I SYMMETRY IN QUANTUM MECHANICS

§1. Symmetries in classical physics

Homogeneity of space

a space is of equal structure at all positions $\vec{r}$;
a space is invariant under translations

Lagrangian $L(\bar{r}_i, \dot{\bar{r}}_i, t)$ - invariant if $\boxed{\bar{r}_i \to \bar{r}_i + \bar{a}}$

$$\delta L = \sum_i \frac{\partial L}{\partial \bar{r}_i} \cdot \delta \bar{r}_i = \bar{a} \cdot \sum_i \frac{\partial L}{\partial \bar{r}_i} = 0 \qquad \underline{\forall\ \vec{a}}$$

hence,
$$\boxed{\sum_i \frac{\partial L}{\partial \bar{r}_i} = 0} \qquad \text{where: } \frac{\partial L}{\partial \bar{r}_i} = \bar{\nabla}_i L = \begin{pmatrix} \frac{\partial L}{\partial x_i} \\ \frac{\partial L}{\partial y_i} \\ \frac{\partial L}{\partial z_i} \end{pmatrix}$$

Using Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0 \text{ , etc.}$$

we get
$$\frac{d}{dt} \sum_i \frac{\partial L}{\partial \dot{x}_i} = \frac{d}{dt} P_x = 0 \to P_x = \text{const.}$$

P_x - x-component of the <u>total momentum</u>

$$\bar{P} = \begin{pmatrix} \sum_i p_{xi} \\ \sum_i p_{yi} \\ \sum_i p_{zi} \end{pmatrix} = \sum_i \bar{p}_i \qquad \boxed{\frac{d\bar{P}}{dt} = 0}$$

Law of momentum conservation in classical mechanics

Homogeneity of time

invariance of the law of nature of isolated systems with respect to translations in time

$$t \to t + t_0$$

i.e. the Lagrangian does not depend on time explicitly

$$L = L(\varphi_i, \dot{\varphi}_i)$$

Hence,

$$\frac{dL}{dt} = \sum_i \frac{\partial L}{\partial \varphi_i} \dot{\varphi}_i + \sum_i \frac{\partial L}{\partial \dot{\varphi}_i} \ddot{\varphi}_i$$

Using Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\varphi}_i} - \frac{\partial L}{\partial \varphi_i} = 0$$

we get

$$\frac{dL}{dt} = \sum_i \dot{\varphi}_i \frac{d}{dt} \frac{\partial L}{\partial \dot{\varphi}_i} + \sum_i \frac{\partial L}{\partial \dot{\varphi}_i} \ddot{\varphi}_i = \sum_i \frac{d}{dt}\left(\dot{\varphi}_i \frac{\partial L}{\partial \dot{\varphi}_i} \right)$$

hence

$$\boxed{\frac{d}{dt}\left(\underbrace{\sum_i \dot{\varphi}_i \frac{\partial L}{\partial \dot{\varphi}_i} - L}_{E} \right) = 0}$$

This expresses a conservation of the total energy (Hamiltonian)

$$E = \sum_i \dot{\varphi}_i \frac{\partial L}{\partial \dot{\varphi}_i} - L = \sum_i \dot{\varphi}_i \pi_i - L = H \qquad \pi_i = \frac{\partial L}{\partial \dot{\varphi}_i}$$

<u>canonical momenta</u>

Systems in which the total energy is conserved are called <u>conservative systems</u>

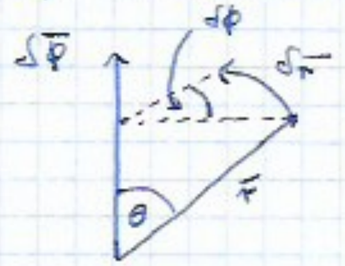
Isotropy of space

- the space has the same structure in all directions
- the mechanical properties of an isolated system remain unchanged if the whole system is arbitrary rotated in space
- the Lagrangian is invariant under rotations

The infinitesimal rotation $\delta\vec{\phi} = \{\delta\phi_x, \delta\phi_y, \delta\phi_z\}$

$d\phi = |\delta\vec{\phi}|$ - characterises the size of the rotation

$\frac{\delta\vec{\phi}}{d\phi}$ - defines the axis of rotation



The radius vector $\bar{r}$ changes under the rotation $\delta\phi$ by $\delta\bar{r}$

$$dr = |\delta\bar{r}| = r\sin\theta\, d\phi$$

and the direction of $\delta\bar{r}$ is perpendicular to the plane spanned by $\delta\bar{\phi}$ and $\bar{r}$

$$\boxed{\delta\bar{r} = \delta\bar{\phi}\times\bar{r}}$$

The velocity vector $\bar{v}_i$ is also changed in this way

$$\boxed{\delta\bar{v}_i = \delta\bar{\phi}\times\bar{v}_i}$$

Since under the rotation the Lagrangian is invariant

$$\delta L = \sum_i \left(\frac{\partial L}{\partial\bar{r}_i}\cdot\delta\bar{r}_i + \frac{\partial L}{\partial\bar{v}_i}\cdot\delta\bar{v}_i\right) = 0$$

canonical momenta

$$\bar{\pi}_i = \frac{\partial L}{\partial \bar{v}_i} = \left\{ \frac{\partial L}{\partial v_{ix}}, \frac{\partial L}{\partial v_{iy}}, \frac{\partial L}{\partial v_{iz}} \right\}$$

and from the Euler-Lagrange equations

$$\dot{\bar{\pi}}_i = \frac{d}{dt}\frac{\partial L}{\partial \bar{v}_i} = \frac{\partial L}{\partial \bar{r}_i}$$

now,

$$\delta L = \sum_i \left(\frac{d}{dt} \bar{\pi}_i \cdot \delta \bar{r}_i + \bar{\pi}_i \cdot \delta \bar{v}_i \right) =$$

$$= \sum_i \left(\dot{\bar{\pi}}_i \cdot \delta \bar{r}_i + \bar{\pi}_i \cdot \delta \bar{v}_i \right) =$$

$$= \sum_i \left(\dot{\bar{\pi}}_i \cdot (\delta \bar{\phi} \times \bar{r}_i) + \bar{\pi}_i \cdot (\delta \bar{\phi} \times \bar{v}_i) \right) =$$

$$= \delta \bar{\phi} \cdot \sum_i \left(\bar{r}_i \times \dot{\bar{\pi}}_i + \bar{v}_i \times \bar{\pi}_i \right) =$$

$$= \delta \bar{\phi} \cdot \frac{d}{dt} \left(\sum_i \bar{r}_i \times \bar{\pi}_i \right) = 0$$

$$\boxed{\begin{aligned} &\bar{A} \cdot (\bar{B} \times \bar{C}) = \\ &= \bar{B} \cdot (\bar{C} \times \bar{A}) = \\ &= \bar{C} \cdot (\bar{A} \times \bar{B}) \end{aligned}}$$

since $\bar{L} = \sum_i \bar{r}_i \times \bar{\pi}_i$ – angular momentum

we proved that $\boxed{\frac{d\bar{L}}{dt} = 0 \Rightarrow \bar{L} = \text{const.}}$

$\boxed{\text{conservation of angular momentum.}}$

§2 Symmetry transformations in Quantum mechanics

translations and rotations in $\mathbb{R}^3$ are associated with operators $\hat{G}$

$$\vec{r} \rightarrow \hat{G}\vec{r} = \vec{r}_T \qquad \hat{G} \text{ acts in } \mathbb{R}^3$$

In quantum mechanics there are unitary operators such that

$$\boxed{\hat{u}\,\psi(\hat{G}\vec{r}) = \psi(\vec{r})}$$

if the physics is invariant under $\hat{G}$ transformation

$$\hat{u}\,|\psi\rangle = |\psi_T\rangle \qquad \hat{u} \text{ acts in } \mathcal{H}$$

e.g. consider translation

$$\vec{r} \rightarrow \vec{r}_T = \vec{r} + \vec{a}$$

$$\psi_T(\vec{r}+\vec{a}) = \psi(\vec{r}) \iff \psi_T(\vec{r}) = \psi(\vec{r}-\vec{a}) =$$
$$= \hat{u}(\vec{a})\,\psi(\vec{r})$$

□

In quantum mechanics symmetry transformations can change vectors $|\psi\rangle$ and operators $\hat{O}$ but averages

$$\langle\psi|\hat{O}|\psi\rangle = \langle\psi_T|\hat{O}_T|\psi_T\rangle$$

and normalized vectors

$$\langle\psi|\psi\rangle = \langle\psi_T|\psi_T\rangle$$

are invariant.

Therefore, $\hat{U}$ must be ~~[illegible]~~ unitary

$$\hat{U}^\dagger \hat{U} = \hat{U}\hat{U}^\dagger = 1$$

Then

$$\langle \psi_T | \psi_T \rangle = \langle \psi | \hat{U}^\dagger \hat{U} | \psi \rangle = \langle \psi | \psi \rangle$$

and from the invariance $\langle \psi | \hat{O} | \psi \rangle = \langle \psi_T | \hat{O}_T | \psi_T \rangle$ we find

$$\underbrace{\langle \psi | \hat{U}^\dagger}_{\langle \psi_T |} \underbrace{\hat{U} \hat{O} \hat{U}^\dagger}_{\hat{O}_T} \underbrace{\hat{U} | \psi \rangle}_{| \psi_T \rangle} = \langle \psi_T | \hat{O}_T | \psi_T \rangle$$

$$\rightarrow \quad \hat{O}_T = \hat{U} \hat{O} \hat{U}^\dagger$$

or $\quad \hat{O}_T \hat{U} = \hat{U} \hat{O}$

In particular, if $\hat{U}$ is symmetry transformation of the Hamiltonian, i.e. $\hat{H}_T = \hat{H}$ then we have

$$\boxed{[\hat{H}, \hat{U}] = 0}$$

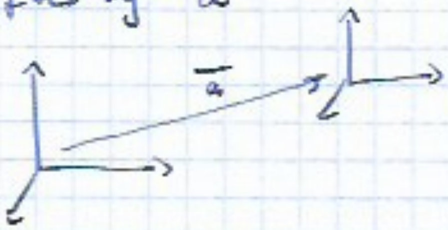
We consider continuous and discrete transformations.

- Continuous transformations → translations, time translations, rotations
- discrete transformations → parity, time reversal

translations

active transformation if all points of space are shifted by vector $\bar{a}$

passive transformation when a coordinate system is shifted by $\bar{a}$



then $\bar{r} \to \bar{r}_T - \bar{a}$

passive view is more convenient

operator $\hat{u}_{\bar{a}}$ transforms $\psi(\bar{r}) \to \psi(\bar{r} - \bar{a})$

$$\hat{u}_{\bar{a}}\,\psi(\bar{r}) = \psi(\bar{r} - \bar{a})$$

Now, we consider infinitesimal translation

$$\psi(\bar{r} - \bar{a}) = \psi(\bar{r}) + \frac{\partial \psi}{\partial \bar{r}}(-\bar{a}) + \dots =$$

$$= \psi(\bar{r}) - \frac{i}{\hbar}\,\bar{a}\cdot\hat{p}\,\psi(\bar{r}) + \dots = \qquad \hat{p} = -i\hbar\nabla_{\bar{r}}$$

$$= \left(1 - \frac{i}{\hbar}\,\bar{a}\cdot\hat{p} + \dots\right)\psi(\bar{r}) =$$

$$= e^{-\frac{i}{\hbar}\bar{a}\cdot\hat{p}}\,\psi(\bar{r})$$

we get $$\boxed{\hat{u}_{\bar{a}} = e^{-i\frac{\bar{a}\cdot\hat{p}}{\hbar}}}$$

$\hat{p}^+ = \hat{p}$

$\hat{u}_{\bar{a}}$ is unitary but not hermitian

$$\hat{u}_{\bar{a}}^{+} = \hat{u}_{\bar{a}}^{-1} \neq \hat{u}_{\bar{a}}$$

If $\hat{H}$ - Hamiltonian is translationally invariant, then

$$[\hat{U}_{\vec{a}}, \hat{H}] = 0$$

From the fact for any smooth function f

$$[\hat{O}, \hat{H}] = 0 \Leftrightarrow [f(\hat{O}), \hat{H}] = 0$$

we read that

$$[\hat{U}_{\vec{a}}, \hat{H}] = 0 \Leftrightarrow \boxed{[\hat{\vec{p}}, \hat{H}] = 0}$$

On the other hand, from the equation of motion

$$i\hbar \frac{d\hat{O}_H}{dt} = [\hat{O}, \hat{H}]_H \qquad \hat{O}_H = e^{\frac{i}{\hbar}\hat{H}t} \hat{O} e^{-i\frac{\hat{H}t}{\hbar}}$$

we find that $\dfrac{d\hat{\vec{p}}}{dt} = 0 \rightarrow \boxed{\hat{\vec{p}} = \text{constant of motion}}$

$\boxed{\text{Momentum conservation law}}$

time translations

$$t \to t_\tau = t + \tau$$

symmetry invariance

$$\Psi_\tau(t_\tau, \vec{r}) = \Psi(t, \vec{r})$$

$$\updownarrow$$

$$\Psi_\tau(t, \vec{r}) = \Psi(t - \tau, \vec{r}) =$$

$$= \Psi(t, \vec{r}) - \frac{\partial}{\partial t}\Psi(t, \vec{r})\,\tau + \dots =$$

$$\boxed{i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi}$$

$$= \Psi(t, \vec{r}) + \frac{i}{\hbar}\left(i\hbar\frac{\partial}{\partial t}\right)\Psi(\vec{r}, t)\cdot\tau + \dots =$$

$$= \Psi(t, \vec{r}) + \frac{i}{\hbar}\,\hat{H}\cdot\tau\,\Psi(\vec{r}, t) + \dots =$$

$$= \left(1 + \frac{i}{\hbar}\hat{H}\cdot\tau + \dots\right)\Psi(\vec{r}, t) =$$

$$= e^{\frac{i}{\hbar}\hat{H}\cdot\tau}\,\Psi(\vec{r}, t)$$

$$\boxed{\hat{U}_t(\tau) = e^{\frac{i}{\hbar}\hat{H}\cdot\tau}}$$

$\hat{H}$ - Hamiltonian

or $\boxed{\hat{U}_t(\tau) = e^{-\tau\frac{\partial}{\partial t}}}$

$$\boxed{\hat{H}|\Psi\rangle = E|\Psi\rangle}$$

note $\psi = \psi(\vec{r})$

$\Psi = \Psi(\vec{r}, t)$

$\psi(\vec{r}) = \langle \vec{r}|\psi\rangle$

$\Psi(\vec{r}) = \langle \vec{r}|\Psi(t)\rangle$

If $\hat{H}$ is time translation invariant

$$\boxed{[\hat{U}_t(\tau), \hat{H}] = 0} \iff \boxed{\frac{\partial \hat{H}}{\partial t} = 0}$$

must not explicitly depend on time.

$\boxed{\text{energy conservation law}}$