Quantum Notes

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CONTENTS

Some notes for quantum

CHAPTER

ONE

INTRODUCTION

Some notes as part of the full theoretical physics notes which are hosted here.

CHAPTER TWO

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2.1 Vocabulary

Vocabulary of physics, the fountain of research ideas.

0. Fine Structure Constant

$\alpha = \frac{k_e e^2}{\hbar c} = \frac{1}{(4\pi\varepsilon_0)}\frac{e^2}{\hbar c} = \frac{e^2 c\mu_0}{2h}$

In electrostatic cgs units, $\alpha = \frac{e^2}{\hbar c}$.

In natural units, $\alpha = \frac{e^2}{4\pi}$.

1. Hydrogen Atom

Potential $V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$.

Energy levels: $E_n = -\left(\frac{Z^2\mu e^4}{32\pi^2\epsilon_0^2\hbar^2}\right)\frac{1}{n^2} = -\left(\frac{Z^2\hbar^2}{2\mu a_\mu^2}\right)\frac{1}{n^2} = \frac{\mu c^2 Z^2\alpha^2}{2n^2}$.

Ground state of hydrogen atom $\psi_{100}(r) = \frac{1}{\sqrt{\pi}}\frac{1}{a^{3/2}}e^{-Zr/a}$.

2.2 Questions

2.2.1 Wedge Product, Cross Prodcut & Commutation relation

2.3 Approximation Methods

2.3.1 Variational Method

Trial functions

Some of the calculable trial functions:

1. $\psi(x) = \cos\alpha x$, for $|\alpha x| < \pi/2$, otherwise 0.
2. $\psi(x) = \alpha^2 - x^2$, for $|x| < \alpha$, otherwise 0.
3. $\psi(x) = C\exp(-\alpha x^2/2)$.
4. $\psi(x) = C(\alpha - |x|)$, for $|x| < \alpha$, otherwise 0.
5. $\psi(x) = C\sin\alpha x$, for $|\alpha x| < \pi$, otherwise 0.

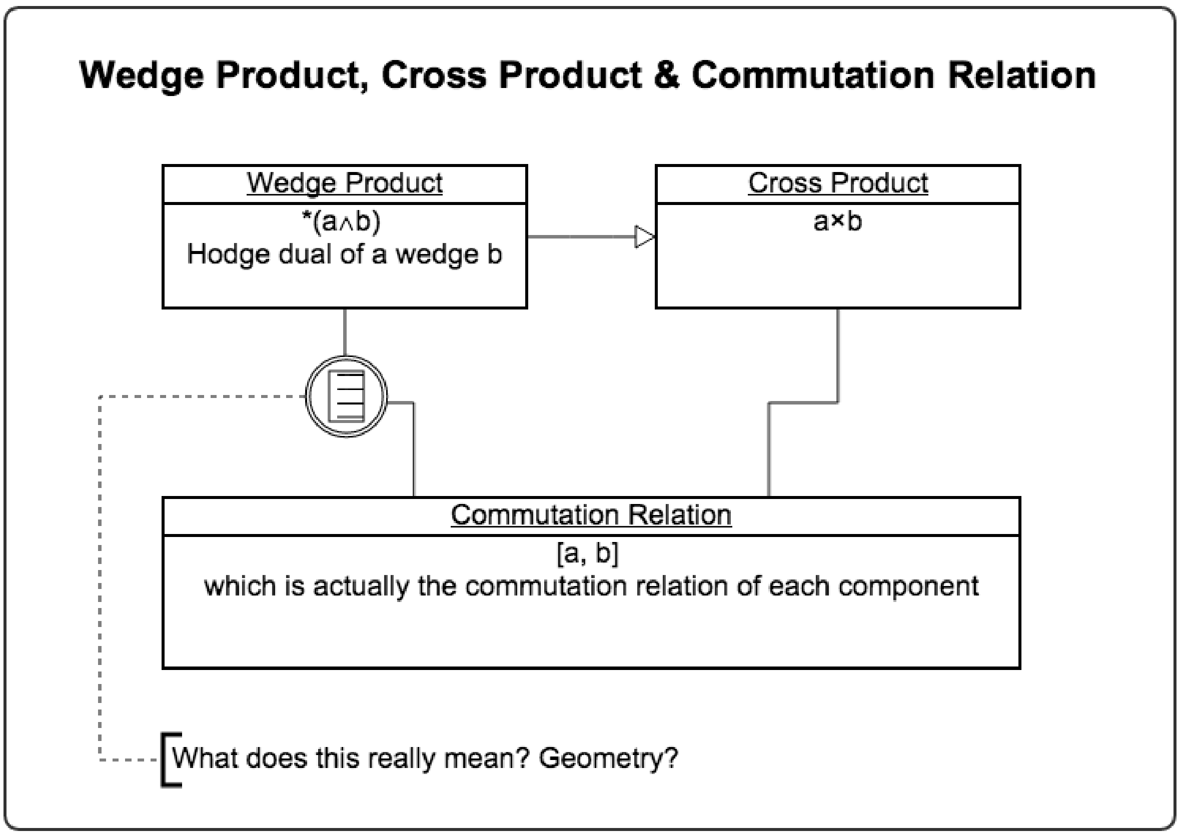


Figure 2.1: Geometry language here?

Procedure

1. Pick a trial function.

Note: How to pick a trial function? For ground state energy, we should pick a function that has the same property as the real ground state. This requires some understanding of the problem we are dealing with.

Things to consider:

(a) The new problem is just a modification of a known solved problem. Then we can easily find out what really is different and interprete the new problem in terms of the old one.

(b) If the Hamiltonian have definite parity, the ground state wave function should pick up some parity which is usually even to make it the lowest energy.

(c) Continious function? A C^∞ Hamiltonian can only have continious functions as solutions for a finite system.

(d) Nodes deteremines the kinetic energy so check the nodes for ground state wave function.

(e) Check the behivior of the wave function at different limits. In most cases, the Shrödinger equation can be reduced to something solvable at some limits.

(f) **One more thing, the trial function should make the problem calculable.**

Why Not General Viriational Method

Why don't we just use a most general variational method to find out the ground state? Because we will eventually come back to the time-independent Shrödinger equation.

Suppose we have a functional form

$$E(\psi^*,\psi,\lambda) = \int dx\psi^* H\psi - \lambda\left(\int dx\psi^*\psi - 1\right)$$

The reason we have this Lagrange multiplier method is that the wave function should be normalized and this multiplier provides the degree of freedom. We would only get a wrong result if we don't include this DoF.

Variation of ψ^*,

$$\delta E = \int dx\delta\psi^* H\psi - \int dx\delta\psi^*\psi = 0$$

Now what?

$$H\psi - \lambda\psi = 0$$

Not helpful.

2.3.2 Variational Method and Virial Theorem

For a potential $V(x) = bx^n$, we can prove that virial theorem is valid for ground state if we use Gaussian trial function $e^{-\alpha x^2/2}$.

A MMA proof is here.

Virial theorem is pretty interesting. It shares the same math with equipartition theorem.

2.3.3 WKB

This is a semi-classical method. It is semi classical because we will use the classical momentum

$$\hbar k(x) = \sqrt{2m(E - V(x))}$$

The following points are important for this method.

0. WKB start from a classical estimation of wave number at a certain energy E which is later quantified by the Bohr-Sommerfeld quantization rule.

1. Conservation law:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \vec{j} = 0$$

   where $\rho = \psi^*\psi$, $\vec{j} = -\frac{\hbar}{2mi}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$. This can be derived from Shrödinger equation easily.

2. Phase: Wave function is generally $A(x)\exp(\phi(x))$. However, $\phi(x)$ should be the area of the phase function starting from some initial point. For example in WKB, $k(x) = \phi'(x)$ and $\phi(x) = \int \phi'(x')dx' = \int k(x')dx'$.

   Using this general wave function and conservation law we find out that $A(x)\ \frac{1}{\sqrt{k(x)}}$. Then we can apply the two boundary conditions. However we will find two different wave functions given by two boundary conditions. Now we should connect them because $\psi(a) = \psi(b)$ exactly. By comparing the two wave functions we can find something like Bohr-Sommerfeld quantization rule.

3. Correction at bouldary: However, this method requires that the potential varies slowly or equivalently the wave number varies slowly. Basicly we are just using the following approximation:

$$A'(x) = 0, k'(x) = 0$$

   For example when taking the derivative of wave function,

$$\psi'(x) = A'(x)e^{i\int\cdots} + A(x)k(x)e^{i\int\cdots} \approx A(x)k(x)e^{i\int\cdots}$$

   where we drop the term with $A'(x)$. That is to say

$$|A'| \ll |Ak| \Rightarrow |k'| \ll k^2$$

   But at boundary where $E = V$, this is obviously not valid because $k = 0$. So we need to fix this problem.

   The solution is to use first order of the potential in a Taylor expansion. Then solve the problem exactly. Finally we connect regions that is far out from the boundary, need the boundary and between the boundary.

If we can have a good boundary condition, then the energy spectrum given by WKB can be very good. Even we don't have a good boundary condtion, the excited states given by this method are always close to the exact ones.

How does it work

2.4 Symmetries in QM

2.4.1 Time and Space Translation

First of all I want to know what is not changed or what is the invariant quantity in a transformation.

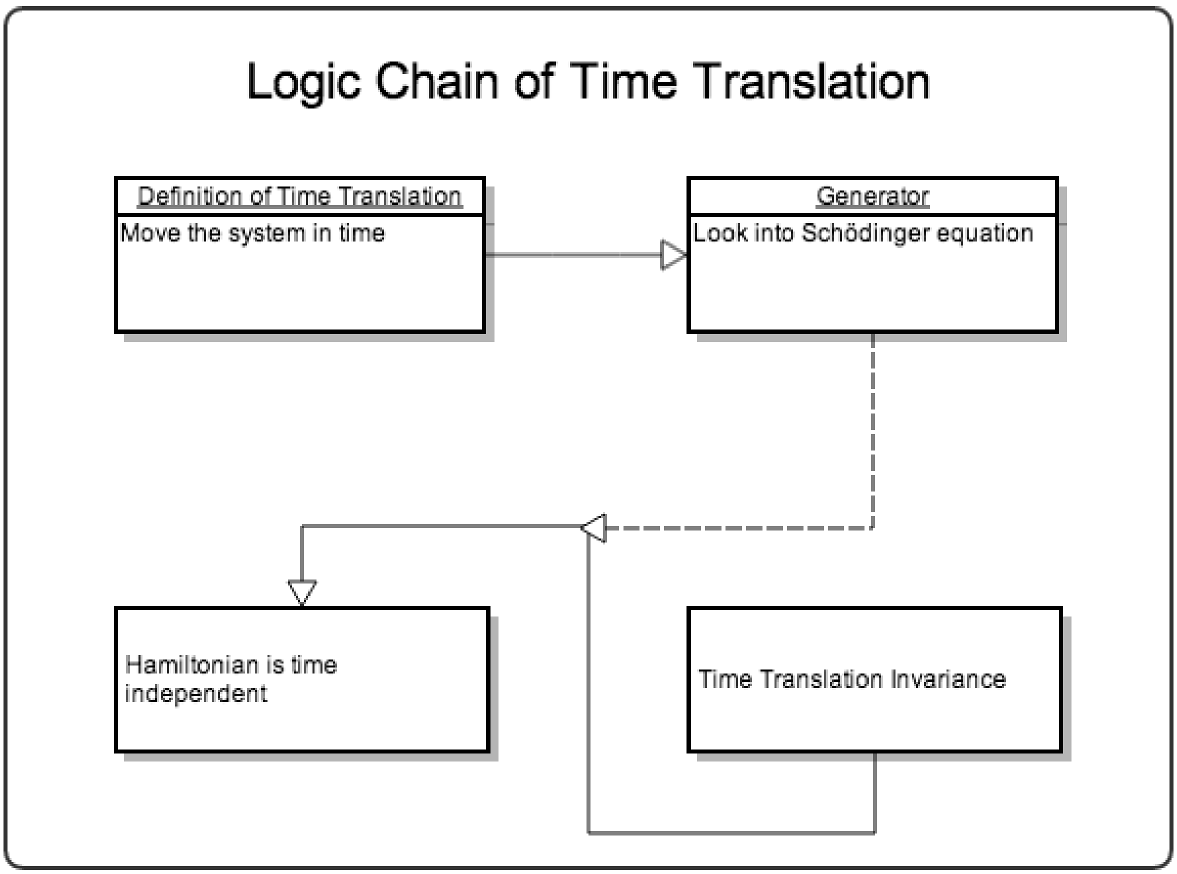
There are three kind of common transformations.

1. Time translation: move the system in time. In this sense time translation is just the time evolution operator or propagator.
2. Space translation: move the system in space.
3. Gauge transformation

The invariance of them corresponds to:

1. Time translation invariance (T.T.I.) means the evolution of the system is not changing under time translations. **Hamiltonian is invariant.**
2. Space translation invariance (S.T.I.) means that the

Time Translation Symmetry



Time translation Gliffy Source

Definition of Time Translation

Move the system in time.

Generator of Time Translation

T.T.I. is generated by Hamiltonian which can be easily understood by looking into Shcrödinger equation.

Hint: Starting from Schrödinger equation,

$$i\hbar\frac{|\psi(t+\Delta t)\rangle - |\psi(t)\rangle}{\Delta t} = H(t)\psi(t)$$

Then we get the state after a evolution of time Δt,

$$|\psi(t+\Delta t)\rangle = \left(\hat{I} - i\frac{\Delta t\hat{H}(t)}{\hbar}\right)|\psi(t)\rangle$$

Time translation symmetry means the state evolution in the same time interval Δt no matter when to start the evolution. Mathematically,

$$|\psi(t_1+\Delta t)\rangle = \left(\hat{I} - i\frac{\Delta t\hat{H}(t_1)}{\hbar}\right)|\psi(t_1)\rangle$$

should get the same final state if we start from some other time t_2,

$$|\psi(t_2+\Delta t)\rangle = \left(\hat{I} - i\frac{\Delta t\hat{H}(t_2)}{\hbar}\right)|\psi(t_2)\rangle$$

That means the two Hamiltonian should be the same. Now we reach the conclusion that Hamiltonian is time independent.

The logic is to prove that Hamiltonian is time independent by using infinitesimal time translation approach. Given that Hamiltonian is time independent, we imediately know that time translation operator is just the propagator with the form

$$\hat{T}_{\Delta t} \equiv \hat{U}(\Delta t) = e^{-i\hat{H}\Delta t/\hbar}$$

All other conclusions come from the fact that Hamiltonian is a constant of motion.

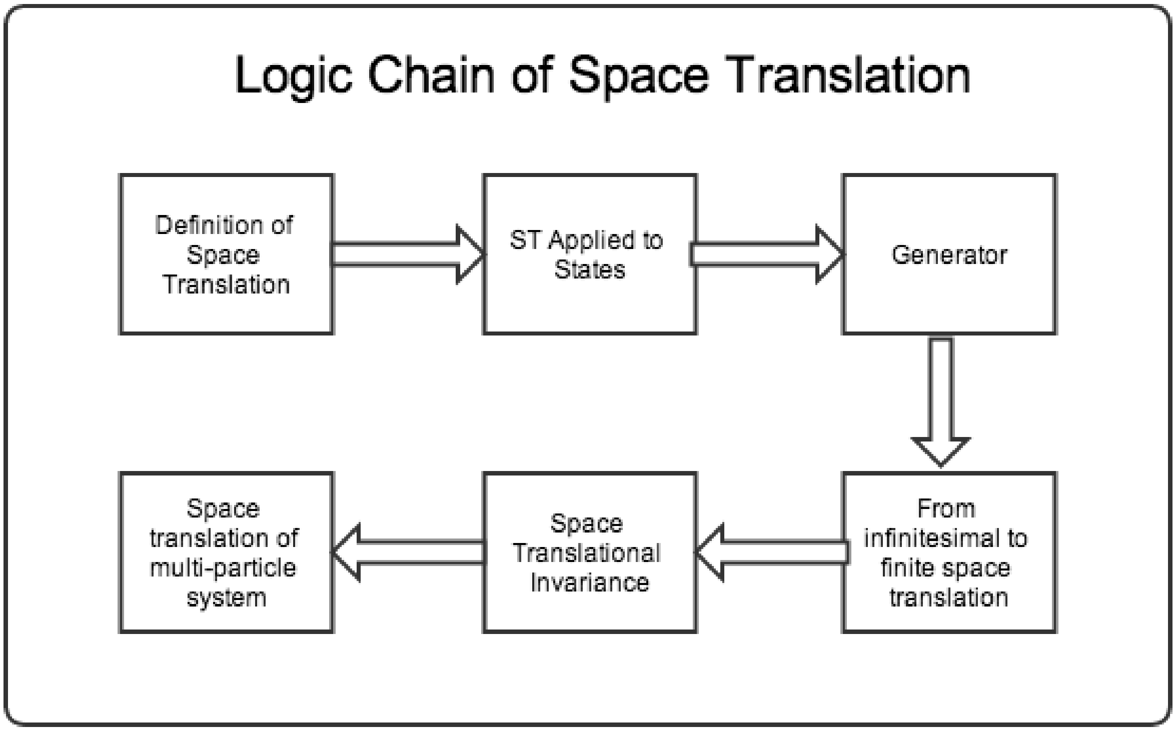
Hint: Ehrenfest theorem tells us that time independent Hamiltonian is a constant of motion.

$$\frac{d}{dt}\langle H\rangle = \frac{1}{i\hbar}\left\langle [\hat{H},\hat{H}]\right\rangle + \left\langle \frac{\partial}{\partial t}H\right\rangle = 0$$

Important: For an isolated system, T.T.I. should always be satisfied because there is nothing more else to change the system but to leave the system with energy conserved.

My concern is if we don't have an Hamiltonian for $T\mathrm{d}S$, we can't actually says this because of what the second law of thermodynamics tells us.

Space Translation Symmetry



Space Translation Gliffy Source

S.T.I. is generated by canonical momentum. This is not so obvious as time translation. To prove this we need to understand what space translation really means.

Definition of Space Translation

Space translation means we change the position of the system by some spatial distance a. In math this means a transformation from $|x\rangle$ to $|x+a\rangle$ where the plus sign is by definition. We invent this space translation operator,

$$\hat{T}_a |x\rangle = |x+a\rangle .$$

Space Translation Applied to States

Next we can obtain the result of space translation operator applied to state in position basis

$$\langle x| \hat{T}_a |\psi\rangle = (\langle x| \hat{T}_a^\dagger) |\psi\rangle = \langle x-a \mid \psi\rangle = \psi(x-a)$$

where we used the relation

$$(\langle x| \hat{T}_a) = (\hat{T}_a^\dagger |x\rangle)^\dagger = (\hat{T}_{-a} |x\rangle)^\dagger = (|x-a\rangle)^\dagger = \langle x-a|$$

which of course is because the normalization of coordinate basis tells us that space translation operator is unitary,

$$\langle x+a \mid x+a\rangle = \langle x| \hat{T}_a^\dagger \hat{T}_a |x\rangle$$

Generator of Space Translation

Similarly to time translation, we can find out the generator out of this definition. For infinitesimal translation,

$$-i\hbar \frac{|\psi(x)\rangle - |\psi(x-\Delta)\rangle}{\Delta} = \hat{p}\,|\psi(x)\rangle$$

i.e.,

$$|\psi(x-\Delta)\rangle = |\psi(x)\rangle - \frac{i\Delta}{\hbar}\,|\psi(x)\rangle$$

which shows that the generator of space translation is momentum operator.

From Infinitesimal to Finite Space Translation

$$\hat{T}_a = \lim_{N\to\infty} \hat{T}^N_{a/N} = \lim_{N\to\infty} \left(1 - \frac{i\hat{p}}{\hbar}\frac{a}{N}\right)^N = exp\left(-\frac{i\hat{p}a}{\hbar}\right)$$

Now we have the explicity expression for space translation operators.

Space Translation on Operators

1. Use the invariant scalar – inner product.
2. Passive vs Active

Space Translational Invariance

Space translational invariance of arbitary operator is

$$\hat{\Omega} = \hat{T}_a^\dagger \hat{\Omega} \hat{T}_a$$

is equivalent to

$$\hat{T}_a \hat{\Omega} = \hat{\Omega}\hat{T}_a \Rightarrow [\hat{T}_a, \hat{O}mega] = 0$$

We say some system has space translational invariance we mean the Hamiltonian is space translational invariant,

$$[\hat{H}, \hat{T}_a] = 0.$$

Such a system has space translational invariance.

Hint: I once thought Hamiltonian is space/time translational invariant is not enough for the statement that the whole system is invariant under space or time translation for all observables. Of course I was wrong. Once the Hamiltonian and initial condition is given the whole system can be determined completely in principle.

2.4.2 Gauge Symmetry

Global Gauge Transformation

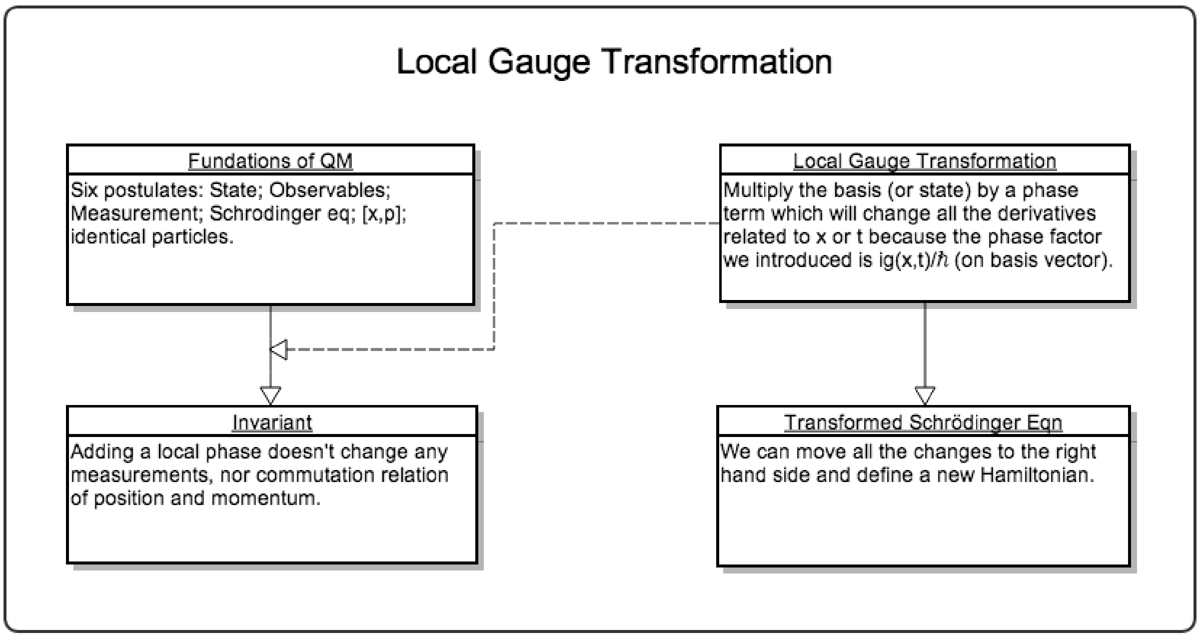
$$|\psi\rangle \to e^{ig\hat{I}}\,|\psi\rangle$$

All quantum states are invariant under such transformation. This is not a nonsene transformation because the two states are different in some sense if we put them in a phase space where the phase factor assigns a position for the state vector in the phase space and we can see the difference directly in this image.

The invariant thing is the probability density which is obvious.

Note: This is global because the phase factor doesn't depend on position and time.

Local Gauge Transformation



Local Gauge Transformation Gliffy Source

What if we have a local phase factor: $g(x,t)$?

One way of implenment this phase factor is to transform the basis, for example:

$$|x\rangle \rightarrow e^{ig(x,t)/\hbar} |x\rangle$$

By changing the basis, we can transform anything on position basis. Since the first principle of QM is Schrödinger equation, we would like to check what happens to that.

It turns out that both space derivative and time derivative of the wave function changed. For both of them,

$$\frac{d}{dw}(\exp(-ig/\hbar)\phi) = \exp(-ig/\hbar)\frac{d}{dw}\phi - i/\hbar\left(\frac{d}{dw}g\right)\phi$$

equivalently, we can just change all the derivatives to

$$\frac{d}{dw} \rightarrow \exp(-ig/\hbar)\frac{d}{dw} - i/\hbar\frac{d}{dw}g$$

where w can be x or t.

2.4.3 Parity

Logic

The only thing we need is the definition:

$$\hat{\Pi}\left|\vec{x}\right\rangle = \left|-\vec{x}\right\rangle$$

Starting from that, we can derive properties.

1. Hermition? **The way to find out something is Hermition or not is to take the Hermitian conjugate of the inner product sandwiched by the operator.**

   We know

   $$\left\langle x\right|\hat{\Pi}\left|x\right\rangle = \delta(x+x')$$

   Take the Hermitian conjugate of the whole expression,

   $$(\left\langle x'\right|\hat{\Pi}\left|x\right\rangle)^\dagger = \delta(x+x')$$

   We know the LHS is $\left\langle x\right|\hat{\Pi}^\dagger\left|x'\right\rangle$. So we have

   $$\left\langle x\right|\hat{\Pi}^\dagger\left|x'\right\rangle = \left\langle x\right|\hat{\Pi}\left|x'\right\rangle$$

   Then we get that parity operator is Hermitian.

2. Inversion? Parity operator is Unitary.

   $$\hat{\Pi}\hat{\Pi}\left|\pi\right\rangle = \hat{\Pi}\pi\left|\pi\right\rangle = \pi^2\left|\pi\right\rangle$$

   By physics we know that parity twice gets back to the original state. So $\pi^2 = 1$. Then we can find inverse parity operator. What's important is that it's unitary.

3. Acts on states? From definition, we need to go to position basis.

   $$\left\langle x\right|\hat{\Pi}\left|\psi\right\rangle = \langle -x \mid \psi\rangle.$$

   We can also find the results on momentum eigenbasis, which is

   $$\left\langle x\right|\hat{\Pi}\left|p\right\rangle = \langle -x \mid p\rangle.$$

   We already know mometum eigen state in postion is some kind of plane wave and it's easily proved that $\langle -x \mid p\rangle = \langle x \mid -p\rangle$.

4. Commutators with any observables? Just sandwich $\hat{\Pi}^\dagger\hat{\Omega}\hat{\Pi}$ then act on arbitary state and put it into position basis.

   As an example, find commutation relation with position operator.

   $$\left\langle x\right|\hat{\Pi}^\dagger\hat{X}\hat{\Pi}\left|\psi\right\rangle = \left\langle -x\right|\hat{X}\hat{\Pi}\left|x\right\rangle = -x\left\langle -x\right|\hat{\Pi}\left|\psi\right\rangle = -x\langle x \mid \psi\rangle$$

which is $\langle x| (-\hat{X}) |\psi\rangle$. This proves the following equation.

$$\hat{\Pi}^\dagger \hat{X} \hat{\Pi} = -\hat{X}$$

which can also be interpreted as passive transformation.

Another example is the commutation relation with (canonical) momentum.

$$\langle x| \hat{\Pi}^\dagger \hat{P} \hat{\Pi} |\psi\rangle = \langle -x| \hat{P} \hat{\Pi} |\psi\rangle = \int \langle -x| \hat{P} |x'\rangle \langle x'| \hat{\Pi} |\psi\rangle \, dx'.$$

By carefully applying parity on position basis, we have

$$\int \langle -x| \hat{P} |x'\rangle \langle -x' \mid \psi\rangle dx' = \int \langle -x| \hat{P} |-x'\rangle \langle x' \mid \psi\rangle dx'$$

Because commutation relation tells us

$$\langle x'| [\hat{X}, \hat{P}] |x\rangle = \langle x'| \hat{X}\hat{P} |x\rangle - \langle x'| \hat{P}\hat{X} |x\rangle = (x' - x) \langle x'| \hat{P} |x\rangle = i\hbar\delta(x' - x)$$

Here comes the keypoint. Recall that

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

we know that

$$(x - x') \langle x| \hat{P} |x'\rangle = i\hbar\delta(x' - x)$$

gives us the expression of momentum in position basis,

$$\langle x'| \hat{P} |x\rangle = -i\hbar\partial_x \delta(x' - x)$$

So to continue our calculation of parity applied to momentum,

$$\int \langle -x| \hat{P} |-x'\rangle \langle x' \mid \psi\rangle dx' = \int \langle x| (-\hat{P}) |x'\rangle \langle x' \mid \psi\rangle dx'$$

So we can prove that mometum actually invserses when parity is applied to it.
