and not in time

The integral is over the path C in configuration space

$$\gamma_{nl}(C) = i \int_C \langle \psi_n(\vec{R}) | \nabla_{\vec{R}} | \psi_n(\vec{R}) \rangle \cdot d\vec{R}$$

◎ Time plays no role, just follow the path

Define :

The Berry Connection $\vec{A}_n(\vec{R})$

$$\vec{A}_n = i \langle \psi_n(\vec{R}) | \nabla_{\vec{R}} | \psi_n(\vec{R}) \rangle$$

N-components one per state

Note on gauge transformations

$$|\psi_n(\vec{R})\rangle = e^{iB(\vec{R})} |\psi_n(\vec{R})\rangle ; B(\vec{R}) \text{ is real}$$

Now let us compute the new Berry connection

$$\vec{A}'_n(\vec{R}) = i \langle \psi_n(\vec{R}) | e^{iB(\vec{R})} \nabla_{\vec{R}} e^{-iB(\vec{R})} | \psi_n(\vec{R}) \rangle$$

$$\vec{A}_n(\vec{R}) = \vec{A}_n(\vec{R}') + \epsilon(-\epsilon) \nabla_{\vec{R}'} B(\vec{R}')$$

$$\vec{A}'_n(\vec{R}') = \vec{A}_n(\vec{R}') + \nabla_{\vec{R}'} B(\vec{R}')$$

This is the gauge transformation of \vec{A}_n

Notice that : Just like a vector potential, \vec{A}_n transforms with a gradient of a function $\rightarrow \vec{A}_n$ transforms like a vector potential in the configuration space $\rightarrow \vec{A}_n$ is a vector potential in configuration space \rightarrow Hence the name Connection.

What happens to Berry's Phase under a gauge transformation

$$\gamma_n(C) = \int_C \vec{A}_n(\vec{R}) \cdot d\vec{R}$$

$$\text{Then } \gamma'_n(C) = \int_C \vec{A}'_n(\vec{R}) \cdot d\vec{R} = \int_C (\vec{A}_n(\vec{R}') + \nabla_{\vec{R}'} B(\vec{R}')) \cdot d\vec{R}$$

$$\gamma'_n(C) = \gamma_n(C) + \int_{\vec{R}_i}^{\vec{R}_f} \nabla_{\vec{R}'} B(\vec{R}') \cdot d\vec{R}$$

$$\gamma'_n(C) = \gamma_n(C) + B(\vec{R}_f) - B(\vec{R}_i)$$

Berry's Phase is not gauge invariant

Since the Berry phase is not gauge invariant \rightarrow it cannot be observed
 \rightarrow But there is a way to fix this

Consider that the motion in configuration space begins and ends at the same point then

$$\gamma'_n(C) = \gamma_n(C) \rightarrow \text{Gauge invariant } (C: \text{closed path})$$

The observable Berry's phase is a geometric phase accumulated by the system in a motion in configuration space where it begins and ends at the same place.

Comments: ① If $|\Psi_{n(t)}\rangle$ can be chosen to be real \rightarrow the geometric phase vanishes

$$\gamma_n(t) = i \int_0^t \langle \Psi_{n(t')} | d\epsilon' | \Psi_{n(t')} \rangle dt'$$

We first need to show that $\langle \Psi | d\epsilon \Psi \rangle$ is purely imaginary

$$\langle \Psi | d\epsilon \Psi \rangle = \int dx \Psi_{G,t}^* d\epsilon \Psi_{G,t} = \int dx d\epsilon [\Psi_{G,t}^* \Psi_{G,t} - d\epsilon \Psi_{G,t}^* \Psi_{G,t}]$$

$$\langle \Psi | d\epsilon \Psi \rangle = d\epsilon \int dx \Psi_{G,t}^* \Psi_{G,t} - \left(\int dx \Psi_{G,t}^* d\epsilon \Psi_{G,t} \right)^*$$

$$\langle \Psi | d\epsilon \Psi \rangle = 0 - \langle \Psi | d\epsilon \Psi \rangle^*$$

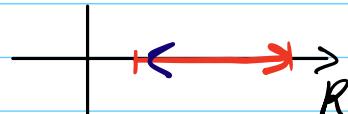
$$\langle \Psi | d\epsilon \Psi \rangle = -\langle \Psi | d\epsilon \Psi \rangle^* \rightarrow \text{Purely Imaginary}$$

Then if $|\Psi_{n(t)}\rangle$ is real $\rightarrow \gamma_n(t) = 0$

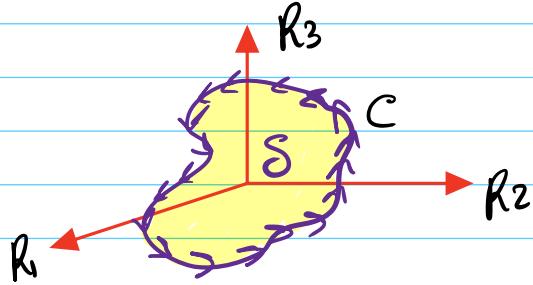
② If the configuration space is one dimensional \rightarrow Berry's phase (closed loop one) vanishes.

$$\gamma_n = \oint \langle \Psi(R) | \frac{d}{dR} | \Psi(R) \rangle dR = 0$$

a closed path in 1D retraces itself



③ 3D



$$\gamma = \oint_C \vec{A} \cdot d\vec{R} = \iint_S (\vec{\nabla} \times \vec{A}) \cdot d\vec{a}$$