Lecture # 9

Main points of # 8

- formulated the scattering problem for classical physics

- introduced cross-section

From now, we will use a system of units with $\hbar = 1$.

PLAN

(08)

- Scattering in quantum mechanics
- Møller operators and S-matrix
- S-matrix and evolution operator in interaction picture of QM
- Properties of S and $\Omega_\pm$, isometric & unitary operators
- Energy conservation and S-matrix
- scattering amplitude, definition

2 Scattering in Quantum mechanics

As previously, take $V(x) \to 0$ at $|\vec{x}| \to \infty$.

Evalution of the wave-packet very far from the scattering center is given by:

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = H_0 \Psi, \quad \text{with } H_0 = \frac{p^2}{2m},$$

$$(***) \quad \Psi(t) \xrightarrow[t \to -\infty]{} U_0(t)|\Psi_{in}\rangle, \quad U_0(t) = \exp\left[-\frac{i}{\hbar} H_0 t\right]$$

and, for $t \to +\infty$,

$$\Psi(t) \to U_0(t)|\Psi_{out}\rangle$$

$|\Psi_{in}\rangle$ is an analogue of $\vec{x}_{in} + \vec{v}_{in} t$

and $|\Psi_{out}\rangle$ is an analogue of $\vec{x}_{out} + \vec{v}_{out} t$

in classical mechanics

Problem of scattering theory: find $|\Psi_{out}\rangle$ as a function of $|\Psi_{in}\rangle$

The mathematical procedure:

(i) Find general solution of Schrödinger eq.

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

(ii) Select solutions with time-asymptotics (***), at $t \to -\infty$

(iii) Find their behaviour at $t \to +\infty$

This will give $|\Psi_{out}\rangle$ as a function of $|\Psi_{in}\rangle$

Remark: $|\Psi(t)\rangle \underset{t\to\infty}{\to} |\Psi\rangle$ means:

$$|\Psi(t) - \Psi|^2 \to 0 \text{ at } t \to \infty.$$

Let us find the (formal) solution of the quantum scattering theory

Solution of the Schrödinger equation is

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi_0) \equiv \underset{\text{evolution operator}}{U(t)}\,\psi_0 \qquad (1)$$

when $t \to +\infty$, $\psi(t) \to U_0(t)|\psi_{out}\rangle$ (2)

when $t \to -\infty$, $\psi(t) \to U_0(t)|\psi_{in}\rangle$

from (1) and (2)

$$\psi_0 = U^+(t)\psi(t) = \lim_{t\to+\infty} U^+(t)U_0(t)|\psi_{out}\rangle$$

Let us denote

$$\lim_{t\to+\infty} U^+(t)U_0(t) = \Omega_- \Rightarrow$$

$$\psi_0 = \Omega_-|\psi_{out}\rangle$$

from (1) and (3):

$$\Psi_0 = U^+ \psi(t) = \lim_{t \to -\infty} U^+(t) U_0(t) |\Psi_{in}\rangle =$$

$$= \Omega_+ |\Psi_{in}\rangle, \quad \text{where } \Omega_+ = \lim_{t \to -\infty} U^+(t) U_0(t)$$

Then, $|\Psi_{out}\rangle = \Omega_-^+ |\Psi_0\rangle = \Omega_-^+ \Omega_+ |\Psi_{in}\rangle$

$$= S |\Psi_{in}\rangle$$

S is called S (scattering)-matrix

$$\Omega_\pm = \lim_{t \to \mp\infty} U^+(t) U_0(t)$$

are called Moller operators.

S-matrix can be related to the evolution operator in the <u>interaction</u> (Dirac) representation of Quantum mechanics.

Reminder: in Dirac representation of quantum mechanics the operators and states are both time-dependent,

$$O_I = e^{\frac{i}{\hbar}H_0 t}\, O_S\, e^{-i\frac{H_0}{\hbar}t}$$

$$\Psi_I = e^{i\frac{H_0 t}{\hbar}} e^{-i\frac{Ht}{\hbar}} |\Psi_S\rangle,$$

where O_S and $|\Psi_S\rangle$ are operators and states in the Schrödinger picture

$$\left(\frac{dO_S}{dt} = 0;\quad -\frac{\hbar}{i}\frac{\partial \Psi_S}{\partial t} = H\Psi_S\right)$$

In our notations:

$$\lim_{t\to-\infty} \Psi_I = \Psi_{in}, \quad \lim_{t\to+\infty} \Psi_I = \Psi_{out},$$

Since $e^{i\frac{H_0 t}{\hbar}} e^{-iHt/\hbar} |\Psi_S\rangle \underset{t\to-\infty}{\longrightarrow} e^{\frac{iH_0 t}{\hbar}} e^{-\frac{iH_0 t}{\hbar}} |\Psi_{on}\rangle =$

$= \Psi_{in}$. The same is for Ψ_{out}.

The evolution operator in interaction picture:

$$\Psi_I(t_1) = \exp\left[i\frac{H_0 t_1}{\hbar}\right] \exp\left[-\frac{iHt_1}{\hbar}\right] |\Psi_S\rangle =$$

$$= e^{\frac{iH_0 t_1}{\hbar}} e^{-\frac{iH t_1}{\hbar}} e^{+\frac{iH t_2}{\hbar}} e^{-\frac{iH_0 t_2}{\hbar}} \psi_I(t_2) \equiv$$

$S(t_1, t_2) \cdot \psi_I(t_2)$, with

$$S(t_1, t_2) = \exp\left[\frac{iH_0 t_1}{\hbar}\right] \exp\left[-\frac{i}{\hbar} H (t_1 - t_2)\right] \exp\left[-\frac{iH_0 t_2}{\hbar}\right]$$

So, $$S = \lim_{\substack{t_1 \to +\infty \\ t_2 \to -\infty}} S(t_1, t_2)$$

So - S-matrix is a limit of the evolution operator in the interaction picture of QM.

<u>Properties of S-matrix and of Møller operators</u>

<u>Questions:</u> S and $\Omega_\pm$ are the limits $t \to \pm\infty$ of unitary operators. Are they unitary? Reminder of definitions.

<u>Definition #1:</u> Operator U is called unitary if

(i) Domain of U, $\mathcal{D}(U) = \mathcal{H}$

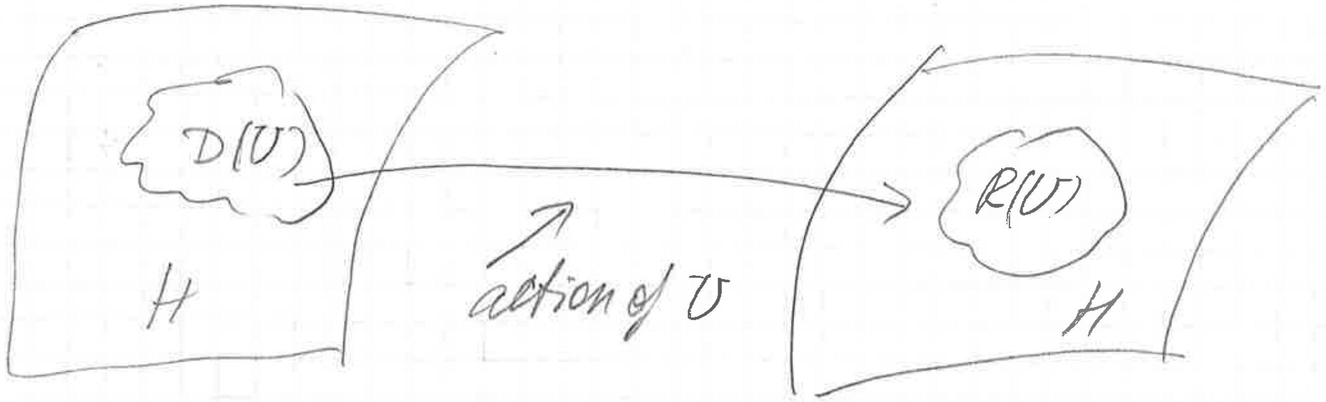
($\mathcal{H}$ is the whole Hilbert space)

Domain of operator : subspace of vectors on which U is defined

(ii) The range of U, $R(U) = H$

Range(image) of operator : the vectors

$U|\psi\rangle$, where $|\psi\rangle \in \mathcal{D}(U)$



(iii) $|U|\psi\rangle| = |\psi\rangle$, i.e. U does not change the norm of a vector.

Definition # 2. Operator U is called isometric, if (i) and (iii) are valid, but (ii) is not necesserily true.

Example: take basis vectors in H, $|1\rangle, |2\rangle, \ldots$ and define operator Ω as:

$\Omega|1\rangle = |2\rangle$; $\Omega|n\rangle = |n+1\rangle$

It is isometric but not unitary, since $R(\Omega) \neq \mathcal{H}$.

Aswers to the questions

(i) S-matrix is unitary and well defined for the following class of potentials:

1) $V(r) = O\left(\frac{1}{r^{3+\varepsilon}}\right)$, $\varepsilon > 0$, $r \to \infty$

This is needed to define rigorously in and out states. If 1) is not satisfied, the motion at $t \to \pm\infty$ is not free (cannot be described by H_0)

2) $V(r) = \left(\frac{1}{r^{3/2-\varepsilon}}\right)$, $r \to 0$

This excludes „falling" to the center trajectories

3) V is a continuous function of $\vec{x}$.

The proof can be found in the book by Taylor.
In what follows we will always assume that these conditions are satisfied.

(ii) Møller operators are <u>isometric</u>, if there are bound states, and are unitary, if there are no bound states.

To see this, let us prove some important relations with Møller operators:

$$H\Omega_+ = \Omega_+ H_0, \quad H\Omega_- = \Omega_- H_0,$$
$$H_0\Omega_+^+ = \Omega_+^+ H, \quad H_0\Omega_-^+ = \Omega_-^+ H$$

Formal proof:

$$e^{iH\tau/\hbar}\cdot\Omega_+ = e^{iH\tau/\hbar}\lim_{t\to-\infty} e^{iHt/\hbar}e^{-iH_0t/\hbar}$$

$$= \lim_{t\to-\infty} e^{iH(t+\tau)/\hbar}e^{-iH_0t/\hbar} =$$

$$\lim_{t\to\infty}\left(e^{iH(t+\tau)/\hbar}e^{-iH_0(t+\tau)/\hbar}\right)e^{+\frac{iH_0\tau}{\hbar}} =$$

$$= \Omega_+ e^{iH_0\tau/\hbar}, \text{ i.e.}$$

$$e^{iH\tau/\hbar}\Omega_+ = \Omega_+ e^{+iH_0\tau/\hbar}$$

take derivative with respect to τ and put τ to zero:

$$H\Omega_+ = \Omega_+ H_0 \quad ; \quad H_0\Omega_+^+ = \Omega_+^+ H$$

exactly in the same way [change limit $t \to -\infty$ to $t \to +\infty$]:

$$H\Omega_- = \Omega_- H_0 \quad ; \quad \Omega_-^+ H = H_0 \Omega_-^+$$

This leads to:

$$\Omega_+^+ H \Omega_+ = H_0$$

$$\Omega_-^+ H \Omega_- = H_0$$

Note: $\pm$ as subscript: $\Omega_\pm$

$+$ as superscript: sign of hermitean conjugation.

Let us consider eigen-vectors of H_0:

$H_0 |\vec{p}\rangle = \frac{\vec{p}^2}{2m}$ (eigenstates of momentum)

or $H_0 |\vec{p}\rangle = E_p |\vec{p}\rangle$, $\quad E_p = \frac{\vec{p}^2}{2m}$

Now,

$$H\Omega_+ |p\rangle = \Omega_+ H_0 |p\rangle = E_p \Omega_+ |p\rangle$$

So, $\Omega_+ |p\rangle$ is an eigenvector of full Hamiltonian with eigenvalue E_p.

Now we cansee that Ω_+ and Ω_- cannot be unitary if there are bound states.

vectors $|\bar{p}\rangle$ span all Hilbert space.

$\Omega_+|\bar{p}\rangle$ are eigenstates of H with positive eigenvalues $\Rightarrow$ bound states of H,
$H\psi = E\psi$, $E<0$ can never be obtained from $\Omega_+|\bar{p}\rangle$.

basisof$R(\Omega_+)$ is composed from $\Omega_+|\bar{p}\rangle \Rightarrow$

range

$$H = R(\Omega_+) \oplus B$$

Hilbert space of bound states.

B and $R(\Omega_+)$ are orthogonal:

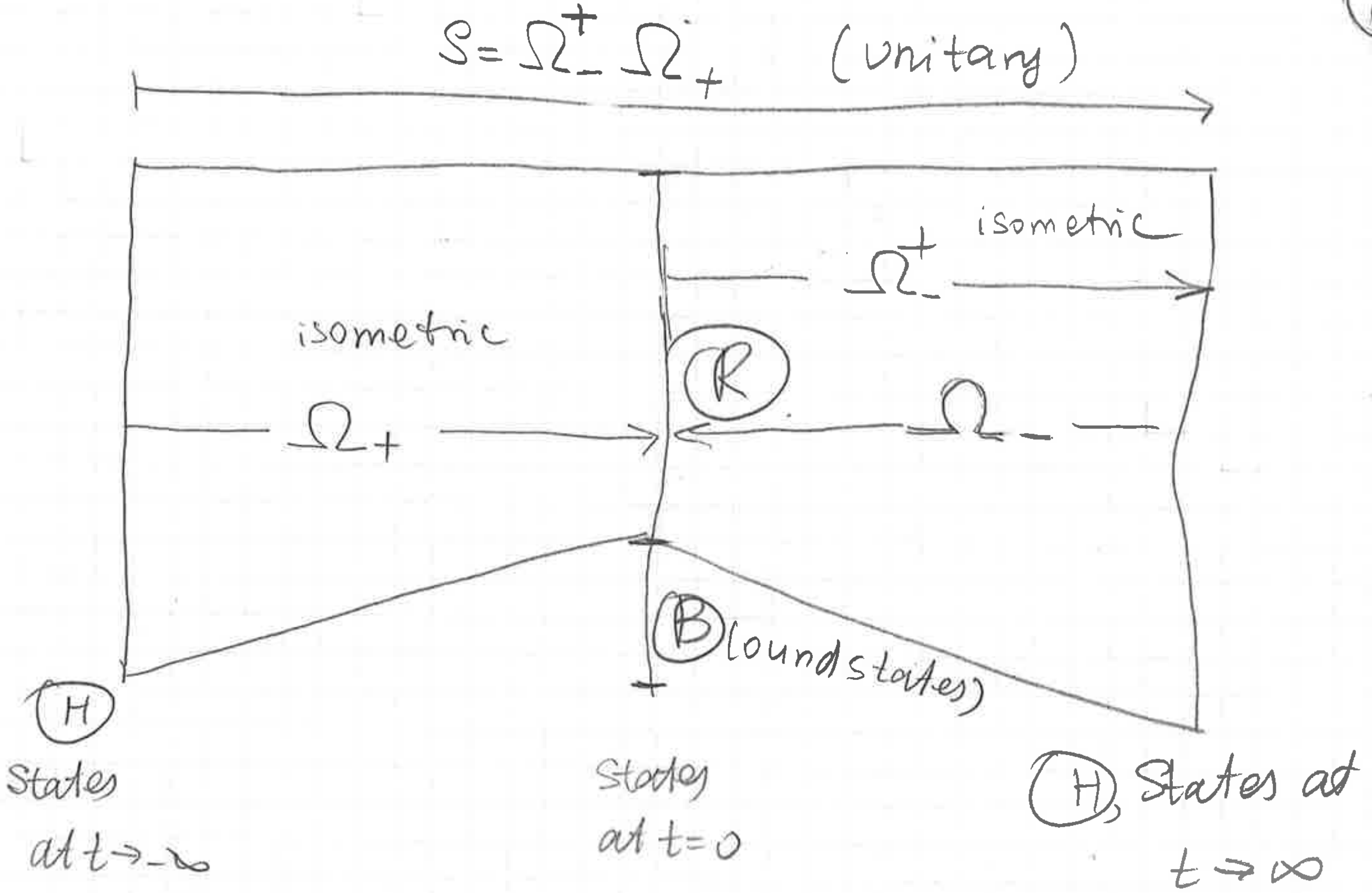
if $\psi_1 \in B$, $\psi_2 \in R(\Omega_+)$, then $\langle\psi_1|\psi_2\rangle = 0$

Simplest proof

$\psi_1 = \sum c_n \psi_n$; $H\psi_n = E_n\psi_n$, $E_n < 0$

$\psi_2 = \sum B_n \tilde{\psi}_n$; $H\tilde{\psi}_n = \tilde{E}_n\tilde{\psi}_n$, $\tilde{E}_n > 0$

$\langle\tilde{\psi}_n, \psi_m\rangle = 0$, as eigenvectors with different eigenvalues.



Overal picture: for the class of potentials for which S-matrix is unitary,

$$R(\Omega_+) = R(\Omega_-) = R$$

Range (image) of Ω_+ and Ω_-

$H = R \oplus B$, where B is the subspace corresponding to the bound states, and $R \perp B$.

Energy conservation and S-matrix

Let us prove an important result:

$[S, H_0] = 0$. Physically almost evident: kinetic energy of in-particles ($t \to -\infty$) is the same as kinetic energy of out-particles, ($t \to +\infty$)

This is based on relations we found in page 7.

Since $S = \Omega_-^+ \Omega_+$, we have

$$[H_0, S] = H_0 \Omega_-^+ \Omega_+ - \Omega_-^+ \Omega_+ H_0 =$$

$$= \Omega_-^+ H \Omega_+ - \Omega_-^+ \Omega_+ H_0 =$$

$$= \Omega_-^+ \Omega_+ H_0 - \Omega_-^+ \Omega_+ H_0 = 0$$

QED: $[H_0, S] = 0$

S-matrix and the scattering amplitude

Since S commutes with H_0, H_0 and S have a common set of eigenvectors, we take them to be $|\vec{p}\rangle$:

$\hat{\vec{p}}|\vec{p}\rangle = \vec{p}|p\rangle$; in x-representation

$$\langle\vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\vec{x}/\hbar}$$

In momentum representation, $\langle\vec{p}'|S|\vec{p}\rangle$, we can relate $|\psi_{out}\rangle$ and $|\psi_{in}\rangle$:

$$\psi_{out}(\vec{p}') = \int \langle\vec{p}'|S|\vec{p}\rangle \psi_{in}(\vec{p})\, d^3\vec{p}$$

Physical interpretation of $\langle p'|S|p\rangle$: amplitude of probability to get a state with momentum $\vec{p}'$ out of the state with momentum $\vec{p}$.

To introduce „scattering" amplitude, consider

$$0 = \langle p' | [H_0, S] | p \rangle = (E_{p'} - E_p) \langle p' | S | p \rangle$$

Therefore,

$$\langle p' | S | p \rangle = \delta(E_{p'} - E_p) \times \text{some function}$$

of momentum p.

If there is no interaction, $S = 1$

So, let's introduce

$$S = 1 + R, \quad [R, H_0] = 0$$

So, $\langle p' | S | p \rangle = \delta^3(\vec{p} - \vec{p}\,') -$

$$- 2\pi i\, \delta(E_p - E_{p'})\, t(\vec{p}\,' \leftarrow \vec{p}) = *$$

The first term, $\sim \delta^3(\vec{p} - \vec{p}\,')$ is the amplitude to pass the center without scattering.

$$* = \delta^3(\vec{p} - \vec{p}\,') + \frac{i}{2\pi m}\, \delta(E_p - E_{p'})\, f(\vec{p}\,' \leftarrow p)$$

f is called scattering amplitude

t and f are related to each other as

$$f(\vec{p}' \leftarrow \vec{p}) = -(2\pi)^2 m \, t(\vec{p}' \leftarrow \vec{p})$$

T is the matrix element of T-matrix, which will be introduced later.

Relation of f and physics (i.e. cross-section):

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\vec{p}' \leftarrow \vec{p})|^2}$$

Differential cross-section is simply the modulus of the scattering amplitude!

This will be proven in the next lecture.