Postulates of QM, Part V

We showed that the basic equation of QM $i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$ follows from the general geometrical principle that time evolution is represented in $\mathcal{H}$ by a unitary transformation.

Now let's generalize further:

Postulate 6''

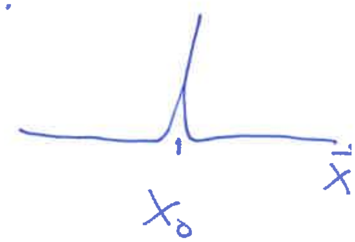
Any geometrical symmetry transformation is represented on $\mathcal{H}$ by a unitary operator.

- Geometrical means that points in $\mathcal{H}$ are caried into other points in $\mathcal{H}$
- ~~Must be~~ If it is to be a symmetry transformation, a necessary condition is that it preserves inner products $\langle\psi|\psi\rangle$ + $\langle\psi|\chi\rangle$, since we have assigned physical significance to these

$\Rightarrow$ Symmetry transformation operators must be unitary

- Let's first discuss general geometrical transformations then ask under what conditions they are symmetries

- Consider first translations in space. Let $|x_0\rangle$ be a state localized at $x = x_0$:



- A translation should carry

$|x_0\rangle \to |x_0 - a\rangle$ where a is a fixed displacement. We will set up this transformation so that it preserves norms. Then we write

$$\mathcal{U}(a)|x_0\rangle = |x_0 - a\rangle$$

The minus sign here is related to the question of whether we are translating the coordinate system to the right or moving the particle to the left. Both are equivalent.

- Since the states $|x_0\rangle$ form a basis for the function space, this equation tells us how $\mathcal{U}(a)$ acts on the whole Hilbert space.

- Another way of writing this is the following. Let $\underset{\sim}{x}$ be the operator associated with measurement of position.

  (Under-tilde will be used from here to distinguish operators from numbers)

- Then if we first act $\underset{\sim}{x}$ on a state & then translate, we will get a different result from the reverse.

This is a statement that $\mathcal{U}(a)\underset{\sim}{x} \neq \underset{\sim}{x}\,\mathcal{U}(a)$ i.e. measuring position then translating gives different result than translating then measuring

$$\mathcal{U}(a)\underset{\sim}{x} = (\underset{\sim}{x} + a)\,\mathcal{U}(a)$$

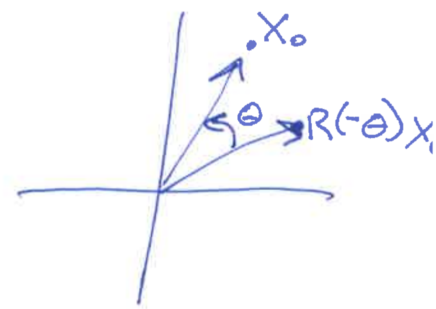
Checking that it works when applied to $|x_0\rangle$:

$$\mathcal{U}(a)\underset{\sim}{x}|x_0\rangle = x_0\,\mathcal{U}(a)|x_0\rangle = x_0\,|x_0-a\rangle \qquad x_0|x_0-a\rangle$$

$$(\underset{\sim}{x}+a)\mathcal{U}(a)|x_0\rangle = (\underset{\sim}{x}+a)|x_0-a\rangle = (x_0-a+a)\,|x_0-a\rangle$$

- In a similar way, we can represent a rotation of θ by a unitary operator $\mathcal{U}(\theta)$

$$\mathcal{U}(\theta)|x_0\rangle = |R(-\theta)x_0\rangle$$



- In both cases, the unitary transformations ~~which~~ are continuously generated.

- We can also discuss discrete transformations e.g. parity $|x\rangle \to |-x\rangle$

- If $\mathcal{U}(\alpha)$ is continuously generated, we saw that we can write it as

$$\mathcal{U}(\alpha) \approx \mathbb{1} + i\alpha G + \mathcal{O}(\alpha^2),$$

for small α, where G is Hermitian

α could be t, a, θ, etc.

$$+ \ \mathcal{U}(\alpha) = e^{i\alpha G} \text{ for finite } \alpha$$

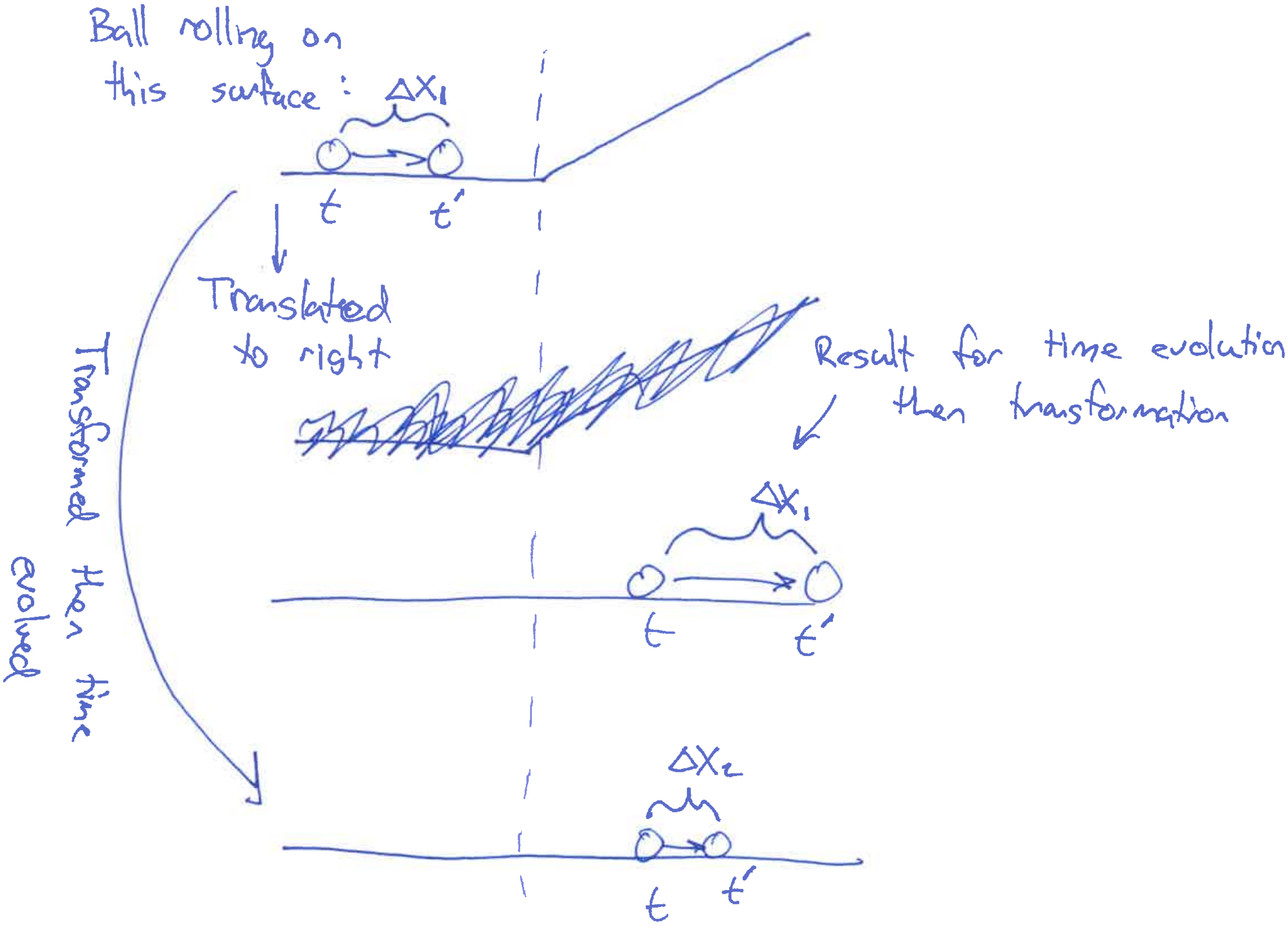
- Now, under what circumstances is $\mathcal{U}$ a symmetry?

- $\mathcal{U}$ is a symmetry if it transforms a solution to the equations of motion (e.g. $|\psi(t)\rangle$) into another solution of the equations of motion, or equivalently if time evolution after applying $\mathcal{U}$ is the same as what would have happened without applying $\mathcal{U}$.

Mathematically

$$
\begin{array}{ccc}
|\psi\rangle & \xrightarrow{\text{time evolve}} & |\psi(t)\rangle \\
\mathcal{U}\downarrow & & \downarrow\mathcal{U} \\
\mathcal{U}|\psi\rangle & \xrightarrow[\text{time evolve}]{} & \text{same thing? If so, } \mathcal{U} \text{ is a symmetry.}
\end{array}
$$

Consider a case where a transform is not a symmetry.



$\Delta X_2 < \Delta X_1$, because it's rolling up the hill.

$\Rightarrow$ In this external potential, translation is not a symmetry.

– But time evolution is just a unitary operator

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

~~For now, we can pretend we don't know that H has anything to do with energy ... will arrive at that conclusion soon. For now it is just the generator of time~~

– So, for some general $\mathcal{U}$ (rotation, translation, etc)

$\mathcal{U}$ is a symmetry if $e^{-\frac{iH}{\hbar}t}\mathcal{U}|\psi\rangle = \mathcal{U}e^{-\frac{iH}{\hbar}t}|\psi\rangle$

– Taking t small, the condition is

$$H\mathcal{U}|\psi\rangle = \mathcal{U}H|\psi\rangle \text{ for any } |\psi\rangle.$$

– In words, apply $\mathcal{U}$ then do a small time step, or do small time step first then apply $\mathcal{U}$, & we get same result.

– It's convenient to define the <u>commutator</u> of $\underset{\sim}{A}, \underset{\sim}{B}$ as $[\underset{\sim}{A}, \underset{\sim}{B}] = \underset{\sim}{A}\underset{\sim}{B} - \underset{\sim}{B}\underset{\sim}{A}$

– So a symmetry is defined by $[\mathcal{U}, H] = 0$

– If $\mathcal{U}$ is continuously generated, we ~~kn~~ can write

$$\mathcal{U}(a) = \mathbb{1} + iaG + \dots$$

- Then the term of order a in the above equation is

$$[G, H] = 0$$

- Conversely, if $[G,H]=0$, G generates a unitary trasformation which is a symmetry
- Interesting! We started talking about unitary transformations & we ended up talking about ~~the~~ properties of ~~the~~ Hermitian operators which are associated with observables. If $\mathcal{U}$ is a symmetry, G must have a special property. Namely, G is a ~~conserved quant~~ conservation law!

- We will prove in two ways:

① Let $|\psi_i\rangle$ be an eigenstate of G : $G|\psi_i\rangle = g_i|\psi_i\rangle$

$$|\psi_i(t)\rangle = e^{-i\frac{H}{\hbar}t}|\psi_i\rangle = \left(1 - i\frac{Ht}{\hbar} + \dots\right)|\psi_i\rangle$$

Is this still an eigenstate of G?

Consider the object

$$0 = \langle\psi_j|[G,H]|\psi_i\rangle$$

$$= \langle\psi_j|GH - HG|\psi_i\rangle = \langle\psi_j|GH|\psi_i\rangle - \langle\psi_j|HG|\psi_i\rangle$$

$$= g_j\langle\psi_j|H|\psi_i\rangle - \langle\psi_j|H|\psi_i\rangle g_i$$

$$= (g_j - g_i)\langle\psi_j|H|\psi_i\rangle$$

$\Rightarrow$ So either $g_i = g_j$ or $\langle\psi_j|H|\psi_i\rangle = 0$
$\quad \& \ \langle\psi_j|e^{-i\frac{H}{\hbar}t}|\psi_i\rangle = 0$

since argument also holds for H^n

- This means that H can only carry $|\psi_i\rangle$ to other states which are also eigenstates of G with same eigenvalue.

- In fact, it is always possible to find a basis that "simultaneously diagonalizes" both G & H (if $[G,H]=0$), such that

$$G|\psi_i\rangle = g_i|\psi_i\rangle \quad , \quad H|\psi_i\rangle = E_i|\psi_i\rangle$$

(2) Other property that should follow from a conservation law is that all matrix elements $\langle \psi | G | \chi \rangle$ are independent of time.

$$\langle \psi(t) | G | \chi(t) \rangle = \langle \psi | e^{i\frac{H}{\hbar}t} G e^{-i\frac{H}{\hbar}t} | \chi \rangle$$

If $[H, G] = 0 \Rightarrow [H^n, G] = 0$

$\Rightarrow \left[e^{i\frac{H}{\hbar}t}, G \right] = 0$

expansion in powers of H

$$= \langle \psi | G | \chi \rangle \quad , \quad t\text{-independent}$$

- In nature, there are three obvious geometrical symmetries:

- <u>Time-translation invariance</u> (Physical laws unchanging in time)

$$\mathcal{U}(\alpha) = e^{itG}$$

Here $G_t = \frac{-H}{\hbar}$

~~3) Def. time energy as a quantity conserved as a result of~~

H is associated with the conserved quantity energy. Fundamental definition of energy.

<u>Space translation invariance</u> (Physical laws unchanging from point to point in space)

Here $U(\vec{a}) \simeq \mathbb{1} + i a G_a$

Define: $G_a = \frac{1}{\hbar} \vec{P}$. This is the fundamental definition of momentum.

<u>Rotational invariance</u> (Laws of physics do not prefer any orientation)

Here $U(\vec{\theta}) \propto \mathbb{1} + i \vec{\theta} \cdot \vec{G}_\theta$

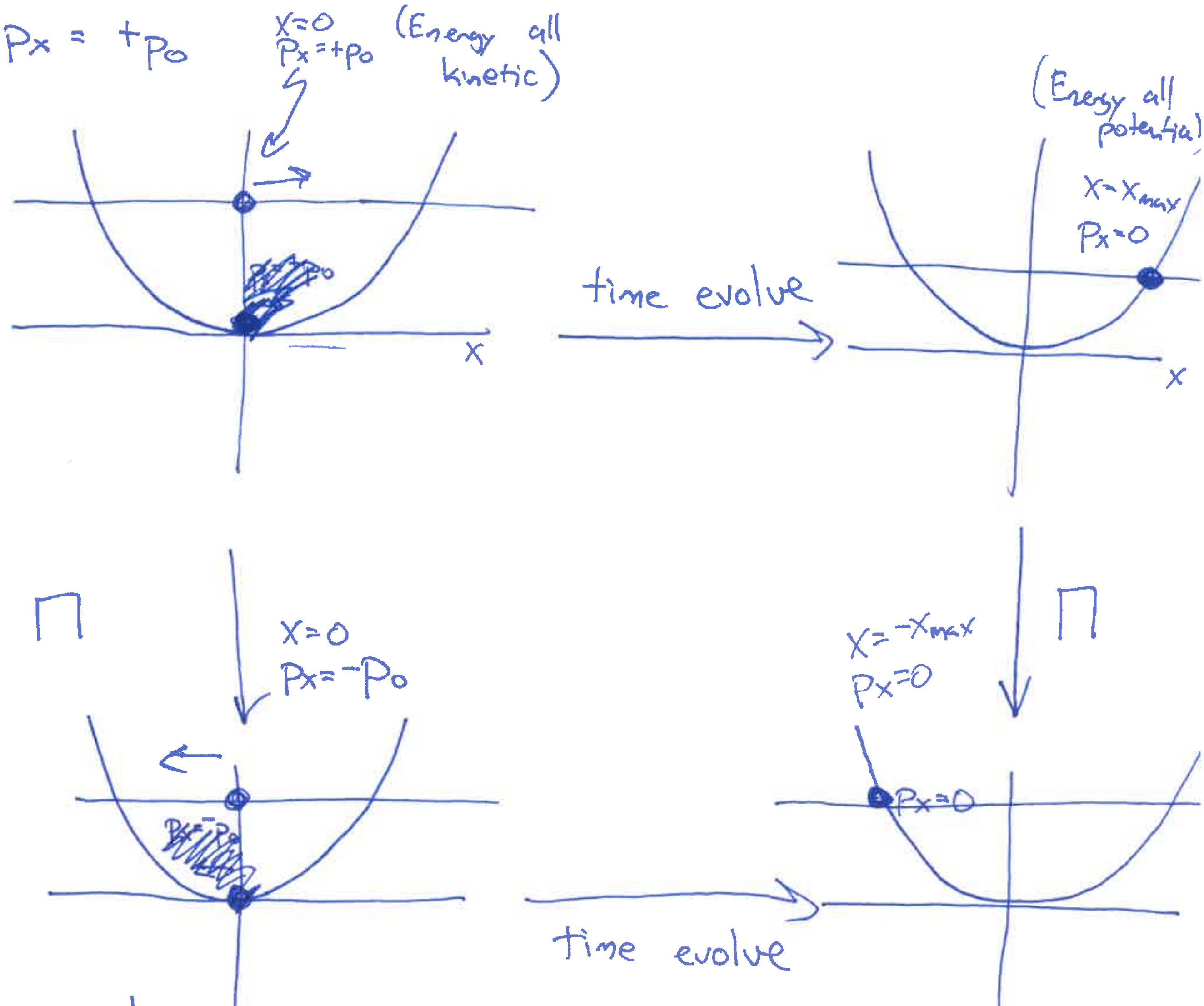
Define $\vec{G}_\theta = \frac{1}{\hbar} \vec{L}$. Fundamental definition of angular momentum.

$\Rightarrow$ Geometrical symmetries explain these most important conservation laws.

More on Symmetries

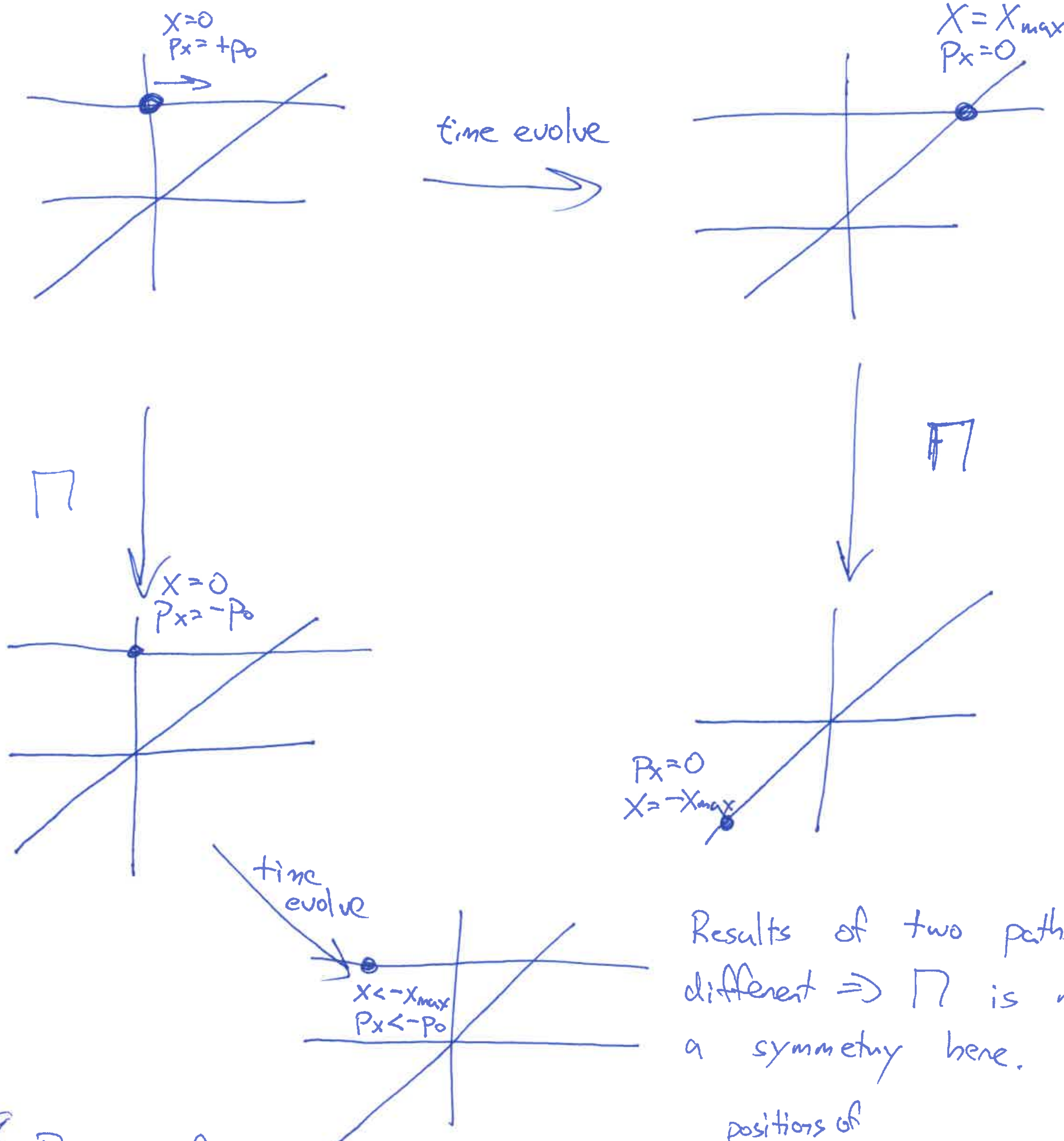
Consider a case where a transformation is a symmetry.

- Π is parity inversion operator, It takes $x \to -x$, $y \to -y$, $z \to -z$, $p_x \to -p_x$, etc.
- Say we have a Π-even potential $V(x) = ax^2$ & initial condition of classical ball at $x=0$ with $p_x = +p_0$



Same outcome following both paths. $\Rightarrow \Pi$ is a symmetry for this external potential.

What about for a non-symmetric external potential?



Results of two paths different $\Rightarrow$ Π is not a symmetry here.

But if we applied Π to all positions of Λ atoms generating the potential, (and if the weak force is not involved), then potential would flip also & we would recover Π symmetry.

Comment on Π transformation

- In classical physics, we need to ~~reverse~~ invert positions & momenta
- In QM, information about momenta is completely contained in $\psi(x,y,z)$. So Π inversion is accomplished by simply inverting coordinates in the position-space wavefunction.
- E.g. $\Pi|\vec{k}_0\rangle$ means

$$e^{i(+k_0x-\omega t)} \overset{\Pi}{\longleftrightarrow} e^{i(-kx-\omega t)}$$

(Invert only x, not k_0 too)

- In the end, we do get a plane wave with reversed momentum, as expected

Further Discussion on Time-Independence

Consider an expectation value $\langle O(t)\rangle = \langle\psi(t)|O|\psi(t)\rangle$, which is a special case of a matrix element $\langle\chi(t)|O|\psi(t)\rangle$. O is independent of time.

There are two ways $\langle O(t)\rangle$ can be time-independent. * Note that $\langle O\rangle$ can be (& often is) nT.D. even though O is not.

① $\psi(t=0)$ is an eigenstate of H, arbitrary $[O, H]$

$$\langle O(t)\rangle = \langle\psi(0)|e^{i\frac{H}{\hbar}t}\, O\, e^{-i\frac{H}{\hbar}t}|\psi(0)\rangle = e^{i\omega t}\langle\psi(0)|O|\psi(0)\rangle e^{-i\omega t}$$

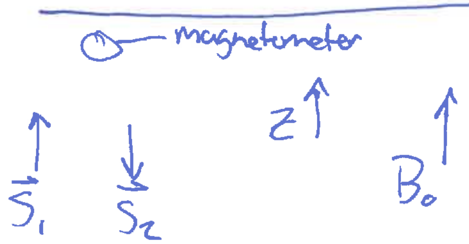
$$= \langle O(t=0)\rangle$$ ~~true for arbitrary $[O, H]$~~

② $[O, H] = 0$, arbitrary $\psi(t=0)$

$$\langle O(t)\rangle = \langle\psi(0)|e^{i\frac{H}{\hbar}t}\, O\, e^{-i\frac{H}{\hbar}t}|\psi(0)\rangle = \langle\psi(0)|O\,\cancel{e^{i\frac{H}{\hbar}t}\, e^{-i\frac{H}{\hbar}t}}|\psi(0)\rangle$$

$$= \langle O(t=0)\rangle$$

Example : Magnetization of 2-spin system



(To look at cases of time-dep./ind. states + measurement expectation values)

$S_1|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$

$$\vec{M} \propto \vec{S} = \vec{S}_1 + \vec{S}_2$$

$$H = \gamma\vec{S}_1\cdot\vec{B} + \gamma\vec{S}_2\cdot\vec{B} = \gamma S_{1z}B_0 + \gamma S_{2z}B_0 = \gamma S_z B_0$$

$$S_z = \hbar \begin{array}{c} |\downarrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\uparrow\uparrow\rangle \\ \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & & 0 \\ 0 & & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array}$$

Degenerate subspace

$\Rightarrow [H, S_{1z}] = 0$

$[H, S_{2z}] = 0$

$[H, S_z] = 0$

$$H = \hbar\gamma B_0 \begin{pmatrix} -1 & & & \\ & 0 & & \\ & & 0 & \\ & & & 1 \end{pmatrix}$$

Can also show for any $\vec{J}$
$[J_z, J^2] = 0$
$J^2 = \vec{J}\cdot\vec{J}$

$\boxed{Q}$ Prepare system in S_z eigenstate $|\uparrow\uparrow\rangle$
Is $|\langle M|\psi(t)\rangle|^2$ constant in time?
$\boxed{A}$ Yes

$\boxed{Q}$ Prepare system in $|\psi(t=0)\rangle = |\psi_i\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle)$

$|\langle\psi_i|\psi(t)\rangle|^2$ constant in time?

$\boxed{A}$ No. Neither final state + initial state are non energy eigenstates.

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-i\Omega t}|\uparrow\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle.$$

When $\Omega t = \pi$,
$|\psi(T)\rangle = \frac{1}{\sqrt{2}}(-|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle)$

$$\langle\psi_i|\psi(t)\rangle = 0$$

Q $|\langle\uparrow\uparrow|\psi(t)\rangle|^2$ const in time?

A Yes → prob. of finding en. eigenstat

Q Thinking of magnetization measurement,

$$\langle M_z(t)\rangle \equiv \langle\psi(t)|M_z|\psi(t)\rangle \quad \text{const in time?}$$

Yes, $[M_z, H] = 0$

Weird superposition of states w/ $M_z = +M_0$ + $M_z = 0$, but average ind. of time. (Each measurement finds either $M_z = 0$ or $+M_0$)

Now add coupling between spins:

$$\cancel{(\vec{S}_1+\vec{S}_2)^2 = S_1^2 + S_2^2 + 2\vec{S}_1\cdot\vec{S}_2}$$

$$H = \gamma S_z B_0 + \alpha \vec{S}_1\cdot\vec{S}_2$$

$$\cancel{(\vec{S}_1+\vec{S}_2)^2 = S_1^2 + S_2^2 + 2\vec{S}_1\cdot\vec{S}_2}$$

$$\cancel{\Rightarrow \vec{S}_1\cdot\vec{S}_2 = \tfrac{1}{2}(S^2 - S_1^2 - S_2^2)}$$

$$= S_{1z}S_{2z} + \tfrac{1}{2}(S_1^+S_2^- + S_1^-S_2^+)$$

Where $S_1^+|\downarrow\downarrow\rangle = \hbar|\uparrow\downarrow\rangle$

$S_1^-|\uparrow\downarrow\rangle = \hbar|\downarrow\downarrow\rangle$

$S_1^-|\downarrow\downarrow\rangle = 0$

etc.

→ H can + does flip individual spins – but ~~only if it ca~~ with certain rules about flips happening together + counteracting each other

Does $[H, M_z] = 0$ still?

Could work out from $[S_{1z}, S_1^-]$ etc,

but can also see from considering M.E.s

$$H|\uparrow\uparrow\rangle = \gamma\hbar B_0|\uparrow\uparrow\rangle + \frac{\alpha\hbar^2}{4}|\uparrow\uparrow\rangle$$

$$H|\uparrow\downarrow\rangle = -\frac{\alpha\hbar^2}{4}|\uparrow\downarrow\rangle + \frac{\alpha\hbar^2}{2}|\downarrow\uparrow\rangle \Rightarrow [H, S_{1z}] \neq 0$$

since H connects states of different S_{1z}

but

$$\boxed{[H, S_z] = 0}$$

(H only connects states within S_z degenerate subspace)

without coupling

No longer degenerate in energy in that subspace degenerate in S_z

$$H = \hbar\gamma B_0 \begin{pmatrix} -1 & & & \\ & 0 & & \\ & & 0 & \\ & & & 1 \end{pmatrix} + \frac{\alpha\hbar^2}{4} \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix}$$

(Can measure S_z then E & get same result if measured in reverse)

$\Rightarrow [H, M_z] = 0$

Q Prepare system in definite magnetization (M_z) state at $t=0$. Will it remain in that state for all time?

A No, not necessarily.

If $|\psi(t=0)\rangle = |\uparrow\uparrow\rangle$, then yes, because there is no S_z degeneracy there. (H can only connect states with same eigenvalue of S_z).

But if $|\psi(t=0)\rangle = |\uparrow\downarrow\rangle$ Not state of definite energy, then time evolution carries us to $|\downarrow\uparrow\rangle$ eventually. Let's look at short times.

$$\mathcal{U}(t) = \mathbb{1} - \frac{it}{\hbar} H$$

$$\mathcal{U}(t)|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle - \left(\frac{it}{\hbar}\frac{\alpha\hbar}{4}\right)\left(-|\uparrow\downarrow\rangle + 2|\downarrow\uparrow\rangle\right)$$

So at $t=0$ we have no $|\downarrow\uparrow\rangle$ mixed in, but the amount grows with t. Can't see from small time expansion, but at some time T, $|\psi(T)\rangle = |\downarrow\uparrow\rangle$.

Q Prepare $|\psi(t=0)\rangle = |\downarrow\uparrow\rangle$. Does $\langle M(t)\rangle$ change in time?

Not state of definite energy.

A No. We just saw that H only mixes in $|\uparrow\downarrow\rangle$, which ~~is~~ has same eigenvalue of $|S_z\rangle$. (This is example of $[O, H] = 0$)

If we choose right basis, we can simultaneously diagonalize H + S_z. That basis is

$|\uparrow\uparrow\rangle$

$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$|\downarrow\downarrow\rangle$

$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

then S_z looks same as before &

$$H = \begin{pmatrix} a & & & \\ & b & & 0 \\ & 0 & c & \\ & & & d \end{pmatrix}$$

Prepare system in one of those states, & of course $\langle M_z\rangle$ is constant, but also $|\psi(t)\rangle$ only has trivial phase winding & system never leaves that state.