Dirac (Interaction) Picture

$$\hat{H}_S(t) = \underbrace{\hat{H}_S^{(0)}}_{\text{time independent unperturbed}} + \underbrace{\hat{H}_S^{(int)}(t)}_{\text{time dependent perturbation}}$$

$$i\hbar \frac{\partial}{\partial t}|\Psi_S(t)\rangle = \hat{H}_S(t)|\Psi_S(t)\rangle = \left\{ \hat{H}_S^{(0)} + \hat{H}_S^{(int)}(t) \right\} |\Psi_S(t)\rangle$$

Basic idea: formally "redo" the dynamics of $\hat{H}_S^{(0)}$ in $|\Psi_S(t)\rangle$

$$|\Psi_D(t)\rangle := e^{+\frac{i}{\hbar}\hat{H}_S^{(0)} t} |\Psi_S(t)\rangle \quad (1) \iff |\Psi_S(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_S^{(0)} t} |\Psi_D(t)\rangle$$

Important: expectation values, i.e. physically observable quantities, do not depend on the choice of the picture

$$\langle \Psi_D(t)| \underbrace{\hat{O}_D(t)}_{\text{Wanted!}} |\Psi_D(t)\rangle \stackrel{!}{=} \underbrace{\langle \Psi_S(t)|}_{=\langle \Psi_D(t)| e^{\frac{i}{\hbar}\hat{H}_S^{(0)} t}} \hat{O}_S \cancel{(t)} \underbrace{|\Psi_S(t)\rangle}_{= e^{-\frac{i}{\hbar}\hat{H}_S^{(0)} t} |\Psi_D(t)\rangle} \quad (1')$$

$$\Rightarrow \hat{O}_D(t) = e^{\frac{i}{\hbar}\hat{H}_S^{(0)} t} \hat{O}_S e^{-\frac{i}{\hbar}\hat{H}_S^{(0)} t} \quad (2)$$

example: $\hat{O}_S = \hat{H}_S^{(0)}$

$$\hat{H}_D^{(0)}(t) = e^{\frac{i}{\hbar}\hat{H}_S^{(0)} t} \hat{H}_S^{(0)} e^{-\frac{i}{\hbar}\hat{H}_S^{(0)} t} = \hat{H}_S^{(0)} \quad (3)$$

$$i\hbar \frac{\partial}{\partial t}|\Psi_D(t)\rangle \stackrel{(1)}{=} \left\{ \cancel{-\hat{H}_S^{(0)} e^{\frac{i}{\hbar}\hat{H}_S^{(0)} t}} + e^{\frac{i}{\hbar}\hat{H}_S^{(0)} t} \left(\cancel{\hat{H}_S^{(0)}} + \hat{H}_S^{(int)}(t) \right) \right\} |\Psi_S(t)\rangle$$

$$\overset{(1')}{=} \underbrace{e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t}\,\hat{H}_S^{(int)}(t)\,e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t}}_{\overset{(2)}{=}\ \boxed{\hat{H}_D^{(int)}}(t)}\,|\psi_D(t)\rangle$$

Dirac picture:

1) Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\hat{O}_D(t) \overset{(2)}{=} e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t}\left\{-\hat{H}_S^{(0)}\hat{O}_S + \hat{O}_S\hat{H}_S^{(0)}\right\}e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t}$$

$$\overset{(2)}{=}\left[\hat{O}_D(t), \hat{H}_S^{(0)}\right]_- \overset{(3)}{=}\left[\hat{O}_D(t), \boxed{\hat{H}_D^{(0)}(t)}\right]_-$$

2) Heisenberg equation

Time Evolution Operator in Dirac Picture:

$$\underbrace{|\psi_D(t_2)\rangle}_{} = \hat{U}_D(t_2,t_1)\,|\psi_D(t_1)\rangle, \quad |\psi_S(t_2)\rangle = \hat{U}_S(t_2,t_1)\,|\psi_S(t_1)\rangle$$

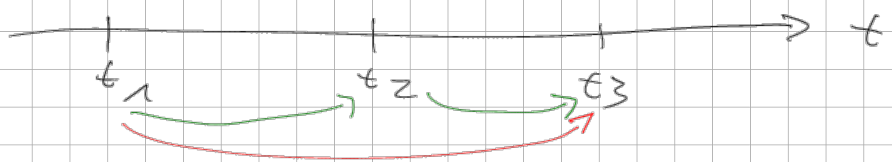
$$= e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}|\psi_S(t_2)\rangle \overset{\downarrow}{=} e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}\,\hat{U}_S(t_2,t_1)\,\underbrace{|\psi_S(t_1)\rangle}_{=e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t_1}|\psi_D(t_1)\rangle}$$

$$\hat{U}_D(t_2,t_1) = e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}\,\hat{U}_S(t_2,t_1)\,e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t_1} \quad (*)$$

Properties of time evolution operator:

1) $\hat{U}_S(t_1,t_1) = 1 \overset{(*)}{\Longrightarrow} \hat{U}_D(t_1,t_1) = 1$

2) Group property:



$$\hat{U}_S(t_3,t_1) = \hat{U}_S(t_3,t_2)\,\hat{U}_S(t_2,t_1) \qquad (**)$$

$$\hat{U}_D(t_3,t_1) \overset{(*)}{=} \boxed{e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t_3}}\,\underbrace{\hat{U}_S(t_3,t_1)}\,\boxed{e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t_1}}$$

$$\overset{(**)}{=} \boxed{\hat{U}_S(t_3,t_2)\,e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}}\,\boxed{e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}\,\hat{U}_S(t_2,t_1)}$$

$$\overset{(*)}{=} \hat{U}_D(t_3,t_2)\,\hat{U}_D(t_2,t_1) \quad \checkmark$$

3) $t_3 = t_1$: $\mathbb{1} \overset{1)}{=} \hat{U}_D(t_1,t_1) \overset{2)}{=} \hat{U}_D(t_1,t_2)\,\hat{U}_D(t_2,t_1)$

$$\Rightarrow \quad \hat{U}_D(t_1,t_2) = \hat{U}_D^{-1}(t_2,t_1)$$

4) $$\hat{U}_D^{+}(t_2,t_1) \overset{(*)}{=} e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t_1}\,\underbrace{\hat{U}_S^{+}(t_2,t_1)}_{=\hat{U}_S^{-1}(t_2,t_1) \overset{3)}{=} \hat{U}_S(t_1,t_2)}\,e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t_2} \overset{(*)}{=} \hat{U}_D(t_1,t_2) \overset{3)}{=} \hat{U}_D^{-1}(t_1,t_2)$$

assumption

$\Rightarrow$ $\hat{U}_D$ is unitary

5) $$i\hbar\frac{\partial}{\partial t_2}\hat{U}_D(t_2,t_1) \overset{(*)}{=} e^{\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}\left\{\cancel{-\hat{H}_S^{(0)}}\cancel{+\hat{H}_S^{(0)}}+\hat{H}_S^{(int)}(t)\right\}\hat{U}_S(t_2,t_1)\,e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t_1}$$

$$= e^{-\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}\,e^{+\frac{i}{\hbar}\hat{H}_S^{(0)}t_2}$$

$$= \hat{H}_D^{(int)}(t_2)\,\hat{U}_D(t_2,t_1)$$

- differential equation for $\hat{U}_D(t_2,t_1)$
- can be rewritten in terms of integral integral

$$\hat u_D^{(n+1)}(t_2,t_1) = \underbrace{1}_{\text{integration constant}} - \frac{i}{\hbar}\int_{t_1}^{t_2} dt_1'\, \hat H_D^{(int)}(t_1')\, \hat u_D^{(n)}(t_1',t_1)$$

$$\frac{d}{dx}\int_{a(x)}^{b(x)} dt\, f(t,x) = b'(x)\, f(b(x),x) - a'(x)\, f(a(x),x) + \int_{a(x)}^{b(x)} dt\, \frac{\partial f(t,x)}{\partial x}$$

Leibniz rule

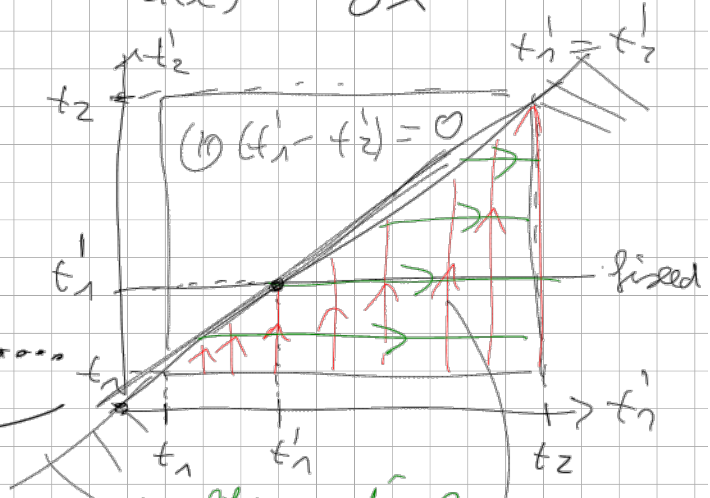
perturbative series for time evolution operators:

$$\hat u_D(t_2,t_1) = 1 - \frac{i}{\hbar}\int_{t_1}^{t_2} dt_1'\, \hat H_D^{(int)}(t_1') + \left(-\frac{i}{\hbar}\right)^2 \underbrace{\boxed{\int_{t_1}^{t_2} dt_1' \int_{t_1}^{t_1'} dt_2'\, \hat H_D^{(int)}(t_1')\, \hat H_D^{(int)}(t_2')}} + \dots$$

$$= \int_{t_1}^{t_2} dt_2' \int_{t_2'}^{t_2} dt_1'\, \hat H_D^{(int)}(t_1')\, \hat H_D^{(int)}(t_2')$$

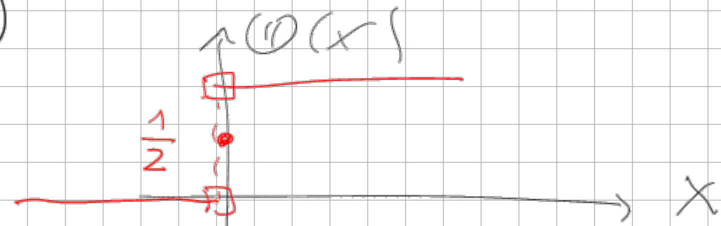
$t_1' \leftrightarrow t_2'$

$$= \int_{t_1}^{t_2} dt_1' \int_{t_1'}^{t_2} dt_2'\, \hat H_D^{(int)}(t_2')\, \hat H_D^{(int)}(t_1')$$



— : alternative

$\Theta(t_1' - t_2') = +1$



$$2\,\boxed{} = 1\,\boxed{} + 1\,\boxed{}$$

$$= \int_{t_1}^{t_2} dt_1' \int_{t_1}^{t_2} dt_2' \underbrace{\left\{ \Theta(t_1' - t_2')\, \hat H_D^{(int)}(t_1')\, \hat H_D^{(int)}(t_2') + \Theta(t_2' - t_1')\, \hat H_D^{(int)}(t_2')\, \hat H_D^{(int)}(t_1') \right\}}$$

$$=: \underbrace{\hat T}_{\text{time ordering operator}} \left(\hat H_D^{(int)}(t_1')\, \hat H_D^{(int)}(t_2) \right)$$

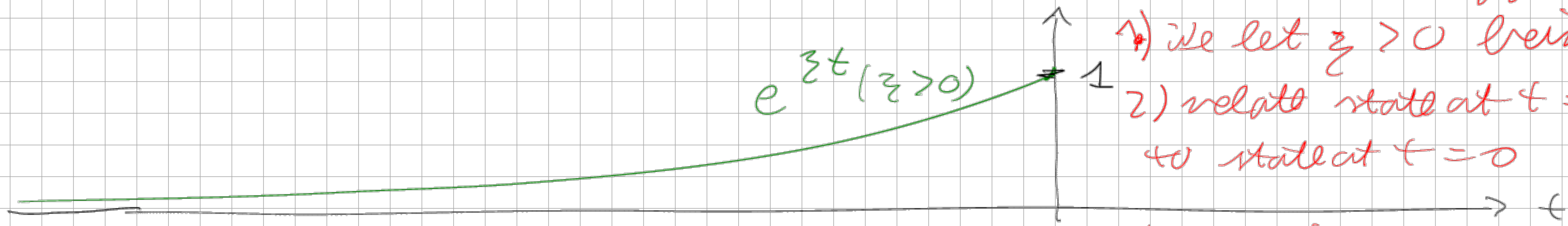
generalizable to any perturbative order:

$$\hat U_D(t_2,t_1) = \hat T\left[\exp\left\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt\, \hat H_D^{(int)}(t)\right\}\right]$$

Formal Scattering Theory

methodology:

1) we let $\xi > 0$ being finite
2) relate state at $t=-\infty$ to state at $t=0$
3) consider limit $\xi \downarrow 0$



$t \to -\infty$ $\hat H_0$

artificial time dependence due to switching on adiabatically the perturbation

$t \to 0$ $\underbrace{\hat H_0 + \hat V}_{\text{time independent}}$

$$\hat H_\xi(t) = \hat H_0 + \hat V e^{\xi t} \quad ; \quad \xi > 0 \quad ; \quad -\infty \le t \le 0$$

$$\lim_{t\to-\infty} \hat H_\xi(t) = \hat H_0 \qquad \lim_{t\to 0} \hat H_\xi(t) = \hat H_0 + \hat V$$

$$\hat H_\xi(t) = \hat H_\xi^{(0)} + \hat H_\xi^{(int)}(t)$$

$$|\Psi_D(t)\rangle = e^{\frac{i}{\hbar}\hat H_0 t}|\Psi_S(t)\rangle, \quad |\Psi_D(0)\rangle = |\Psi_S(0)\rangle = \underbrace{|\Psi\rangle}_{\text{after scattering}}$$

$$\hat V_D(t) = \hat H_D^{(int)}(t) = e^{\frac{i}{\hbar}\hat H_0 t}\, \hat V e^{\xi t}\, e^{-\frac{i}{\hbar}\hat H_0 t}$$

integral equation:

$$i\hbar \frac{\partial}{\partial t}|\Psi_D(t)\rangle = \hat H_D^{(int)}(t)\,|\Psi_D(t)\rangle$$

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

$t \to 0$, $t_0 = -\infty$

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

scattering problem

$$\hat{H}_0 |\phi\rangle = E\, |\phi\rangle, \quad E > 0 \qquad \hat{H}|\psi\rangle = E\,|\psi\rangle$$

initial state before scattering

final state after scattering

elastic scattering

free solution of unperturbed Schrödinger equation

plane wave

$$|\psi_D(t\to-\infty)\rangle = |\phi\rangle$$

adiabaticity parameter

$$|\psi_\xi\rangle = \hat{u}_D(0,-\infty)|\phi\rangle = |\phi\rangle - \frac{i}{\hbar}\int_{-\infty}^{0} dt\, e^{\frac{i}{\hbar}\hat{H}_0 t}\, \hat{V} e^{\xi t}\, \cancel{e^{-\frac{i}{\hbar}\hat{H}_0 t}}\, \underbrace{|\psi_D(t)\rangle}$$

$$\cancel{e^{\frac{i}{\hbar}\hat{H}_0 t}}\, |\psi_S(t)\rangle$$

$$\underbrace{e^{-\frac{i}{\hbar}Et}\, |\psi_S(0)\rangle}_{=|\psi\rangle}$$

Now: $\xi \downarrow 0$

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

$$\lim_{\xi\downarrow 0}\int_{-\infty}^{0} dt\, e^{\frac{i}{\hbar}(\hat{H}_0 - E - i\hbar\xi)t}\, \hat{V}\, |\psi\rangle \qquad (\xi > 0)$$

adiabaticity parameter = convergence factor

$$|\psi\rangle = |\phi\rangle - \frac{i}{\hbar} \lim_{\varepsilon \downarrow 0} \underbrace{\left. \frac{e^{\frac{i}{\hbar}(\hat{H}_0 - E - i\varepsilon\hbar)t}}{\frac{i}{\hbar}(\hat{H}_0 - E - i\varepsilon\hbar)} \right|_{-\infty}^{0}}_{\frac{1}{\frac{i}{\hbar}(\hat{H}_0 - E - i\varepsilon\hbar)}} \hat{V} |\psi\rangle$$

$$|\psi\rangle = |\phi\rangle + \underline{\lim_{\varepsilon \to 0}} \frac{-1}{\hat{H}_0 - E \boxed{- i\varepsilon\hbar}} \hat{V} |\psi\rangle$$

Lippmann-Schwinger equation

scattering state