$$i \frac{d}{dt} |\Psi(t)\rangle_I = i \frac{d}{dt}\left[e^{iH_0 t} |\Psi(t)\rangle_S \right]$$

$$= e^{iH_0 t}\left[-H_0 + H\right] |\Psi(t)\rangle_S$$

$$= e^{iH_0 t} H'(t) e^{-iH_0 t} |\Psi(t)\rangle_I$$

[NB- rewrote RHS in terms of interaction picture to get closed equation]

$H'_I(t) = e^{iH_0 t} H'(t) e^{-iH_0 t}$ by usual defn of Int. Picture, although H' already depended on t in S. Picture

$$i \frac{d}{dt} |\Psi(t)\rangle_I = H'_I(t) |\Psi(t)\rangle_I$$

"slow" t-evolution since only involves $H'(t)$ - we can write formally exact solution in terms of time-ordered exponential but we only need results to linear order in H' [$\propto \vec{A}$]

$$|\Psi(t)\rangle_I = |\Psi(-\infty)\rangle_I - i\int_{-\infty}^{t} dt'\, H'_I(t')\, |\Psi(-\infty)\rangle_I$$

[obeys S.E., correct initial state]

- physical assumptions: $H'(t)$ "turned off" at $t \to -\infty$ before measurement (at $t=0$)

- for periodic vector potential case we replace $H'(t) \to e^{\eta t} H'(t)$ with $\eta \to 0^+$ (for measurement at $t=0$)

& - wait long enough for transient to die out - calculate $\langle J(t=0)\rangle$ & take $\eta \to 0^+$ at end.

- also assume $|\Psi(t)\rangle_I$ approaches ground state of H_0 at $t \to -\infty$ when $H'(t) \to 0$

NB: if $H'=0$ $|\Psi(t)\rangle_I = |\Psi(t)\rangle_H$

[this is for zero temperature]

at $H'=0$ $|\Psi(t)\rangle_H$ is t-independent $= |\Psi(0)\rangle_S$

- ie system in ground state before we turn on E-field - reasonable
- at finite temperature, we will assume system is in mixed state corresponding to a thermal ensemble governed by H_0 at $t \to -\infty$ [Boltzmann dist]
- consider $T=0$ first:
- $\frac{12}{11}$ let $|\Psi_0\rangle$ be ground state of H_0 (in Heisenberg Rep.)

$$H'(t) = -\frac{e}{c}\int d^3r\ \vec{j}(r)\cdot\vec{A}\ [\times e^{\eta t}]$$

- calculate ${}_S\langle\Psi_0|\, j_S(t)\,|\Psi_0\rangle_S$

NB $|\Psi_0(t)\rangle_S$ is exact eigenstate of H but we work to first order in $\vec{A}$ only.

$$\langle j\rangle = {}_I\langle\Psi_0(t)|\ j_I(t)\ |\Psi_0(t)\rangle_I$$

$\langle \vec{j}(t) \rangle = \langle \Psi_0 | \vec{j}_I(t) | \Psi_0 \rangle$

$+ \frac{ie}{c} \int d^3r' \int_{-\infty}^{t} dt' \langle \Psi_0 | [\vec{j}_I(\vec{r}, t),$
$\vec{j}_I(\vec{r}', t') \cdot \vec{A}(\vec{r}', t')] | \Psi_0 \rangle + O(A^2)$

$|\Psi_0\rangle$ is grnd state of H_0 [Heis Rep]

$A \to e^{\eta t} A \quad , \eta \to 0^+$

- since we have an explicit factor of $\vec{A}$ in 2nd term we can evaluate $\vec{j}_I$ at $H' = 0$ in which case it becomes Heisenberg Rep

- we expect 1st term $\langle \Psi_0 | \vec{j}_I(t) | \Psi_0 \rangle = 0$

then $= \langle \Psi_0 | e^{iH_0 t} \vec{j}(\vec{r}) e^{-iH_0 t} | \Psi_0 \rangle$

$= \langle \Psi_0 | \vec{j}(t) | \Psi_0 \rangle$ in Schroed. Rep

$|\Psi_0\rangle$ is grnd state for $H' = 0$, no current

$$\langle j^a(\vec{r},t)\rangle = \frac{ie}{c}\sum_b \int d^3\vec{r}\,' \int_{-\infty}^{t} dt' \langle \Psi_0 | [j^a(\vec{r},t), j^b(\vec{r}\,',t')] | \Psi_0\rangle \, A^b(\vec{r}\,',t')$$

NB - matrix element evaluated at $H'=0$

so interaction picture → Heisenberg picture

- this motivates def'n of retarded Green's function

$$\langle j^a(\vec{r},t)\rangle = -\frac{e'}{c}\sum_b \int d^3r' \int_{-\infty}^{\infty} dt' \, G^{ab}_{ret}(\vec{r}-\vec{r}\,', t-t') \, A^b(\vec{r}\,',t')$$

where $G^{ab}_{ret}(\vec{r}-\vec{r}\,', t-t') \equiv i\,\theta(t-t')\langle \Psi_0 | [j^a(\vec{r},t), j^b(\vec{r}\,',t')] | \Psi_0\rangle$

- NB 1) - it is convenient to extend t' integral from $-\infty$ to ∞ so that it gives a simple Fourier transform when $A \propto e^{i\omega t'}$

- but this requires step function $\theta(t) = 1,\ t \geq 0$
$= 0,\ t < 0$

in def'n of $G(t-t')$

- physical significance of step function is that current at time t only depends on $\vec{A}(t')$ at earlier times - causality

⇒ name retarded

2) H_0 is time and space translationally invariant ⇒ $\langle \; \rangle$ is a function only of $\vec{r}-\vec{r}'$, $t-t'$, as written

3) recall we actually insert factor of $e^{\eta t'}$ with $\eta \to 0^+$

- instead we can insert a factor of $e^{-\eta(t-t')}$ in def'n of retarded GF

$$G^{ab}(\vec{r}, t) = -e^{-\eta t}\, i\,\theta(t) \langle \Psi_0 | [\, j^a(\vec{r}, t),\, j^b(\vec{0}, 0)] | \Psi_0 \rangle$$

$$\eta \to 0^+$$

$$e^{-\eta t} \to 1, \quad e^{\eta(t'-t)} \approx e^{\eta t'}$$

- this is general def'n of retarded Green's function for any pair of Hermitean bosonic operators j^a, j^b

- retarded GF can be used to predict many other types of phenomena besides elec. conductivity

- e.g. a quantum magnetic system may be described by the Heisenberg model

$$H = J \sum_{\vec{R}, \vec{\delta}} \vec{S}_R \cdot \vec{S}_{\vec{R}+\vec{\delta}} - \vec{B}_0 \cdot \sum_{\vec{R}} \vec{S}_R$$

- in electron spin resonance experiment a small oscillating (micro-wave) field is also applied $\delta H = - \vec{B}_1(t) \cdot \sum_{\vec{R}} \vec{S}_R$

rate of adsorption of radiation is proportional to $G^{ab}_{\vec{R}-\vec{R}'}(t-t') \equiv -i\,\theta(t-t')$

$$\langle \Psi_0 | [S^a_{\vec{R}}(t), S^b_{\vec{R}'}(t')] | \Psi_0 \rangle$$

- nuclear magnetic resonance experiments:
- shift and width of nuclear ~~Zeeman~~ spin transitions is determined by weak hyperfine couplings of nuclear to atomic spin

$$\sum_{a,b,\vec{R},\vec{R}'} I^a_{\vec{R}} S^b_{\vec{R}'} f_{ab}(\vec{R}, \vec{R}')$$

- NMR signal given by GF of atomic spins
- thermal conductivity of a metal
  - measure heat current produced by small temperature gradient - determined by retarded GF of energy current operator
- it is also very convenient to define retarded GF for fermionic operators (electrons, ...)
  - defined the same way except with anti-commutator

$$G^{ret}_{\sigma\sigma'}(\vec{r}-\vec{r}', t-t') = -i\theta(t-t')\langle\Phi_0|\{\Psi_\sigma(\vec{r},t), \Psi^\dagger_{\sigma'}(\vec{r}',t')\}|\Phi_0\rangle$$

- for interacting electrons, current GF can be expressed in terms of electron GF + other terms
- photo-emission experiments are analysed in terms of electron GF

for a non-Hermitean bosonic operator U:

$G \equiv -i\theta \langle \Psi_0 | [U, U^\dagger] | \Psi_0 \rangle$

- it is usually more convenient to work with Fourier transform of retarded GF

$$G_{ret}(\vec{q},\omega) = \int d^3\vec{r} \int_{-\infty}^{\infty} dt \, e^{i\vec{q}\cdot\vec{r} + i\omega t} \, G_{ret}(\vec{r}, t)$$

[for homogeneous case $G(\vec{r},\vec{r}'; t,t') = G(\vec{r}-\vec{r}'; t-t')$]

- return to electrical conductivity

$$\langle j^a(\vec{r},t) \rangle = -\frac{e}{c} \sum_b \int d^3\vec{r}' \int_{-\infty}^{\infty} dt' \, G^{ab}(\vec{r}-\vec{r}', t-t') \, A^b(\vec{r}', t')$$

Fourier transform:

$$j^a(\vec{q},\omega) = \int d^3\vec{r} \, e^{i\vec{q}\cdot\vec{r}} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \, j^a(\vec{r},t)$$

by convolution theorem

$$\langle j^a(\vec{q},\omega) \rangle = -\frac{e}{c} \sum_b G^{ab}_{ret}(\vec{q},\omega) \, A^b(\vec{q},\omega)$$

[Proof: suppressing $\vec{r}$-dependence

$$\int_{-\infty}^{\infty} dt\, e^{i\omega t} \int_{-\infty}^{\infty} dt'\, G(t-t')\, A(t')$$

$$= \int_{-\infty}^{\infty} dt\, e^{i\omega t} \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} e^{-i\omega_1 (t-t')}$$

$$\int_{-\infty}^{\infty} \frac{d\omega_2}{2\pi} e^{-i\omega_2 t'}\, G(\omega_1)\, A(\omega_2)$$

$$= \int d\omega_1 d\omega_2\, \delta(\omega-\omega_1)\, \delta(\omega_1-\omega_2)\, G(\omega_1)\, A(\omega_2)$$

$$= G(\omega)\, A(\omega) \quad]$$

- we also must include 2^{nd} term in

$$\langle J^{a(2)} \rangle (\vec{r}, t) = -\frac{e^2}{mc} \langle \rho \rangle (\vec{r}, t)\, A^a(\vec{r}, t)$$

$$\langle \rho \rangle = n_0 \text{ - electron density}$$

NB $|\psi_0\rangle$ is unperturbed ground state to 1^{st} order in A

all together $\langle J^a \rangle (\vec{q}, \omega) = -\frac{1}{c} \sum_b \left[G^{ab}_{ret}(\vec{q}, \omega) + \frac{n_0 e^2}{m} \delta^{ab} \right] A^b(\vec{q}, \omega)$

- we wish to express $\langle J^a \rangle$ in terms of electric field, not vector potentials

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

$$\vec{E}(\vec{q},\omega) = \frac{i\omega}{c}\vec{A}(\vec{q},\omega)$$

or, including convergence factor: $\vec{A}(t) \to e^{\eta t}\vec{A}(t)$
$(\eta \to 0^+)$

$$\vec{E} = \frac{(i\omega - \eta)}{c}\vec{A}(\vec{q},\omega)$$

$$\langle J^a\rangle(\vec{q},\omega) = \sum_b \sigma^{ab}(\vec{q},\omega)\, E^b(\vec{q},\omega)$$

conductivity =

$$\sigma^{ab}(\vec{q},\omega) = \frac{i}{\omega + i\eta}\left[G^{ab}_{ret}(\vec{q},\omega) + \frac{n_0 e^2}{m}\delta^{ab}\right]$$

$(\eta \to 0^+)$, normally $\vec{q} = 0$, since $q = \frac{\omega}{c}$ for E-field

- remark: to get dc conductivity we then take $\omega \to 0$

- normally $G^{ab} \to -\frac{n_0 e^2}{m}\delta^{ab} + O(\omega)$

so limit is finite

G^{ab}_{ret} is calculated, in general, including not only e-e interactions but also ionic potential + disorder potential + phonons - vibrations of ions

- for simple jellium model it can be shown that $G_{ret}(\omega) = 0$ ~~as $\omega \to 0$~~

$$\sigma^{ab} = \frac{i}{\omega + i\eta} \frac{n_0 e^2}{m} \delta^{ab}$$

$$\text{Re}\,\sigma = \delta(\omega) \frac{\pi n_0 e^2}{m}$$ - ballistic transport

- this follows because there is no momentum relaxation in jellium model
- if we start a current flowing it won't stop due to momentum conservation for electrons
- collisions conserve total momentum [HW?]
- with a static potential $\delta H = \int d^3x\, \rho(x)\, U(x)$

"Umklapp scattering" processes occur

where electron momentum is not conserved during e-e scattering - momentum ~~lost~~ loss = reciprocal lattice vector

$\Rightarrow$ momentum transferred to lattice

- <u>finite temperature</u>

- now we calculate

$$\langle \vec{J} \rangle(\vec{r},t) = \frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n} \langle \Psi_n | \vec{J} | \Psi_n \rangle$$

$\left(\mathcal{Z} = \sum e^{-\beta E_n} \right)$

- we can follow same steps - go to interaction picture, treat $\vec{A}$ in 1st order

- basic assumption is now that in infinite past, before E-field was turned on, system was in thermal equilibrium state for unperturbed Hamiltonian, H_0

- formula for conductivity is <u>identical</u> if we modify def'n of retarded GF to

$$G^{ab}_{ret}(\vec{r},t) = -i\frac{\theta(t)}{Z}\sum_n e^{-\beta E_n} \langle\Psi_n| [j^a(\vec{r},t), j^b(\vec{0},0)] |\Psi_n\rangle$$

171 - ($q=0$ for conductivity), $\beta \equiv \frac{1}{T}$, ($k_B=1$)

- we generally work in grand canonical ensemble: $H \to H - \mu\hat{N}_e$ where μ = chemical potential, $\beta = \frac{1}{k_BT} \to \frac{1}{T}$

$E \to E - \mu N_e$ - time evolution of operators calculated with $H - \mu\hat{N}_e$

$\Omega = \sum_n e^{-\beta(E_n - N_n)}$ [sum over all numbers of electrons and all states]

- following Mahan I will write $E_n - N_n$ as simply E_n

$\mathcal{E}_{\vec{k}i} \to \mathcal{E}_{\vec{k}i} - \mu$. [at low T, $\mu \to \mathcal{E}_F$]

- also write $|\Psi_n\rangle$ as simply $|n\rangle$

- remark:

$$G^{ab}_{ret}(\vec{r},t) = \frac{-i\theta(t)}{Z}\, \mathrm{tr}\, e^{-\beta H}[j^a(\vec{r},t), j^b(\vec{0},0)]$$

Spectral resolution of GF's

- convenient for understanding physical significance & for applications
- also useful for establishing connection with Matsubara or imaginary time GF that we will discuss next [very useful in Feynman path integral]
- Consider retarded GF at finite T for a general operator $U(t)$
- eg - could be $j^{a}_{\vec{q}}(t)$ or $C_{\vec{q}}(t)$ [suppress $\vec{q}$]

$$G(t) = -i e^{\beta \Omega} \sum_n e^{-\beta E_n} \langle n | [U(t), U^+(0)] | n \rangle$$

- or for fermionic case $[\,,\,] \to \{\,,\,\}$

$$e^{\beta \Omega} = 1/Z$$

E_n are exact eigenvalues of interacting Hamiltonian [but not including E-field or other small perturbations]

- ~~Now insert a complete set of s~~

- for non-interacting electrons, general state $|m\rangle$ is $|\vec{k}_1 \sigma_1, \vec{k}_2 \sigma_2, - \vec{k}_N \sigma_N\rangle$

but with interactions these are not eigenstates — use exact ones [in principle]

$$I = \sum_m |m\rangle\langle m|$$

$$G(t) = -i\,\Theta(t)\, e^{\beta\Omega} \sum_{n,m} e^{-\beta E_n} \left[\langle n|U(t)|m\rangle\langle m|U^+(0)|n\rangle \right.$$

$$\left. - \langle n|U^+(0)|m\rangle \langle m|U(t)|n\rangle \right]$$

$$\langle n|U(t)|m\rangle = \langle n| e^{iHt} U e^{-iHt} |m\rangle$$

$$= e^{i(E_n - E_m)t} \langle n|U|m\rangle$$

NB — $U(t)$ is Heisenberg rep, U is short-hand for $U_H(0) = U_S$

(3 K)

$$G_{ret}(t) = -i\, e^{\beta\Omega}\, \theta(t) \sum_{n,m} e^{-\beta E_n} \Big[|\langle n|U|m\rangle|^2 e^{i(E_n-E_m)t}$$

$$\mp |\langle m|U|n\rangle|^2 e^{i(E_m-E_n)t} \Big]$$

[$-$ for bosons, $+$ for fermions]

- we now switch $n \leftrightarrow m$ in 2^{nd} term

so that we have common factors of $|\langle n|U|m\rangle|^2$

$e^{i(E_n-E_m)t}$

$$G_{ret}(t) = -i\, e^{\beta\Omega}\, \theta(t) \sum_{n,m} |\langle n|U|m\rangle|^2 e^{i(E_n-E_m)t}$$

$$\left(e^{-\beta E_n} \mp e^{-\beta E_m}\right)$$

- for fermions, only difference is in last factor $\rightarrow$ $\left(e^{-\beta E_n} + e^{-\beta E_m}\right)$

$$G_{ret}(\omega) = -i\, e^{\beta\Omega} \sum_{n,m} |\langle n|U|m\rangle|^2 \left(e^{-\beta E_n} \mp e^{-\beta E_m}\right)$$

$$\int_0^\infty dt\; e^{i(\omega+i\eta)t}\, e^{i(E_n-E_m)t}$$

NB 1) $0 \le t \le \infty$ only due to $\theta(t)$ in def'n of retarded GF

2) re-inserted $e^{-\eta t}$ factor in precise def'n of G_{ret}

$$G_{ret}(\omega) = e^{\beta\Omega} \sum_{n,m} \frac{|\langle n|U|m\rangle|^2 \left(e^{-\beta E_n} \mp e^{-\beta E_m}\right)}{\omega + E_n - E_m + i\eta} \quad (*)$$

[limit $\eta \to 0^+$ implicit]

Im G_{ret} [as Re σ determined by it] is especially simple & important - ~~called spectral density function~~

$$\mathrm{Im}\, \frac{1}{x+i\eta} = \mathrm{Im}\left(\frac{-i\eta}{x^2+\eta^2}\right) = -\pi\,\delta(x)$$

$$\mathrm{Im}\, G_{ret}(\omega) = -\pi\, e^{\beta\Omega} \sum_{n,m} |\langle n|U|m\rangle|^2 \left(e^{-\beta E_n} \mp e^{-\beta E_m}\right) \delta(\omega + E_n - E_m)$$

using $E_m = E_n + \omega$ we can write this

$$\mathrm{Im}\, G_{ret}(\omega) = -\pi\, e^{\beta\Omega}\left(1 \mp e^{-\beta\omega}\right) \sum_{n,m} |\langle n|U|m\rangle|^2 e^{-\beta E_n} \delta(\omega + E_n - E_m)$$

- can rewrite pre-factor in terms of Bose & Fermi distribution functions

$$n_B(\omega) = \frac{1}{e^{\beta\omega} - 1}, \quad n_F(\omega) = \frac{1}{e^{\beta\omega}+1}$$

$$1 - n_B(\omega) = -\frac{1}{e^{-\beta\omega} - 1}$$

$$1 ~~\beta~~ - n_F(\omega) = \frac{1}{e^{-\beta\omega} + 1}$$

Im $G_{ret}(\omega)$ gets a contribution from every pair of states $|n\rangle, |m\rangle$ whose energies differ by ω and which have non zero matrix element $\langle n|U|m\rangle \neq 0$

$$E_m - E_n = \omega$$

$T \to 0$ limit, Boltzmann factors force either $|n\rangle$ or $|m\rangle$ to be the groundstate [which, depends on sign of ω]

for $\omega > 0$ $\quad e^{-\beta\omega} \to 0$ as $\beta \to \infty$ $(T \to 0)$

$$e^{\beta\Omega} e^{-\beta E_n} \to \delta_{n,0}$$

$$\text{Im}\, G_{ret}(\omega)\Big|_{T=0} = -\pi \sum_m |\langle 0|U|m\rangle|^2 \, \delta(\omega + E_0 - E_m)$$

— only excited states with $E_m = E_0 + \omega$ $(\omega > 0)$ contribute, with ~~$\langle 0|U|m\rangle \neq 0$~~ $\langle m|U^\dagger|0\rangle \neq 0$

for $\omega < 0$, $|m\rangle$ must be the ground state

$$\mathrm{Im}\, G^{ret}_{T=0}(\omega) = \pm \pi \sum_n |\langle 0|U^+|n\rangle|^2 \delta(\omega + E_n - E_0)$$

↗ Boson/fermion

$$E_n = E_0 - \omega > E_0$$

all excited states contribute with ~~$\langle 0|U^+|n\rangle \neq 0$~~ $\langle n|U|0\rangle \neq 0$

$$E_n = E_0 - \omega > 0$$

- So, by looking at both $\omega > 0$ and $\omega < 0$ at $T=0$ we probe matrix elements ~~$\langle 0|U|m\rangle$~~ $\langle m|U^+|0\rangle$ and ~~$\langle 0|U^+|n\rangle$~~ $\langle n|U|0\rangle$ respectively
- in general both may be non-zero and different
- eg if $U = C_{\vec{q}}$, $U^+|0\rangle$ gives particle states and $U|0\rangle$ gives hole states
- photo-emission - sudden approx. ⇒ GF of C_q

<u>Matsubara</u> (Imaginary time) <u>Green's functions</u>

- Retarded GF is directly related to ~~eq~~ experiments but difficult to calculate