Many-Body Theory SoSe 2011 Jan von Delft $\boxed{GF1}$

Green's Functions – Formalism

Q: Why study GF? (Rickayzen, Ch. 1)

A: GF is response to a perturbation – contains information about dynamics of system

1. Oldest example (George Green)

Electrostatics: what is general solution to Poisson-Eq?

$$\nabla^2 \phi(\vec{r}) = -\frac{\rho(\vec{r})}{\varepsilon_0} \quad (1)$$

Let $G(\vec{r}-\vec{r}\,')$ be solution of

$$\underbrace{\nabla^2 G(\vec{r}-\vec{r}\,')}_{\text{response at } \vec{r}} = - \underbrace{\frac{\delta(\vec{r}-\vec{r}\,')}{\varepsilon_0}}_{\text{perturbation at } \vec{r}\,'} \quad (2)$$

$\boxed{GF2}$

Solution to (1.1): $$\phi(\vec{r}) = \int d\vec{r}\,' \, G(\vec{r}-\vec{r}\,')\rho(\vec{r}\,') \quad (1)$$

Check: $$\nabla^2 \phi(\vec{r}) \overset{(1.2)}{=} \int d\vec{r}\,' \left(-\frac{\delta(\vec{r}-\vec{r}\,')}{\varepsilon_0}\right)\rho(\vec{r}\,') \quad (2)$$

$$= -\frac{\rho(\vec{r})}{\varepsilon_0} = (1.1) \checkmark \quad (3)$$

Knowledge of GF $\Rightarrow$ solution of diff. eq.

What is GF for (1.2)? Fourier-transformation shows:

$$\tilde{G}(\vec{k}) = \frac{1}{\varepsilon_0 k^2} \implies G(\vec{r}-\vec{r}\,') = \frac{1}{4\pi\varepsilon_0|\vec{r}-\vec{r}\,'|} \quad (4)$$

2. Example: Kubo Formula for linear response of a quantum system

GF3

Consider $\hat{H} = \underbrace{\hat{H}_0}_{\text{"simple"}} + \underbrace{\hat{H}_1}_{\text{"perturbation"}}$ (1)

Kubo formula for response of an expectation value to perturbation

(proof: later) $\langle \hat{A} \rangle = \langle \hat{A} \rangle_0 + \delta\langle \hat{A} \rangle$ (2)

operators in interaction representation

commutator

$$\delta\langle \hat{A}(t)\rangle \overset{\text{Kubo}}{=} \int_{t_0}^{\infty} dt' \underbrace{\left(-i/\hbar\right)\theta(t-t')\left\langle\left[\hat{A}(t), \hat{H}_1(t')\right]\right\rangle}_{\mathcal{G}^R(t,t') \, = \, \text{"retarded GF"}} \quad (3)$$

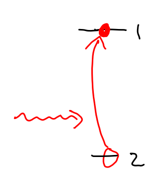
thermal exp. value

3. Energy absorption rate

GF4

Suppose $\hat{H}' = e^{i\omega t}\hat{X}^\dagger + e^{-i\omega t}\hat{X}$ (1)

$X^\dagger = \underbrace{c_1^\dagger c_2}_{\text{operator}} \underbrace{A(\omega)}_{\text{"c-number"}}$



Absorption rate by golden rule:

$$w_{n\leftarrow m} = \frac{2\pi}{\hbar} \left|\langle n|\hat{X}^\dagger|m\rangle\right|^2 \delta\left(\hbar\omega - (E_n - E_m)\right) \quad (2)$$

(3)

with $\hat{H}_0|n\rangle = E_n|n\rangle$ a complete set of many-body eigenstates.

For total absorption rate, average over initial states, sum over final states:

partition function

Boltzmann factor

$$W(\omega) = \frac{2\pi}{\hbar Z} \sum_{m,n} e^{-\beta E_m} \left|\langle n| X^\dagger |m\rangle\right|^2 \frac{1}{\hbar}\delta\left[\omega - (E_n - E_m)/\hbar\right] \quad (4)$$

$$W(\omega) = \frac{2\pi}{\hbar Z} \sum_{nm} e^{-\beta E_m} \langle m|\hat{X}|n\rangle \int \frac{dt}{2\pi\hbar} e^{i\left[\omega - \frac{E_n}{\hbar} + \frac{E_m}{\hbar}\right]t} \langle n|\hat{X}^\dagger|m\rangle \qquad \boxed{GF5} \tag{5}$$

$$= \frac{2\pi}{\hbar Z} \sum_m e^{-\beta E_m} \int \frac{dt}{2\pi\hbar} e^{i\omega t} \langle m| \underbrace{e^{iHt/\hbar}\, \hat{X}\, e^{-iHt/\hbar}}_{\hat{X}(t)} |n\rangle\langle n| \underbrace{\hat{X}^\dagger}_{\hat{X}^\dagger(0)} |m\rangle \tag{6}$$

Heisenberg pict.

$\mathbb{1} = \sum_n |n\rangle\langle n|$

$$= \frac{2\pi}{\hbar} \int \frac{dt}{2\pi\hbar} e^{i\omega t} \underbrace{\frac{1}{Z}\sum_m e^{-\beta E_m} \langle m|\hat{X}(t)\,\hat{X}^\dagger(0)|m\rangle}_{\hbar i \mathcal{G}^>_{XX}(t) \equiv \langle \hat{X}(t)\hat{X}^\dagger(0)\rangle_T} \tag{7}$$

thermal exp. value

$$= \frac{2\pi}{\hbar} \int \frac{dt}{2\pi}\, i\, \mathcal{G}^>_{XX}(t) = \frac{2\pi}{\hbar}\, i\, \mathcal{G}^>_{XX}(\omega) \tag{8}$$

This is a different type of GF than the retarded one of (3.3), but they are related to each other. It will be useful to develop such relations in great generality.

$\boxed{GF6}$

Green's functions are very useful objects.
- They represenent relevant information about dynamics in a <u>compact</u> form.
- "Overly detailed information", such as the specific form of all eigenstates and specific values of eigenenergies, are not needed or computed.

It will be very useful to develop systematic methods for
- expressing observables (like current, absorption rate) i.t.o. GFs
- computing GFs (e.g. by perturbation theory in small parameter, or numerically)
- relating various types of GFs to each other,
- expressing complicated GFs in terms of simpler ones,
- ...

Review of some basics

GF7

Thermal expectation value

$$\langle \hat{A} \rangle = \mathrm{Tr}\left[\hat{\rho}\,\hat{A}\right] = \sum_n \langle n|\,\hat{\rho}\,\hat{A}\,|n\rangle \qquad (1)$$

complete orthonormal basis: $\mathbb{1} = |n\rangle\langle n|$

Density matrix: $$\hat{\rho} = \begin{cases} \frac{1}{Z}\, e^{-\beta \hat{H}} & \text{(canonical)} \quad (2) \\ \frac{1}{Z}\, e^{-\beta(\hat{H}-\mu\hat{N})} & \text{(grand-canonical)} \quad (3) \end{cases}$$

$$\beta = \frac{1}{k_B T}, \qquad Z = \mathrm{Tr}\,\hat{\rho} = \begin{cases} \sum_n e^{-\beta E_n} & (4) \\ \sum_n e^{-\beta(E_n-\mu N_n)} & (5) \end{cases}$$

$$\langle \hat{A} \rangle = \frac{\sum_n e^{-\beta(E_n-\mu N_n)}\,\langle n|\hat{A}|n\rangle}{\sum_n e^{-\beta(E_n-\mu N_n)}}$$

Schrödinger, Heisenberg, Interaction pictures (Messiah, Ch. 8)

GF8

There are several equivalent ways of representing expectation values:

quantum time evolution

$$\bar{A}(t) = \langle \psi_s(t_0)|\, U^{\dagger}(t,t_0)\, \hat{A}_s(t)\, \hat{U}(t,t_0)\, |\psi_s(t_0)\rangle \qquad (1)$$

explicit or external time dependence [eg. velocity operator : $\hat{v}(t) = \frac{1}{m}\left[-i\hbar\vec{\nabla} - e\vec{A}(t)\right]$]

vector potential

quantum time evolution can be encoded in:

(i) $|\psi\rangle \Rightarrow$ Schrödinger picture : $|\psi_S(t)\rangle = \hat{U}(t,t_0)\,|\psi_s(t_0)\rangle \qquad (2)$

or

(ii) $\hat{A} \Rightarrow$ Heisenberg picture $\quad \hat{A}_H(t) = \hat{U}^{\dagger}(t,t_0)\,\hat{A}_s(t)\,\hat{U}(t,t_0) \qquad (3)$

or

(iii) both $\Rightarrow$ interaction picture

$$\begin{cases} |\psi_I(t)\rangle = \hat{U}_I(t,t_0)\,|\psi_s(t_0)\rangle & (4) \\ \hat{A}_I(t) = e^{i\hat{H}_0(t-t_0)}\,\hat{A}_s(t)\,e^{-i\hat{H}_0(t-t_0)} & (5) \end{cases}$$

Here: $\hat{U}(t,t_0)$ = time-evolution operator; satisfies $\boxed{GF9}$

- group properties: $\hat{U}(t,t) = \mathbb{1} \quad \forall\, t$ (1)

$$\hat{U}(t,t'')\hat{U}(t'',t') = \hat{U}(t,t') \quad \forall\, t, t', t'' \qquad (2)$$

$$t = t' \overset{(2)}{\Longrightarrow} U(t,t'')\,\hat{U}(t'',t) \overset{(1)}{=} \mathbb{1} \Longrightarrow \hat{U}(t'',t) = \hat{U}^{-1}(t,t'') \qquad (3)$$

- unitarity: $\hat{U}^{\dagger}(t,t') = \hat{U}^{-1}(t,t') \overset{(3)}{=} \hat{U}(t',t)$ (4)

Schrödinger eq: completely general ($\hat{H}_s$ could contain explicit time-dependence, as in (4.1))

$$i\hbar\, \partial_t \hat{U}(t,t') = \hat{H}_s(t)\, U(t,t') \qquad (5a)$$

$$(5a)^{\dagger} \qquad -i\hbar\, \partial_t \hat{U}^{\dagger}(t,t') = U^{\dagger}(t,t')\,\hat{H}_s(t) \qquad (5b)$$

Solution for time-independent Hamiltonian:

$$\hat{H} \equiv \hat{H}_s \neq \hat{H}_s(t) \qquad \hat{U}(t,t') = e^{-i\hat{H}(t-t')/\hbar} \qquad (6)$$

(i) Schrödinger picture: $\boxed{GF10}$

$$\bar{A}(t) \overset{(8.1)}{=} \langle\psi(t_0)|\, U^{\dagger}(t,t_0)\,\hat{A}_s(t)\,\hat{U}(t,t_0)\,|\psi(t_0)\rangle \overset{(2)}{=} \langle\psi_s(t)|\,\hat{A}_s(t)\,|\psi_s(t)\rangle \qquad (1)$$

where $|\psi_s(t)\rangle = U(t,t_0)\,|\psi_s(t_0)\rangle$ (2)

$\hat{A}_s(t)$ has no quantum time evolution. If it also has no external time evolution, $\hat{A}_s \neq \hat{A}_s(t)$, then $\hat{A}_s$ is fully time-independent

(ii) Heisenberg picture:

$$\bar{A}(t) \overset{(8.1)}{=} \langle\psi(t_0)|\, U^{\dagger}(t,t_0)\,\hat{A}_s(t)\,\hat{U}(t,t_0)\,|\psi(t_0)\rangle = \langle\psi_H|\,\hat{A}_H(t)\,|\psi_H\rangle \qquad (3)$$

where $\hat{A}_H(t) = \hat{U}^{\dagger}(t,t_0)\,\hat{A}_s(t)\,\hat{U}(t,t_0)$, $\quad |\psi_H\rangle = |\psi_s(t_0)\rangle$ (4)

Heisenberg eq: $\boxed{\text{GF11}}$

$$i\hbar \frac{d}{dt}\hat{A}_H(t) = \hat{U}^{\dagger}(t,t_0)\Big[\hat{A}(t,t_0)\overset{(5a)}{\hat{H}(t)} - \overset{(5b)}{\hat{H}(t)\hat{A}_s(t)} + \underbrace{\frac{\partial}{\partial t}\hat{A}_s(t)}_{\equiv(\partial_t\hat{A})_s(t)}\Big]\hat{U}(t,t_0) \tag{1}$$

$U(t,t_0)\,U^{\dagger}(t,t_0)$ $\qquad$ $U(t,t_0)\,U^{\dagger}(t,t_0)$

$$= \left[\hat{A}_H(t), \hat{H}_H(t)\right] + (\partial_t\hat{A})_H(t) \tag{2}$$

If in Schrödinger picture $\hat{H}_s$ has no explicit t-dependence, $\hat{H}_s \neq \hat{H}(t)$

then (9.6) holds, hence

$$\hat{A}_H(t) \overset{(10.4)}{=} e^{i\hat{H}(t-t_0)/\hbar}\,\hat{A}_s(t)\,e^{-i\hat{H}(t-t_0)/\hbar} \tag{3}$$

(iii) Interaction picture: $\boxed{\text{GF12}}$

Useful if $\quad \hat{H}_s(t) = \hat{H}_0 + \hat{H}'(t)$ $\quad$ time dependence possible (but not necessary) $\qquad$ (1)

$\hat{H}_0$: time-independent

then, construct representation where $\hat{H}_0$ governs quantum time evolution of operators

$\hat{H}_1(t)$ " " " " " states:

$$\bar{A}(t) \overset{(8.1)}{=} \langle\psi_s(t_0)|\underbrace{U^{\dagger}(t,t_0)\,e^{-i\hat{H}_0(t-t_0)}}\;\underbrace{e^{+i\hat{H}(t-t_0)}\hat{A}_s(t)\,e^{-i\hat{H}_0(t-t_0)}}\;\underbrace{e^{+i\hat{H}_0(t-t_0)}\hat{U}(t,t_0)}|\psi_s(t_0)\rangle \tag{2}$$

$$\equiv \underbrace{\langle\psi_s(t_0)|\hat{U}_I^{\dagger}(t,t_0)}_{\langle\psi_I(t)|}\;\hat{A}_I(t)\;\underbrace{\hat{U}_I(t,t_0)|\psi_s(t_0)\rangle}_{|\psi_I(t)\rangle}$$

Define:
$$\hat{A}_I(t) \equiv e^{i\hat{H}_0(t-t_0)/\hbar}\,\hat{A}_s(t)\,e^{-i\hat{H}_0(t-t_0)/\hbar} \tag{3}$$

$\Rightarrow$
$$\hat{U}_I(t) \equiv e^{i\hat{H}_0(t-t_0)/\hbar}\,\hat{U}(t,t_0) \tag{4}$$

$$|\psi_I(t)\rangle \equiv \hat{U}_I(t,t_0)\,|\psi_s(t_0)\rangle \tag{5}$$

Eq. of motion for $\mathcal{U}_I$: $\boxed{\text{GF13}}$

$$i\hbar \frac{\partial}{\partial t}\hat{\mathcal{U}}_I(t,t_0) \overset{(12.4)}{=} \underbrace{e^{i\hat H_0(t-t_0)/\hbar}\big[\underbrace{-\hat H_0 + \hat H_S(t)}_{(12.1)\ \hat H'(t)}\big]\, e^{-i\hat H_0(t-t_0)}}_{(12.3)\ \hat H_I'(t)}\ \overset{(9.5a)}{}\underbrace{e^{i\hat H_0(t-t_0)}\ \hat{\mathcal{U}}(t,t_0)}_{(12.4)\ \hat{\mathcal{U}}_I(t,t_0)} \qquad (1)$$

$$= \hat H_I'(t)\ \hat{\mathcal{U}}_I(t,t_0) \qquad (2)$$

Solution (by inspection) note: $t_1 \geq t_2 \geq \dots \geq t_{n-1} \geq t_n$ (3)

$$\hat{\mathcal{U}}_I(t,t_0) = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n\ \hat H_I'(t_1)\,\hat H_I'(t_2)\dots \hat H_I'(t_n) \qquad (4)$$

include all possible time orders, and compensate

$$= \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \dots \int_{t_0}^{t} dt_n\ \mathcal{T}\left[\hat H_I'(t_1)\,\hat H_I'(t_2)\dots \hat H_I'(t_n)\right] \qquad (5)$$

↑ time-ordering operator: orders operators in order of decreasing times, as in (3)

$$\equiv \mathcal{T}\, e^{-i/\hbar \int_{t_0}^{t} dt'\, H_I'(t')} \qquad (6)$$

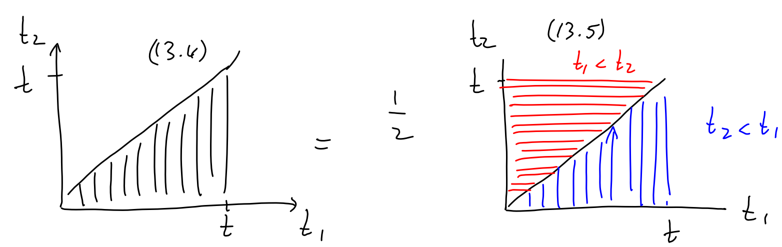
↳ "time-ordered exponential"

THIS IS COMMON STARTING POINT FOR PERTURBATION THEORY IN H_I

$\boxed{\text{GF14}}$

$n = 2$:

$(t_0 = 0)$



$$\mathcal{T}\left[\hat H_I'(t_1)\,\hat H_I'(t_2)\right] \equiv \begin{cases} \hat H_I'(t_1)\,\hat H_I'(t_2) & \text{for } t_1 > t_2 \\ \hat H_I'(t_2)\,\hat H_I'(t_1) & \text{for } t_2 > t_2 \end{cases} \qquad (1)$$

$$\frac{1}{2}\int_0^t dt_1 \int_0^t dt_2\ \mathcal{T}\left[\hat H_I'(t_1)\,\hat H_I'(t_2)\right] \qquad (2)$$

$$= \frac{1}{2}\left[\int_0^t dt_1 \int_0^{t_1} dt_2\ \hat H_I'(t_1)\,\hat H_I'(t_2) + \underbrace{\int_0^t dt_1 \int_{t_1}^{t} dt_2}_{= \int_0^t dt_2 \int_0^{t_2} dt_1\text{, then rename } t_1 \leftrightarrow t_2}\ \hat H_I'(t_2)\,\hat H_I'(t_1)\right] \qquad (3)$$

$$= \int_0^t dt_1 \int_0^{t_1} dt_2\ \hat H_I'(t_1)\,\hat H_I'(t_2) \qquad (4)$$

Imaginary time

GF15

Thermal averaging : $\rightsquigarrow$ factors of $e^{-\beta \hat{H}}$ (with $\hat{H} \neq \hat{H}(t)$) (1)

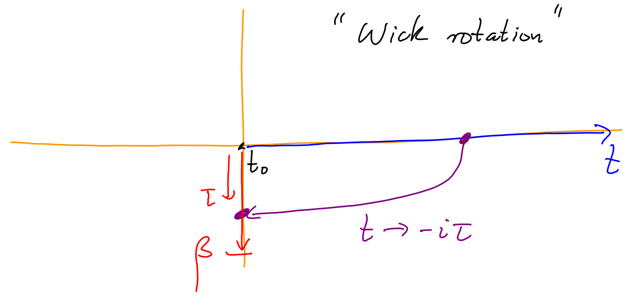
time evolution : $\rightsquigarrow$ factors of $e^{-i\hat{H}t/\hbar} \xrightarrow{t \to -i\tau} e^{-\hat{H}\tau/\hbar}$ (2)

Calculations are simpler if only one type of exponent occurs. So, it is convenient to make an analytic continuation

"Wick rotation"

$$t \to -i\tau \qquad (3)$$

$$\partial_t \to i\partial_\tau \qquad (4)$$



Price to pay: at end of calculation we must continue back, which may require considerable mathematical care.

Then, imaginary time propagator is defined as [(9.5a), with (15.4)]

GF16

$$\underbrace{-\hbar\,\partial_\tau}_{(15.4)\ i\partial t \to i(i\partial_\tau) = -\partial_\tau} \hat{\tilde{U}}(\tau,\tau') \equiv \hat{\tilde{H}}_s(\tau)\,\hat{\tilde{U}}(\tau,\tau') \qquad (1) \qquad \hbar\, i\partial_t \hat{U}(t,t') \overset{(9.5a)}{=} \hat{H}_s(t)\,\hat{U}(t,t')$$

(tildes will often be dropped...)

For time-independent $\hat{H}_s = \hat{H}$ (as is the case in the thermal factor $e^{-\beta\hat{H}}$)

solution is: $$\hat{\tilde{U}}(\tau,\tau') = e^{-(\tau-\tau')\hat{H}/\hbar} \qquad \left(\text{cf. } \hat{U}(t,t') = e^{-iH(t-t')/\hbar}\right) \qquad (2)$$

($t \to -it$)

Properties: $\hat{\tilde{U}}(\tau,\tau) = \mathbb{1}$ (3), $\hat{\tilde{U}}(\tau,\tau'')\,\hat{\tilde{U}}(\tau'',\tau') = \hat{\tilde{U}}(\tau,\tau')$ (4)

but $\hat{\tilde{U}}^{\dagger}(\tau,\tau') \neq \hat{\tilde{U}}^{-1}(\tau,\tau')$ (5)

Analogously: $$\hat{A}_I(\tau) \overset{(12.3)}{=} e^{\hat{H}_0(\tau-\tau_0)/\hbar}\,\hat{A}_s(\tau)\,e^{-\hat{H}_0(\tau-\tau_0)/\hbar} \qquad (6)$$

$$-\partial_\tau \hat{\tilde{U}}_I(\tau,\tau') \overset{(13.2)}{=} \hat{H}'_I\,\hat{\tilde{U}}_I(\tau,\tau') \qquad (7)$$