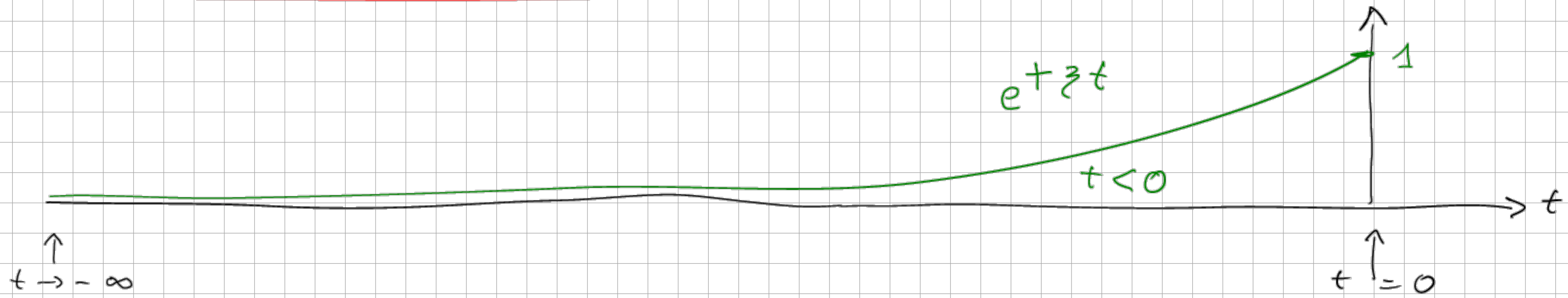
Formal Scattering Theory – Lippmann-Schwinger Equation



$\hat{H}_0$ $\qquad\qquad$ $\hat{H}_0 + \hat{V}$

$$(\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle$$

scattering state

$\xi > 0$

$$\hat{H}_\xi(t) = \hat{H}_0 + \hat{V} e^{\xi t} \quad ; \quad -\infty \leq t \leq 0$$

$$\hat{H}_S(t) = \hat{H}_S^{(0)} + \hat{H}_S^{(int)}(t)$$

Note: We let $\xi > 0$ finite, consider first states at $t = -\infty$ and $t = 0$ and only at the end we consider the limit $\xi \downarrow 0$

$$|\psi_D(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_S(t)\rangle \quad \Rightarrow \quad |\psi_D(0)\rangle = |\psi_S(0)\rangle = \underline{\underline{|\psi\rangle}}$$

$$\hat{V}_D(t) = \hat{H}_D^{(int)}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t} \underbrace{\hat{V} e^{+\xi t}}_{=\hat{H}_S^{(int)}(t)} e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

$$i\hbar \frac{\partial}{\partial t}|\psi_D(t)\rangle = \hat{H}_D^{(int)}(t)|\psi_D(t)\rangle$$

$$|\psi_D(t)\rangle = \underbrace{|\psi_D(t_0)\rangle} - \frac{i}{\hbar}\int_{t_0}^{t} d\tau \underbrace{\hat{H}_D^{(int)}(\tau)}_{e^{\frac{i}{\hbar}\hat{H}_0 \tau}\hat{V} e^{\xi\tau} e^{-\frac{i}{\hbar}\hat{H}_0 \tau}} |\psi_D(\tau)\rangle$$

$$\lim_{t_0 \to -\infty} \hat{H}_\xi(t) = \hat{H}_0 \qquad \Bigg| \qquad \lim_{t \to 0} \hat{H}_\xi(t) = \hat{H}_0 + \hat{V} = \hat{H}$$

$$\hat{H}_0 |\phi\rangle = E|\phi\rangle, \quad |\Psi_D(t_0 \to -\infty)\rangle = |\phi\rangle \qquad \Bigg| \qquad \hat{H}|\Psi\rangle = E|\Psi\rangle$$

$E > 0$ — elastic scattering

free solution of Schrödinger equation | scattering solution

$$|\Psi\rangle = |\phi\rangle - \frac{i}{\hbar}\int_{-\infty}^{0} dt\, e^{\frac{i}{\hbar}\hat{H}_0 t}\, \hat{V}\, e^{\xi t}\, \cancel{e^{-\frac{i}{\hbar}\hat{H}_0 t}}\, \underbrace{|\Psi_D(t)\rangle}_{\cancel{e^{+\frac{i}{\hbar}\hat{H}_0 t}}\, |\Psi_S(t)\rangle}$$

Now $\xi \downarrow 0$

$$|\Psi\rangle = |\phi\rangle - \frac{i}{\hbar}\lim_{\xi\downarrow 0}\int_{-\infty}^{0} dt\, e^{\frac{i}{\hbar}\hat{H}_0 t}\, \hat{V}\, e^{\xi t}\, \underbrace{\lim_{\xi\downarrow 0} |\Psi_S(t)\rangle}$$

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

$$e^{-\frac{i}{\hbar}Et} = \Big\{\, \underline{e^{-\frac{i}{\hbar}\hat{H}t}}\, \underbrace{|\Psi_S(0)\rangle}_{=|\Psi\rangle}$$

$$|\Psi\rangle = |\phi\rangle + \underbrace{\left(-\frac{i}{\hbar}\right)\lim_{\xi\downarrow 0}\int_{-\infty}^{0} dt\, e^{\frac{i}{\hbar}(\hat{H}_0 - E - i\hbar\xi)t}}_{\text{green operator}}\, \hat{V}\, |\Psi\rangle$$

convergence factor

$$= -\cancel{\frac{i}{\hbar}}\lim_{\xi\downarrow 0} \frac{e^{\frac{i}{\hbar}(\hat{H}_0 - E - i\hbar\xi)t}}{\cancel{\frac{i}{\hbar}}(\hat{H}_0 - E - i\hbar\xi)}\Bigg|_{-\infty}^{0} = \lim_{\xi\downarrow 0} \frac{-1}{\hat{H}_0 - E - i\cancel{\hbar}\xi}$$

- $i\xi$ important to avoid singular behaviour

• Green operator depends only on $\hat{H}_0$

$\Rightarrow$ $|\psi\rangle = |\phi\rangle + \hat{G}_0 \hat{V} |\psi\rangle$ Lippmann-Schwinger representation

self-consistent equation for scattering state

spatial representation:

$$\langle \vec{x} | \psi \rangle = \langle \vec{x} | \phi \rangle + \langle \vec{x} | \hat{G}_0 \int d^3x' \, |\vec{x}'\rangle \underbrace{\langle \vec{x}' | \hat{V} | \psi \rangle}_{= V(\vec{x}') \langle \vec{x}' | \psi \rangle}$$

$$\psi(\vec{x}) = \phi(\vec{x}) + \int d^3x' \underbrace{\langle \vec{x} | \hat{G}_0 | \vec{x}' \rangle}_{= G_0(\vec{x};\vec{x}')} V(\vec{x}') \, \psi(\vec{x}')$$

$= G_0(\vec{x};\vec{x}')$ Green function

$$= \int d^3q \, \langle \vec{x} | \lim_{\varepsilon \downarrow 0} \frac{-1}{\underbrace{\hat{H}_0}_{= \frac{\hbar^2 \vec{q}^2}{2\mu}} - E - i\varepsilon} |q\rangle \underbrace{\langle \vec{q} | \vec{x}' \rangle}_{\frac{1}{(2\pi)^{3/2}} e^{-i\vec{q}\vec{x}'}}$$

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

$$|q\rangle \lim_{\varepsilon \downarrow 0} \frac{-1}{\frac{\hbar^2 q^2}{2\mu} - E - i\varepsilon}$$

$$= \lim_{\varepsilon \downarrow 0} \int \frac{d^3q}{(2\pi)^3} \frac{-1}{\frac{\hbar^2 q^2}{2\mu} - \frac{\hbar^2 k^2}{2\mu} - i\varepsilon} = \frac{2\mu}{\hbar^2} \lim_{\varepsilon \downarrow 0} \int \frac{d^3q}{(2\pi)^3} \frac{-1}{q^2 - k^2 - i\varepsilon}$$

$\Rightarrow$ recovering of previous Green function, but this time with Feynman $i\varepsilon$-prescription

T-matrix: $|\psi\rangle = \underline{|\phi\rangle} + \hat{G}_0 \hat{V} |\psi\rangle$

Lippman-Schrödinger has to be solved for each input (free) state solution → disadvantage

$$|\psi\rangle = \underbrace{|\phi\rangle}_{0.} + \underbrace{\hat{G}_0 \hat{V} |\phi\rangle}_{1.} + \underbrace{\hat{G}_0 \hat{V} \hat{G}_0 V |\phi\rangle}_{2.} + \underbrace{\hat{G}_0 \hat{V} \hat{G}_0 \hat{V} \hat{G}_0 \hat{V} |\phi\rangle}_{3.} + \dots$$

→ Born series

$$= \Big\{ 1 + \hat{G}_0 \underbrace{\left[\hat{V} + \hat{V} \hat{G}_0 \hat{V} + \hat{V} \hat{G}_0 V \hat{G}_0 \hat{V} + \dots \right]}_{= \hat{T}} \Big\} |\phi\rangle$$

$= \hat{T}$ transfer matrix

$$|\psi\rangle = \{ 1 + \hat{G}_0 \hat{T} \} |\phi\rangle$$

$\hat{T}$ follows from a Lippman Schrödinger equation

$$\hat{T} = \hat{V} + \hat{V} \hat{G}_0 \hat{T}$$

$$= \underbrace{\boxed{\hat{V}}}_{\text{(first) Born approximation}} + \hat{V} \hat{G}_0 \hat{V} + \hat{V} \hat{G}_0 \hat{V} \hat{G}_0 V + \dots$$

(first) Born approximation

Remark: spatial representation ⇒ nonlocal

$$T(\vec{x}, \vec{x}') = V(\vec{x})\, \delta(\vec{x} - \vec{x}') + \int d^3x''\, V(\vec{x})\, G_0(\vec{x}, \vec{x}'')\, T(\vec{x}''; \vec{x}') + \dots$$

Organizational Remark: start of exercises on 7.12. is ~~8.25~~

8 Feynman Formulation Quantum Mechanics

Motivation:

- 1942, PhD of Richard Feynman
  → different formulation of quantum mechanics: path integral
- corresponding publication delayed by Second World War
  R. P. Feynman, Space-Time Approach to Non-Relativistic Quantum Mechanics
  Rev. Mod. Phys. 20, 367 (1948)

8.1 Propagator Notion:

1926 Schrödinger formulation of quantum mechanics

here: 1D, wave function $\Psi(x,t)$ is a solution of initial value problem

$$\begin{cases} \text{Schrödinger equation} & i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \hat{H}(x)\Psi(x,t)\,; \quad \hat{H}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \\ \text{initial value} & \Psi(x_0,t_0) = \Psi_0(x_0,t_0) \end{cases}$$

Formal solution necessitates a basis

eigenvalue problem: $\hat{H}(x)\,\phi_n(x) = E_n\,\phi_n(x)$

orthonormality: $\int_{-\infty}^{+\infty} dx\, \phi_n^*(x)\,\phi_{n'}(x) = \delta_{nn'}$

completeness: $\sum_n \phi_n^*(x)\,\phi_n(x') = \delta(x-x')$

$$\hookrightarrow \quad \Psi(x,t) = \sum_n c_n(t)\,\phi_n(x)$$

$\underbrace{}_{\text{may dependent on time}}$

insert Schrödinger equation

$$\sum_n i\hbar \frac{\partial}{\partial t} c_n(t)\, \phi_n(x) = \sum_n \underbrace{\hat{H}(x)\phi_n(x)}_{=E_n \phi_n(x)} c_n(t) = \sum_n E_n\, \phi_n(x)\, c_n(t) \quad \Big| \int_{-\infty}^{+\infty} dx\, \phi_{n'}^*(x) \cdot$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} c_{n'}(t) = E_{n'}\, c_{n'}(t) \quad \Rightarrow c_{n'}(t) = c_{n'}(t_0)\, e^{-\frac{i}{\hbar} E_n (t-t_0)}$$

$$\Rightarrow \Psi(x,t) = \sum_n \underbrace{c_n(t_0)}_{\text{yet unknown}}\, e^{-\frac{i}{\hbar} E_n(t-t_0)}\, \phi_n(x)$$

implement initial value: $\Psi(x,t_0) = \sum_n c_n(t_0)\, \phi_n(x) \overset{!}{=} \Psi_0(x,t_0) \quad \Big| \int_{-\infty}^{+\infty} dx\, \phi_{n'}^*(x) \cdot$

$$\Rightarrow c_{n'}(t_0) = \int_{-\infty}^{+\infty} dx_0\, \Psi_0(x_0,t_0)\, \phi_{n'}^*(x_0)$$

Solution of initial value problem:

$$\Psi(x,t) = \int_{-\infty}^{+\infty} dx_0 \underbrace{\left\{ \sum_n \phi_n^*(x_0)\, e^{-\frac{i}{\hbar} E_n (t-t_0)}\, \phi_n(x) \right\}}_{= G(x,t;x_0,t_0)} \Psi_0(x_0,t_0)$$

spectral representation of a propagator

propagator

- for any initial wave function this yield $\Psi(x,t)$ at a later time
- $\Psi_0(x_0,t_0) = \delta(x_0 - x_0') \Rightarrow \Psi(x,t) = G(x,t;x_0',t_0)$
- propagators are more fundamental than wave function

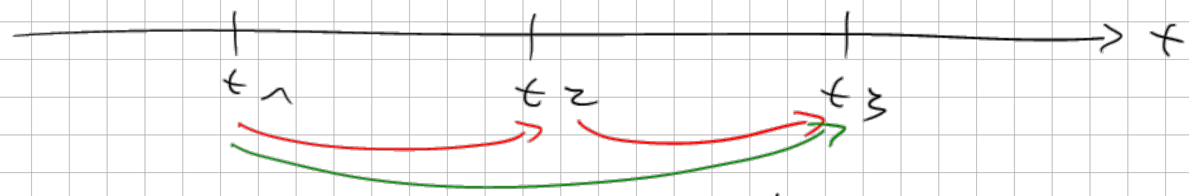
8.2 Propagator Properties:

- propagator solves this initial value problem:

$$\begin{cases} i\hbar \dfrac{\partial}{\partial t} G(x,t;x_0,t_0) = \hat{H}(x)\, G(x,t;x_0,t_0) \\ G(x,t_0;x_0,t_0) = \delta(x-x_0) \end{cases}$$

- spectral representation: see above
- homogeneity in time: $G(x,t+\tau;x_0,t_0+\tau) = G(x,t;x_0,t_0)$

  $\tau = -t_0$: $G(x,t-t_0;x_0,0) = G(x,t;x_0,t_0)$

- 

$$\psi(x_3,t_3) = \int_{-\infty}^{+\infty} dx_2\, G(x_3,t_3;x_2,t_2) \underline{\int_{-\infty}^{+\infty} dx_1}\, G(x_2,t_2;x_1,t_1)\, \psi(x_1,t_1)$$

$$= \underline{\int_{-\infty}^{+\infty} dx_1}\, G(x_3,t_3;x_1,t_1)\, \underline{\psi(x_1,t_1)}$$

$\Rightarrow$ group property:

$$G(x_3,t_3;x_1,t_1) = \int_{-\infty}^{+\infty} dx_2\, G(x_3,t_3;x_2,\boxed{t_2})\, G(x_2,\boxed{t_2};x_1,t_1)$$

but not on left-hand side $\qquad$ t_2 at right-hand side

Intermediate result: The group property is the starting point to determine the path!