## Time-Reversal in QM

In Newtonian physics: $m\ddot{\vec{r}} = -\vec{\nabla} V(\vec{r})$.

If $\vec{r}(t)$ is a solution, then so is $\vec{r}(-t)$.

(Take $t \to -t$ ; $\frac{d^2}{d(-t)^2} = \frac{d^2}{dt^2}$ .)

Maxwell's equations also have a time-reversal symmetry:

$$\left.\begin{aligned} &\vec{\nabla}\cdot\vec{E} = 4\pi\rho \\ &\vec{\nabla}\cdot\vec{B} = 0 \\ &\vec{\nabla}\times\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \\ &\vec{\nabla}\times\vec{B} - \frac{1}{c}\frac{\partial\vec{E}}{\partial t} = \frac{4\pi}{c}\vec{J} \end{aligned}\right\} \text{ invariant under } \left\{\begin{aligned} &t \to -t \\ &\vec{E} \to \vec{E} \\ &\vec{B} \to -\vec{B} \\ &\rho \to \rho \\ &\vec{J} \to -\vec{J} \end{aligned}\right.$$

If $\vec{E}(\vec{r},t)$, $\vec{B}(\vec{r},t)$, $\rho(\vec{r},t)$, $\vec{J}(\vec{r},t)$ is a solution, then

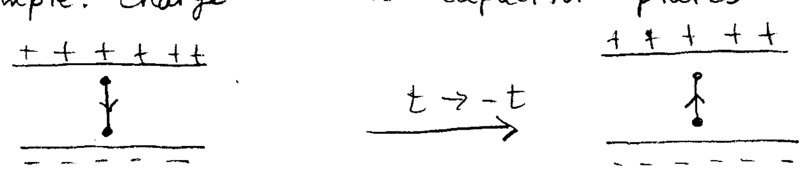
so is $\vec{E}(\vec{r},-t)$, $-\vec{B}(\vec{r},-t)$, $\rho(\vec{r},-t)$, $-\vec{J}(\vec{r},-t)$.

Also, if a test charge $q$ is present,

$$\vec{F} = q\left[\vec{E} + \frac{1}{c}\vec{v}\times\vec{B}\right], \quad \text{so} \quad \vec{v} \to -\vec{v}.$$

Think of time-reversal as watching a movie run backwards.
If the backwards movie obeys same laws of physics,
then $H$ is invariant under time reversal.

Example: charge between capacitor plates



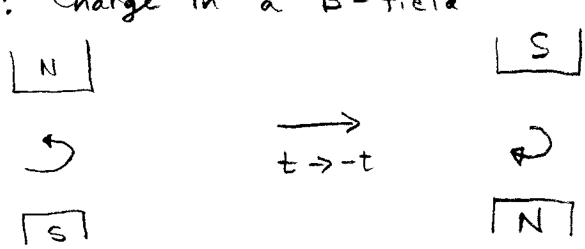

if $v_0$ is down, charge accelerates down

if $v_0$ is up, charge accelerates up

$t \to -t$
$\vec{E} \to \vec{E}$
$\rho \to \rho$
$\vec{v} \to -\vec{v}$

✓

**Example**: Charge in a $\vec{B}$-field




$t \to -t$
$\vec{B} \to -\vec{B}$
$\vec{v} \to -\vec{v}$

✓

For the Schrodinger equation (position representation)

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

Now, take the complex conjugate:

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

So if $\Psi(\vec{r},t)$ solves the original equation, then $\Psi^*(\vec{r},-t)$ does also.

(Note $\Psi(\vec{r},-t)$ <u>not</u> a solution, because $\frac{\partial}{\partial t} \neq \frac{\partial}{\partial(-t)}$.)

Time-reversal is represented by an <u>anti-unitary</u> operator $\Theta$.
very weird

First, define an operator $K$ to satisfy:

1) $K c|\alpha\rangle = c^* K|\alpha\rangle$ where $|\alpha\rangle$ is <u>any</u> ket

2) $K|a\rangle = |a\rangle$ for $|a\rangle$ = members of a fixed basis of kets.

*** Tricky Danger !!! *** <u>The definition of $K$ depends on the choice of basis.</u>

To illustrate:

$$\underset{\text{any ket}}{K|\alpha\rangle} = K \underset{\text{basis}}{\sum_a} |a\rangle\langle a|\alpha\rangle = K \sum_a \underset{\text{numbers}}{(\langle a|\alpha\rangle)} |a\rangle = \sum_a \langle a|\alpha\rangle^* |a\rangle$$

<u>Claim</u> An antiunitary operator has the form: $\Theta = \underset{\text{unitary}}{U} K$.

For time-reversal,

$$|\Psi\rangle \to \Theta|\Psi\rangle = \text{time-reversed state}$$

If $|\Psi\rangle = |\vec{p}\rangle$, then $\Theta|\vec{p}\rangle = \underset{\text{possible phase}}{e^{i\delta}} |-\vec{p}\rangle$

Suppose at time $t=0$, state is $|\psi(0)\rangle$.

At time $\delta t$, state is $\left(1 - i\frac{H\delta t}{\hbar}\right)|\psi(0)\rangle = |\psi(\delta t)\rangle$

Now consider $\Theta|\psi(0)\rangle$ = time-reversed state at $t=0$.

Then: $\left(1 - i\frac{H\delta t}{\hbar}\right)\Theta|\psi(0)\rangle = \Theta|\psi(-\delta t)\rangle = \Theta\left(1 + i\frac{H\delta t}{\hbar}\right)|\psi(0)\rangle$

So $-iH\Theta|\psi(0)\rangle = \Theta iH|\psi(0)\rangle$ . (True for any $|\psi(0)\rangle$.)

$= -i\Theta H|\psi(0)\rangle$

because $\Theta$ contains $K$.

So $\boxed{H\Theta = \Theta H}$

[What would have gone wrong if we tried to make $\Theta$ unitary?

Then $\Theta iH = i\Theta H \implies H\Theta = -\Theta H$.

So $H\Theta|n\rangle = -\Theta H|n\rangle = -E_n\Theta|n\rangle$, so $\Theta|n\rangle$ has energy $-E_n$.

Disaster: for a free particle, $E \geq 0$. ]

Consider an energy eigenstate $|n\rangle$. Then:

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

So $|n\rangle$ and $\Theta|n\rangle$ have the <u>same</u> energy.

Another consequence of the boxed equation:

$\Theta H \Theta^{-1} = H$ (we say $H$ is even under time-reversal).

A momentum e-state $|\vec{p}\rangle$ should have $\vec{p} \to -\vec{p}$ under time-reversal.

So $\vec{P}\,\Theta|\vec{p}\rangle = -\vec{p}\,\Theta|\vec{p}\rangle$ $\quad(\Theta|\vec{p}\rangle = e^{i\delta}|-\vec{p}\rangle)$

$= -\Theta\vec{P}|\vec{p}\rangle = -\Theta\vec{P}\underbrace{\Theta^{-1}\Theta}_{=1}|\vec{p}\rangle$

So $\Theta \vec{P} \Theta^{-1} = -\vec{P}$ (momentum is odd).

More generally, any Hermitian observable is even or odd.

$$\Theta \vec{R} \Theta^{-1} = +\vec{R} \quad \text{(position is even)} \iff \Theta|\vec{r}\rangle = |\vec{r}\rangle$$

(up to a phase, chosen by convention $=1$)

Since $\vec{L} = \vec{R} \times \vec{P}$, it must be odd:

$$\Theta \vec{L} \Theta^{-1} = -\vec{L}.$$

This also follows (for any angular momentum) from:

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

$i$ odd! $\Theta i \Theta^{-1} = -i$.

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

Wave functions: $|\psi\rangle = \int d^3\vec{r}\ |\vec{r}\rangle \underbrace{\langle r|\psi\rangle}_{\psi(\vec{r})}$, at some fixed $t$.

Then $\Theta|\psi\rangle = \int d^3\vec{r}\ \underbrace{\Theta|\vec{r}\rangle}_{=|\vec{r}\rangle}(\langle\vec{r}|\psi\rangle)^* = \int d^3\vec{r}\ |\vec{r}\rangle\, \psi^*(\vec{r})$

So $\langle\vec{r}|\Theta|\psi\rangle = \psi^*(\vec{r})$

Look at the angular part in an $(l,m)$ basis:

$$Y_{lm}(\theta,\phi) \to [Y_{lm}(\theta,\phi)]^* = (-1)^m Y_{l,-m}(\theta,\phi)$$

If $\psi_{\alpha,l,m} = R_\alpha(r)\, Y_{lm}(\theta,\phi)$, then

assume real

$$\Theta|\alpha, l, m\rangle = (-1)^m |\alpha, l, -m\rangle$$

Note that, doing this twice:

$\Theta^2 |\alpha, l, m\rangle = |\alpha, l, m\rangle$, so $\Theta^2 = +1$.

But, this is only for spinless states.

For spin-½ states $|+\rangle \equiv |m_s = \tfrac{1}{2}\rangle$ $\quad |-\rangle \equiv |m_s = -\tfrac{1}{2}\rangle$,

$\Theta |+\rangle = \eta |-\rangle$, and $\Theta |-\rangle = -\eta |+\rangle$, where $\eta$ = arbitrary phase,
(proof in Sakurai)

More generally,

$$\Theta \left( c_+ |+\rangle + c_- |-\rangle \right) = \eta c_+^* |-\rangle - \eta c_-^* |+\rangle.$$ Do it again...

So $$\Theta^2 \left( c_+ |+\rangle + c_- |-\rangle \right) = -|\eta|^2 c_+ |+\rangle - |\eta|^2 c_- |-\rangle$$
$$= -\left( c_+ |+\rangle + c_- |-\rangle \right)$$

So $\Theta^2 = -1$ (for spin-$\frac{1}{2}$) (Note: different conventions exist for $\eta$, but don't matter here.)

More generally, for total angular momentum $j$,

$$\Theta^2 |j\rangle = (-1)^{2j} |j\rangle$$ (+1 for integer $j$, −1 for half-integer $j$)

## Kramers Degeneracy

Suppose $[H, \Theta] = 0$, and consider energy eigenstates $|n\rangle$ and $\Theta |n\rangle$. We showed they have the same energy $E_n$.

But, are they the same state?

If they are, then $\Theta |n\rangle = e^{i\delta} |n\rangle$, for some phase angle $\delta$.

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

So, if non-degenerate, then $\Theta^2 |n\rangle = |n\rangle$.

But, we also said $\Theta^2 = -1$ for systems with odd $j$.

**So, if $j$ = odd, <u>every</u> energy eigenstate must have at least degeneracy 2.**

This includes all states with an odd number of electrons

True even when $H$ is very complicated.

We assumed $[H, \Theta] = 0$. But, is it true?

Systems with an external $\vec{E}$:

H includes $V(\vec{R}) = e\Phi(\vec{R})$ real function of even operator.

So $[H, \Theta] = 0$. Previous results apply.

Systems with an external $\vec{B}$:

H contains $\vec{S}\cdot\vec{B}_{ext}$ or $\vec{p}\cdot\vec{A}_{ext} + \vec{A}_{ext}\cdot\vec{p}$ where $\vec{A}_{ext} = \vec{\nabla}\times\vec{B}_{ext}$

Since $\vec{S}$, $\vec{p}$ are odd,

$[H, \Theta] \neq 0$ (Note $\vec{B}_{ext}$ is even under time-reversal; not part of the system.)

Systems with H containing complex phases

In the Standard Model of particle physics, the weak nuclear force has a tiny amount of time-reversal violation.

negligible for atomic, molecular, solid state

$[H_{universe}, \Theta] \neq 0$.

This is also known as CP violation.

charge conjugation (replace each particle by antiparticle)

parity

A deep theorem says $CP = \Theta$ in all theories that satisfy a few basic properties.

CP violation first discovered experimentally in 1964 by Cronin & Fitch in decays of neutral kaons.