~~Sat~~ Greens Functions, Propagators, and Time Evolution

Sakurai ~~p~~ 2.6 p.116-122
P.W. Anderson, Basic Notions of Condensed Matter Physics, p.108

Time evolution as operator:

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

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

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

Time evolution operator

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

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

$$\langle x''|U(t''-t')|x'\rangle = \underbrace{\langle x''|e^{-iHt''/\hbar}\, e^{iHt'/\hbar}|x'\rangle}$$

wrong way in time?

Propagator ≡ Greens Function Bad Notation

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

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

No

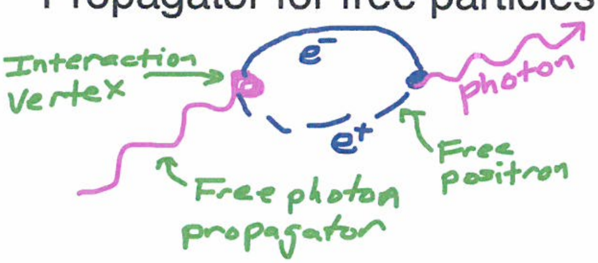
$\langle x''|E_n\rangle = \psi(x)$

$\underbrace{\langle E_n|x'\rangle = \psi^*(x')}$

evolves w $e^{iEt/\hbar}$

- $|x\rangle$-basis version of $U(\tau)$
- Time evolution of initial state $\delta(x-x')$ for time $t''-t'$
  $\psi(x'',t'') = K(x'',t'';x',t')$ [Add]
  - Satisfies Schrödinger
  - ~~$\psi(x'',t'') = \langle x''|x'\rangle = \delta(x''-x')$~~ Can be integrated to solve Schrödinger [Add]
- 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

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

$$\langle x'' | e^{-iH(t''-t')/\hbar} | x' \rangle \qquad 1 = \int dp \, |p\rangle\langle p|$$

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

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

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

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

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

$$\cdots$$

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

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 $p = \hbar k$

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

Simple Harmonic Oscillator

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

* Feynman's PhD thesis: from path integrals

Feynman's thesis centered around propagator for the <u>forced</u> harmonic oscillator

$$\mathcal{L}(t) = \frac{1}{2}\left(m\dot{\cancel{x}}^2 + \frac{1}{2} m\omega^2 \cancel{x}^2\right) - f(t)\, q$$

going from $\cancel{x} = a$ at t_a to $\cancel{x} = b$ at t_b,

$$K(b, t_b; a, t_a) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin\omega t}}\; e^{-\frac{i}{\hbar} S_{cl}(b,a)}$$

$S_{cl}(b,a)$ = <u>Classical</u> action for going from $a, t_a \to b, t_b$

$$= \frac{m\omega}{\sin\omega t}\Big\{ \frac{1}{2}\left(x_a^2 + x_b^2\right)\cos\omega T - x_b x_a$$

$$+ \frac{x_a}{m\omega}\int_{t_a}^{t_b} dt\, f(t) \sin\omega(t_b - t)$$

$$+ \frac{x_b}{m\omega}\int_{t_a}^{t_b} dt\, f(t) \sin\omega(t - t_a)$$

$$- \frac{1}{m^2\omega^2}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} ds\, f(t) f(s) \sin\omega(t_b - t)\, \sin\omega(s - t_a)\Big\}$$

<u>This</u> was the formula I integrated by parts (twice), and convolved with Gaussian ground states at x_a, t_a & x_b, t_b.

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

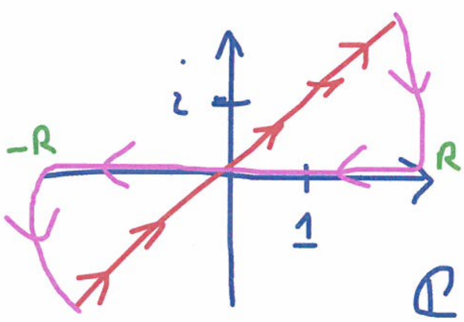
$$\int_{-\infty}^{\infty} e^{-(Ax^2+Bx)}dx = \sqrt{\frac{\pi}{A}}\; e^{-B^2/4A}$$

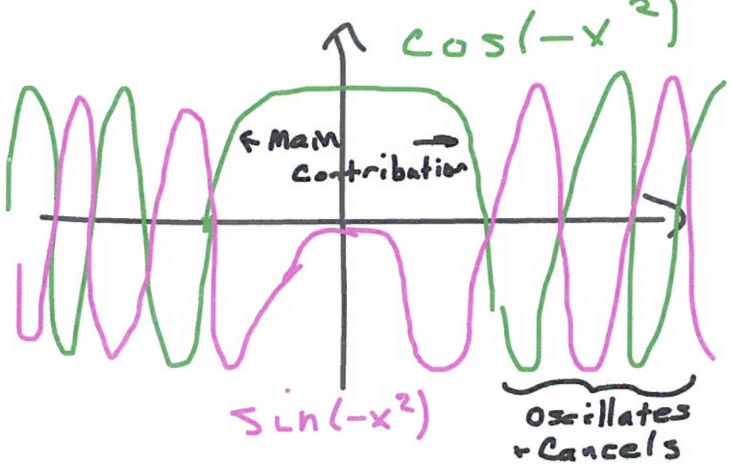
$$e^{-A\left(x+\frac{B}{2A}\right)^2} e^{-B^2/4A}, \quad \text{completing the square}$$

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

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|.

Warning! $\int_{-\infty}^{\infty} x^2 e^{-iAx^2}dx$ arcs don't go to zero! Small negative imaginary part to A.

More info on propagators:

* Like free propagator expand in 1 = sum |p><p|, expand in sum |E><E|:

$$K(x'', t; x, 0) = \langle x''|\, e^{-iHt/\hbar}\, \mathbb{1}\, |x'\rangle$$

$$= \sum_{\alpha,\beta} \langle x''|E_\alpha\rangle \underbrace{\langle E_\alpha| e^{-iHt/\hbar} |E_\beta\rangle}_{e^{iE_\alpha t/\hbar}\ \delta_{\alpha\beta}} \langle E_\beta|x\rangle$$

$$= \sum_\alpha \langle x''|E_\alpha\rangle\langle E_\alpha|x\rangle e^{-iE_\alpha t/\hbar} = \sum_\alpha \psi_\alpha(x'')\psi_\alpha^*(x)\, e^{-iE_\alpha t/\hbar}$$

Basic Notions of Condensed Matter Physics p. 108)

* 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: $\mathrm{Tr}(G(E)) = \int \langle x|G|x\rangle dx = \int K(E,x,x)\,dx$

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

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

or even easier ($\mathrm{Tr}_x = \mathrm{Tr}_\alpha$):

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

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

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

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

→ Specific Heat, Excitations, ...

Note: $G(E)$ knows all eigenvalues of H and all eigenfunctions ψ_α

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

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

(determines ψ_α up to phase)

Also: <u>Local</u> density of states

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

* Used for STM, etc. $\quad G(x',x) = \langle a(x')a^\dagger(x)\rangle$
* Green's fcts deal collectively w/ eigenstates
* Greens fcts deal w/ many body $\langle \mathrm{Soup}|a(x')a^\dagger(x)|\mathrm{Soup}\rangle$

Brief peek at Feynman diagrams & Dyson eqn

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

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

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

How to Taylor expand? Matrices don't commute?

Claim: $G_0 + G_0 I (G_0 + G_0 I G_0 + \dots)$

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

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

$\frac{1}{1-\delta} = 1 + \delta + \delta^2 + \delta^3 + \dots$

$\frac{1}{x - \delta} = \frac{1}{x}\left(\frac{1}{1 - \delta/x}\right)$

$= \frac{1}{x}\left(1 + \frac{\delta}{x} + \frac{\delta^2}{x^2} + \dots\right)$

$\delta \Leftrightarrow I$

$x \Rightarrow E - H_0 + i\epsilon$

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

Dysonvers

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

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

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

Does $(E - H_0)^{-1}(E - H_0 - I)$

non-commuting