# Greens Functions, Propagators, and Time Evolution

Time evolution as operator:

$$i\hbar \frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle \;\rightarrow |\psi(t_0+dt)\rangle = \left(\mathbb{1} - \frac{i}{\hbar} H\,dt\right)|\psi(t_0)\rangle$$

$$\rightarrow |\psi(t_0+\tau)\rangle = \underbrace{\left(\mathbb{1} - \frac{i}{\hbar}H\,dt\right)^{\tau/dt}}_{\left(e^{-iH\,dt/\hbar}\right)^{\tau/dt}} |\psi(t_0)\rangle$$

$$= e^{-iH\tau/\hbar}\,|\psi(t_0)\rangle$$

<u>Time evolution operator</u>

$$U(\tau) = e^{-\frac{i}{\hbar}H\tau}$$

"$U$" because unitary: $U(\tau)\underbrace{U^{+}(\tau)}_{U(-\tau)} = \mathbb{1}$

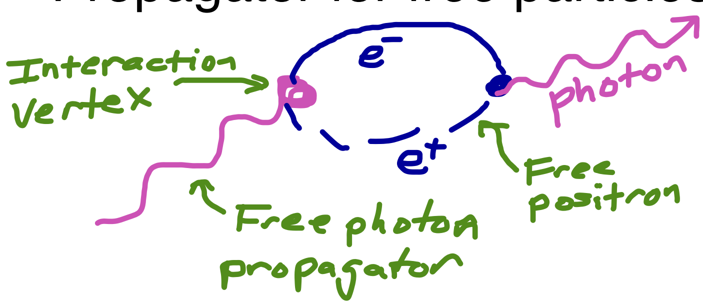
<u>Propagator</u> $\equiv$ <u>Greens Function</u>

$$K(x'',t'';x',t') = \langle x'',t''|x',t'\rangle = \langle x''|U(t''-t')|x'\rangle$$

$$= \langle x''|e^{-iH(t''-t')/\hbar}|x'\rangle$$

- $|x\rangle$-basis version of $U(\tau)$
- Time evolution of initial state $\delta(x-x')$ for time $t''-t'$
  $\psi(x'',t'') = K(x'',t'';x',t')$
  - Satisfies Schrödinger
  - $\psi(x',t') = \langle x''|x'\rangle = \delta(x''-x')$
- Not easy to calculate for interacting systems
- Calculated by Path Integrals (next)

Propagator for free particles is basis for Feynman diagrams




$$H = \underbrace{H_0}_{\text{Free Particles}} + \underbrace{H_1}_{\text{Interactions}}$$

## Free particle propagator, one dimension

$$H = \frac{p^2}{2m}$$

$$\langle x'' | \mathbb{1} e^{-iH(t''-t')/\hbar} \mathbb{1} | x' \rangle$$

$\mathbb{1} = \int |p\rangle\langle p|\, dp$ twice

$$= \int dp\, \langle x'' | p \rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t''-t')} \langle p | x' \rangle$$

$\leftarrow p' = p$

$$= \int dp\, \frac{e^{ipx''/\hbar}}{\sqrt{2\pi\hbar}} e^{-ip^2/2m\hbar\,(t''-t')} e^{-ipx'/\hbar}/\sqrt{2\pi\hbar}$$

Exercise 2.2b

$\langle x | k \rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$

$\rightarrow \langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$

since $p = \hbar k$

$\langle p' | p \rangle = \delta(p'-p)$

$= \frac{\delta(k'-k)}{\hbar} = \frac{\langle k' | k \rangle}{\hbar}$

$$= \frac{1}{2\pi\hbar} \int dp\, \exp \underbrace{\left[ -i \frac{(t''-t')}{2m\hbar} p^2 + \frac{i(x''-x')}{\hbar} p \right]}$$

complete square: $Ap^2 + Bp = A\left(p^2 + \frac{B}{2A}\right)^2 - \frac{B^2}{4A}$

$$= \frac{1}{2\pi\hbar} e^{-\left(\frac{i(x''-x')}{\hbar}\right)^2 / 4\left(-\frac{i(t''-t')}{2m\hbar}\right)} \int_{-\infty}^{\infty} dp\, \underbrace{e^{-i\frac{(t''-t')}{2m\hbar}\left[p - \frac{(x''-x)}{\hbar} / 2\left(\frac{t''-t'}{2m\hbar}\right)\right]^2}}_{\text{Gaussian}}$$

$\bullet \bullet \bullet$

$$= \sqrt{\frac{m}{2\pi i\hbar(t''-t')}} \exp\left[\frac{im(x''-x')^2}{2\hbar(t''-t')}\right]$$

## Simple Harmonic Oscillator

$$K(x'', t''; x', t') = \sqrt{\frac{m\omega}{2\pi\hbar \sin(\omega(t''-t'))}} \exp\left[\frac{im\omega}{2\hbar \sin(\omega(t''-t'))} * \left\{ (x''^2 + x'^2)\cos(\omega(t''-t')) - 2x''x' \right\}\right]$$

* Feynman's PhD thesis: from path integrals

# Gaussian Integrals and Cauchy's Theorem

$$\int_{-\infty}^{\infty} \exp(-x^2/2) = \sqrt{2\pi}$$

$$\left(\int e^{-x^2/2}dx\right)\left(\int e^{-y^2/2}dy\right) = \int dx\, dy\; e^{-(x^2+y^2)/2} = \int_0^\infty 2\pi r\, dr\; e^{-r^2/2}$$
$$= -2\pi e^{-r^2}\Big|_0^\infty = 2\pi$$

$$\int_{-\infty}^{\infty} e^{-Ax^2}dx = \sqrt{\frac{\pi}{A}} \qquad y = \sqrt{A}\,x, \quad dx = dy/\sqrt{A}$$

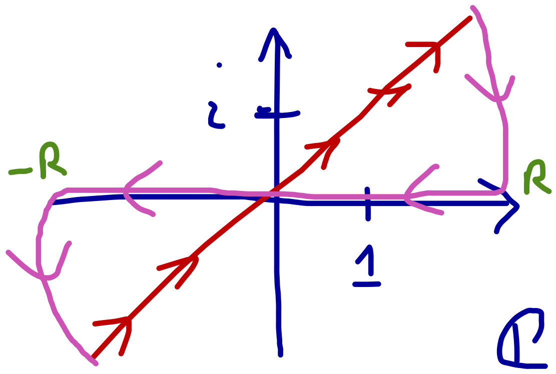
$$\int_{-\infty}^{\infty} x e^{-Ax^2} dx = 0 \qquad \int_{-\infty}^{\infty} x^2 e^{-Ax^2} dx = -\frac{d}{dA}\left(\int e^{-Ax^2}\right) = \frac{1}{2}\sqrt{\frac{\pi}{A^3}}$$
odd

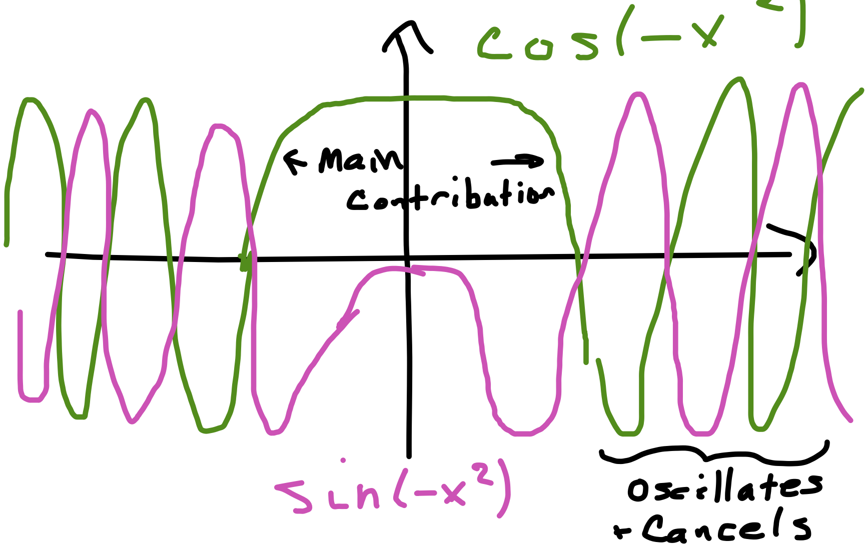
$$\int_{-\infty}^{\infty} e^{-(Ax^2+Bx)} dx = \sqrt{\frac{\pi}{A}}\; e^{B^2/4A}$$
$$= e^{-A(x+\frac{B}{2A})^2}\, e^{B^2/4A}$$, completing the square

$$\int_{-\infty}^{\infty} e^{-iAx^2}dx = \int_{-\sqrt{i}\infty}^{\sqrt{i}\infty} e^{-Az^2}\frac{dz}{\sqrt{i}} = \sqrt{\frac{\pi}{iA}}$$

Seems easy? $z = \sqrt{i}\,x$, $\frac{dz}{\sqrt{i}} = dx$, same formula $A \to iA$?

Path in $\mathbb{C}$




Cauchy's Theorem: Integral around closed loop in complex plane zero if no singularities inside. (Exercise?)
Close the contour. Real axis = diagonal plus arcs; check arcs go to zero at large |x|.

More info on propagators:

* Like free propagator expand in 1 = sum Ip><pl, expand in sum IE><El:

$$K(x'', t; x, 0) = \langle x'' | \mathbb{1}\, e^{-iHt/\hbar}\, \mathbb{1} | x' \rangle$$
$$= \sum_{\alpha,\beta} \langle x'' | E_\alpha \rangle \underbrace{\langle E_\alpha | e^{-iHt/\hbar} | E_\beta \rangle}_{e^{iE_\alpha t/\hbar}\ \delta_{\alpha\beta}} \langle E_\beta | x \rangle$$
$$= \sum_\alpha \langle x'' | E_\alpha \rangle \langle E_\alpha | x \rangle e^{-iE_\alpha t/\hbar}$$

* Advisor (PW Anderson) wrote:
  Green's function solves (E-H) G = delta(x'', x') = "1"
  => G = 1/(E-H)

Write $G(E, x'', x') =$ 'positive time' Fourier transform

$$= -i \int_0^\infty \frac{dt}{\hbar}\, e^{i(E+i\varepsilon)t/\hbar} \underbrace{K(x'', t; x', 0)}_{\sum_\alpha \langle x'' | E_\alpha \rangle e^{-iE_\alpha t/\hbar} \langle E_\alpha | x \rangle}$$

$$-i \int_0^\infty \frac{dt}{\hbar}\, e^{i(E-E_\alpha)t/\hbar}\, e^{-\varepsilon t/\hbar}$$
$$= \frac{1}{E - E_\alpha + i\varepsilon}$$

$$= \sum_\alpha \frac{\langle x'' | E_\alpha \rangle \langle E_\alpha | x' \rangle}{E - E_\alpha + i\varepsilon}$$
$$= \langle x'' | G(E) | x' \rangle$$

$$G(E) = \sum_\alpha \frac{|E_\alpha\rangle \langle E_\alpha|}{E - E_\alpha + i\varepsilon} = \frac{1}{E - H + i\varepsilon}$$

making sense of his terse derivation!

Notice: $Tr(G(E)) = \int \langle x|G|x\rangle dx = \int K(E,x,x)\,dx$

$$= \sum_\alpha \int \frac{\langle x|E_\alpha\rangle\langle E_\alpha|x\rangle dx}{E-E_\alpha+i\varepsilon} \quad = \int |\psi|^2 = 1$$

$$= \sum_\alpha \frac{1}{E-E_\alpha+i\varepsilon}$$

or even easier ($Tr_x = Tr_\alpha$):

$$Tr(G(E)) = \sum_\beta \sum_\alpha \frac{\langle E_\beta|E_\alpha\rangle\langle E_\alpha|E_\beta\rangle}{E-E_\alpha+i\varepsilon} = \sum_\alpha \frac{1}{E-E_\alpha+i\varepsilon}$$

Now, exercise 2.2(c): $\frac{1}{x-i\varepsilon} = P.V.\frac{1}{x} + i\pi\,\delta(x)$

$$Im\left(\frac{1}{E-E_\alpha+i\varepsilon}\right) = -\pi\,\delta(E-E_\alpha)$$

$$-\frac{1}{\pi} Im(Tr(G(E))) = \sum_\alpha \delta(E-E_\alpha) = \text{Density of States}$$

$\rightarrow$ Specific Heat, Excitations, ...

Note: $G(E)$ knows all eigenvalues of $H$ and all eigenfunctions $\psi_\alpha$

$$G(E,x'',x') = \langle x''|G(E)|x'\rangle = \sum_\alpha \frac{\langle x''|E_\alpha\rangle\langle E_\alpha|x'\rangle}{E-E_\alpha+i\varepsilon} \quad \begin{matrix} \} \text{ Residue} \\ \} \text{ Pole at } E_\alpha - i\varepsilon \end{matrix}$$

$$\text{Residue} = \langle x''|E_\alpha\rangle\langle E_\alpha|x'\rangle$$
$$= \psi_\alpha(x'')\,\psi_\alpha^*(x')$$

(determines $\psi_\alpha$ up to phase)

Also: Local density of states

$$g(E|x) = \sum |\psi_\alpha(x)|^2\,\delta(E-E_\alpha)$$
$$= -\frac{1}{\pi} Im\, G(E,x,x)$$

# Brief peek at Feynman diagrams & Dyson eqn

$$H = \underbrace{H_0}_{\text{Free Particles}} + \underbrace{I}_{\text{Interactions (small)}}$$

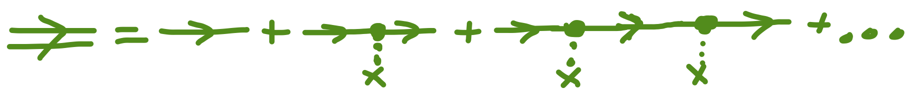
$G_0 = \dfrac{1}{E - H_0}$ known

Taylor expand $G = \dfrac{1}{E - H_0 - I} = G_0 + \dots$

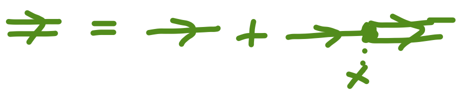
How to Taylor expand? Matrices don't commute?

Claim:

$$G = G_0 + G_0 I G_0 + G_0 I G_0 I G_0 + \dots$$ (Feynman)



$$G = G_0 + G_0 I G$$ (Dyson)



Check: $GG^{-1} = G(E - H_0 - I)$

$$= (G_0 + G_0 I G)(E - H_0 - I)$$

$$= \left(\frac{1}{E - H_0} + \frac{1}{E - H_0} I \frac{1}{E - H_0 - I}\right)(E - H_0 - I)$$

$$= \frac{E - H_0 - I}{E - H_0} + \frac{I}{E - H_0} = \mathbb{1} \checkmark$$