⑦ # Response functions from linear response (Kubo)

External field $S \to S + \int dx\, \hat{M}(x) \cdot h(x)$ $\boxed{\text{or } S \to S + \int d\tau\, \Delta H}$ with ΔH perturbation

$x = (\vec{r}, \tau)$; $\hat{M}$ is observable $= \psi^{+}_{(\vec{r}\tau)} \hat{M} \psi(\vec{r}\tau)$

h is external field

e) Magnetic susceptibility $M(x) = \vec{M}(\vec{r}, \tau) = \psi^{+}_{s}(\vec{r},\tau) \vec{\sigma}_{ss'} \psi_{s'}(\vec{r}\tau)$. The external field $h = -\vec{B}$

h) Optical conductivity $M(x) = \frac{1}{c} \vec{j}(\vec{r}, \tau)$ and $h(x) = \vec{A}(\vec{r}, \tau)$ vector potential

Recall

$$H = \int \psi^{+}(\vec{r}) \frac{1}{2m} (\underbrace{-i\hbar \vec{\nabla}}_{\vec{p}} - e\vec{A})^2 \psi(\vec{r})\, d^3r + \mu_B \vec{B} \cdot \int \psi^{+}_{s} \vec{\sigma}_{ss'} \psi_{s'} + H_{int}$$

$$= H^0 + \frac{ie\hbar}{2m} \int \psi^{+} (\vec{\nabla} \cdot \vec{A} + \vec{A} \cdot \vec{\nabla}) \psi\, d^3r + \text{small terms} \left(\frac{1}{\alpha}\right)$$

by parts

$$\underbrace{(\psi^{+} \psi \vec{A})\Big|}_{\text{boundary vanishes}} - \int (\vec{\nabla} \psi^{+})\, \vec{A}\, \psi\, d^3r$$

$$H = H^0 - \int \vec{A} \cdot \frac{e i\hbar}{2m} \left\{ (\vec{\nabla} \psi^{+}) \psi - \psi^{+} (\nabla \psi) \right\} d^3r = H^0 - \int \vec{A} \cdot \vec{j}\, d^3r$$

$$\vec{j} = \frac{e\hbar}{2mi} \left(\psi^{+} \nabla \psi - (\nabla \psi^{+}) \psi \right)$$

Need to find change of the observable M at point x_1 due to disturbance at earlier time $x_2 = (r_2, t_2)$

First sloppy derivation of the response:

$$\langle M(x_1) \rangle = \frac{1}{Z} \int D[\psi^{+}\psi]\, e^{-S_0 - \int dx\, M(x) h(x)}\, M(x_1) \approx \frac{\int D[\psi^{+}\psi]\, e^{-S_0} \left(M(x_1) - \int dx_2\, M(x_2) M(x_1) h(x_2) \right)}{\int D[\psi^{+}\psi]\, e^{-S_0} \left(1 - \int dx_2\, M(x_2) h(x_2) \right)}$$

$$\langle M(x_1) \rangle \approx \frac{Z_0 \left\{ \langle M(x_1) \rangle^0 - \int dx_2\, h(x_2) \langle T_\tau M(x_2) M(x_1) \rangle^0 \right\}}{Z_0 \left\{ 1 - \int dx_2\, h(x_2) \langle M(x_2) \rangle^0 \right\}} = \langle M(x_1) \rangle^0 + \int dx_2\, h(x_2) \left\{ \langle M(x_2) \rangle^0 \langle M(x_1) \rangle^0 - \langle M(x_2) M(x_1) \rangle^0 \right\}$$

$$\langle M(x_1) \rangle \approx \langle M(x_1) \rangle^0 + \int dx_2\, h(x_2)\, \chi(x_2 x_1) \quad ; \quad \chi(x_2, x_1) = \langle M(x_2) \rangle^0 \langle M(x_1) \rangle^0 - \langle M(x_2) M(x_1) \rangle^0$$

connected correlation function

⑧ More careful real time derivation of causal response

$$\langle M(t)\rangle^0 = \frac{Tr(e^{-\beta H^0} M(t))}{Tr(e^{-\beta H^0})}$$

We will work in the interaction representation

- Operators have time dependence $O(t) = e^{iH^0 t}\, O\, e^{-iH^0 t}$
- Wave function have the rest of time dependence $|\Psi(t)\rangle = e^{iH_0 t}\, e^{-i(H_0+\Delta H)t}\, |\Psi(0)\rangle$

So that $\langle\Psi(t)|O(t)|\Psi(t)\rangle = \langle\Psi(0)|\, e^{i(H_0+\Delta H)t}\, \underbrace{e^{-iH_0 t}\, e^{iH_0 t}}_{=1}\, O\, \underbrace{e^{-iH_0 t}\, e^{iH_0 t}}_{=1}\, e^{-i(H_0+\Delta H)t}\, |\Psi(t)\rangle$

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = e^{iH_0 t}[iH_0 - i(H_0+\Delta H)]\, e^{-i(H_0+\Delta H)t}|\Psi(t)\rangle = -i\Delta H(t)\,|\Psi(t)\rangle$$ therefore

formally $\quad |\Psi(t)\rangle = T_t\, e^{-i\int_0^t \Delta H(t')dt'}\, |\Psi(0)\rangle \quad$ i.e., $\quad U(t,0) = T_t\, e^{-i\int_0^t \Delta H(t')dt'}$

Why?

Because of causality the response is after the cause.

$$\frac{\partial}{\partial t}U(t) = -i\Delta H(t)\, U(t)$$

$$U(t) - U(0) = -i\int_0^t \Delta H(t')\, U(t')\, dt' \quad \text{where } U(0)=1$$

recursively inserting $U(t)$ back, we get

$$U(t) = 1 - i\int_0^t dt_1\, \Delta H(t_1) + (-i)^2\int_0^t dt_1\, \Delta H(t_1)\int_0^{t_1} dt_2\, \Delta H(t_2) + \cdots = \sum_{m=0}^{\infty}(-i)^m \int_0^t dt_1\, \Delta H(t_1)\int_0^{t_1} dt_2\, \Delta H(t_2)\cdots\int_0^{t_{m-1}} dt_m\, \Delta H(t_m)$$

$$= \sum_{m=0}^{\infty}\frac{(-i)^m}{m!}\, T_t \int_0^t dt_1\, \Delta H(t_1)\int_0^t dt_2\, \Delta H(t_2)\cdots\int_0^t dt_m\, \Delta H(t_m)$$

$$= T_t\, e^{-i\int_0^t dt_1\, \Delta H(t_1)}$$

Now we say that at $t=-\infty$ there was no external force, but was gradually switched on, so that at time t we have:

$$\langle M(t)\rangle = \frac{1}{Z} Tr\left(e^{-\beta H^0}\, U(-\infty,t)\, M(t)\, U(t,-\infty)\right)$$

$$\text{where } U(t,-\infty) = T_t\, e^{-i\int_{-\infty}^t dt_1\, \Delta H(t_1)}$$

$$\text{and } M(t) = e^{iH_0 t} M e^{-iH_0 t}$$

⑨

$$\langle M(t)\rangle = \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H^0} T_t\, e^{+i\int_{-\infty}^{t} dt_1\, \Delta H(t_1)} M(t)\, e^{-i\int_{-\infty}^{t} dt_2\, \Delta H(t_2)}\right)$$

$$\langle M(t)\rangle \approx \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H_0}\left(1+i\int_{-\infty}^{t} dt_1\, \Delta H(t_1)\right)M(t)\left(1-i\int_{-\infty}^{t} dt_2\, \Delta H(t_2)\right)\right)$$

$$\approx \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H_0}\left(M(t) - i\int_{-\infty}^{t}[M(t), \Delta H(t_1)]dt_1\right)\right)$$

$$= \langle M(t)\rangle^0 - i\int_{-\infty}^{\infty}\Theta(t_1<t)\langle[M(t), \Delta H(t_1)]\rangle^0 dt_1 = \langle M(t)\rangle^0 - i\int_{-\infty}^{\infty} dt_1\, h(t_1)\,\Theta(t_1<t)\langle[M(t), M(t_1)]\rangle^0$$

Since $\Delta H(t) = M(t)\, h$

$$\langle M(t)\rangle - \langle M(t)\rangle^0 \approx \int_{-\infty}^{\infty} dt_1\, \chi(t,t_1)\, h(t_1)$$

where $\chi(t,t_1) = -i\Theta(t-t_1)\langle[M(t), M(t_1)]\rangle_0$

Conclusion: The measurable response function is the retarded susceptibility:

$\chi_M = \langle\langle M; M\rangle\rangle^R$ i.e., $\chi_M(t,t_1) = -i\Theta(t-t_1)\langle[M(t), M(t_1)]\rangle_0$

It can be obtained from Matsubara $\chi(i\omega) = -\int_0^{\beta}\langle T_\tau M(\tau) M(0)\rangle e^{i\omega\tau} d\tau$

by analytic continuation $\chi^R(\omega) = \chi(i\omega \to \omega + i\delta)$

Examples: Optical conductivity

$\Delta H = -\vec{A}\cdot\vec{j}$

$\Delta H = \frac{1}{i\omega}\vec{E}\cdot\vec{j}$

from Maxwell in Coulomb gauge ($\vec{\nabla}\cdot\vec{A}=0$ and $\vec{E} = -\frac{\partial\vec{A}}{\partial t}$)

$\vec{E} = -i\omega\vec{A}$

$h = \vec{E}$

$M = -\frac{i}{\omega}\vec{j}$

$$\langle j\rangle = \int_{-\infty}^{t}\sigma(t,t_1)\,\vec{E}(t_1)\,dt_1$$

$$\langle -\tfrac{i}{\omega} j\rangle = \left(-\tfrac{i}{\omega}\right)^2 \langle\langle j; j\rangle\rangle E$$

$$\sigma_{\vec{q}}(\omega) = -i\int_{-\infty}^{t}\Theta(t-t_1)\langle[j(\vec{r},t), j(\vec{r}_1,t_1)]\rangle e^{i\omega(t-t_1) - i\vec{q}(\vec{r}-\vec{r}_1)} dt_1\, d^3r_1 \left(-\frac{i}{\omega}\right)$$

$$\sigma_q(\omega) = \frac{1}{\omega}\int_0^{\infty}\Theta(t)\langle[j(\vec{r},t), j(0,0)]\rangle e^{i\omega t - i\vec{q}\vec{r}} dt\, d^3\vec{r}$$

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Example charge response

start with: $\Delta H = -\int \underbrace{V_{ext}(\vec{r})}_{\substack{\text{associate } h \\ \text{with}}} \underbrace{M(\vec{r})}_{M}\, d^3r$

Recall: $\langle M(x_1)\rangle \approx \langle M(x_1)\rangle^0 + \int dt_2\, h(x_2)\, \chi(x_2 x_1)$; $\chi(x_2,x_1) = \langle M(x_2)\rangle^0 \langle M(x_1)\rangle^0 - \langle M(x_2) M(x_1)\rangle^0$

connected correlation function

In this case:

$$M([V_{ext}]\,\vec{r},\tau) = M([V_{ext}=0],\vec{r},\tau) - \int V_{ext}(\vec{r}'\tau')\,\chi(\vec{r}'\tau',\vec{r},\tau) \Rightarrow \Big|\ \delta M(\vec{r},\tau) = -\int V_{ext}(\vec{r}',\tau')\,\chi(\vec{r}'\tau',\vec{r}\,\tau)$$

with $\chi(\vec{r}'\tau',\vec{r}\,\tau) = -\langle T_\tau M(\vec{r}'\tau')\, M(\vec{r}\,\tau)\rangle^0 + \langle M(\vec{r}',\tau')\rangle^0 \langle M(\vec{r},\tau)\rangle^0$

How is this related to dielectric constant? We usually want to express charge response in terms of

$$\delta V_{tot}(x_1) \underset{\text{definition}}{\equiv} \int \varepsilon^{-1}(x_1\, x_2)\, V_{ext}(x_2)\, dt_2 \qquad \text{(definition)}$$

interaction that charge particle feels

screening by dielectric function of the material

external potential (electric field)

$$\delta V_{tot}(x_1) = \delta V_{ext}(x_1) + \int V_c(x_1, x_3)\, \delta M(x_3)\, dx_3 = \delta V_{ext} - \int V_c(x_1 x_3)\, \chi(x_3, x_2)\, V_{ext}(x_2)\, dt_2\, dt_3$$

bare interaction between electrons $= \frac{1}{|\vec{r}_1 - \vec{r}_2|}$

electrons rearrange in the solid, and contribute to the potential change

Hence:

$$\delta V_{tot}(x_1) = \int \Big[\delta(x_1 - x_2) - \int V_c(x_1\, x_3)\, \chi(x_3, x_2)\, dt_3\Big]\, V_{ext}(x_2)\, dt_2$$

Finally using definition (definition) we get:

$$\varepsilon^{-1}(x_1, x_2) = \delta(x_1 - x_2) - \int V(x_1, x_3)\, \chi(x_3, x_2)\, dt_3$$

By Fourier transform: $\varepsilon^{-1}_{q\omega} = 1 - V_q\, \chi_q(\omega)$ where $\chi_q(i\omega) = -\int_0^\beta \int \langle T_\tau M(\vec{r},\tau)\cdot M(0,0)\rangle\, e^{i\omega\tau - i\vec{q}\cdot\vec{r}}\, d^3r\, d\tau$

Note that from Maxwell relations we also have

$$\varepsilon = \varepsilon_0 + 4\pi i\, \frac{\sigma(\omega)}{\omega}$$

dielectric constant

optical conductivity

(11) Back to the Single particle Green's function

Very important because:

It is the lowest order correlation function with the simplest analytic structure
It appears as the basic building block of Feynman diagrammatic technique.

$$\langle\langle A; B\rangle\rangle^R = -i\Theta(t_1-t_2)\langle [\overset{\psi}{\overset{\shortparallel}{A}}(\vec r_1 t_1), \overset{\psi^+}{\overset{\shortparallel}{B}}(\vec r_2, t_2)]_+\rangle$$

$$G^R_{\mathbf{k}}(\omega) = \iint_0^\infty dt\,(-i)\langle[\psi(\vec r_1,t),\psi^+(0,0)]\rangle\, e^{i\omega t - i\vec k\cdot\vec r}\, d^3r$$

$$G_{\mathbf{k}}(i\omega) = \iint_0^\beta d\tau\, e^{i\omega\tau}(-1)\langle T_\tau\, \psi(\vec r_1,\tau)\psi^+(0,0)\rangle\, e^{i\omega\tau - i\vec k\cdot\vec r}\, d^3r$$

We proved $\int G^R_{\mathbf{k}}(\omega)\,d\omega = 1$ and $G_{\mathbf{k}}(z) = \int \frac{A_{\mathbf{k}}(\omega)}{z-\omega}d\omega$ where $A_{\mathbf{k}}(\omega) = -\frac{1}{\pi}\mathrm{Im}\, G_{\mathbf{k}}(\omega)$

and $A_{\mathbf{k}}(\omega)$ is positive spectral function.

Noninteracting system: $\boxed{A_{\mathbf{k}}(\omega) = \delta(\omega-\varepsilon_{\mathbf{k}})}$ and $\boxed{G^R_{\mathbf{k}}(\omega) = \frac{1}{\omega-\varepsilon_{\mathbf{k}}+i\delta}}$

From definition $A(\omega) \equiv \sum_{mn} \delta(\omega+E_m-E_n)\langle m|c_{\mathbf{k}}|n\rangle\langle n|c^+_{\mathbf{k}}|m\rangle\left(\frac{e^{-\beta E_m}}{Z} + \frac{e^{-\beta E_n}}{Z}\right) \to \delta(\omega-\varepsilon_{\mathbf{k}})$

$|m\rangle = \prod_{k_i} c^+_{k_i}|0\rangle \qquad E_n = E_m + \varepsilon_{\mathbf{k}}$

$|n\rangle = c^+_{\mathbf{k}} \prod_{k_i\neq k} c^+_{k_i}|0\rangle \qquad \langle n|c^+_{\mathbf{k}}|m\rangle = 1$

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Which quantities can be computed from $G_2(\omega)$?

1) Density $\quad n(\vec r) = \lim_{\substack{\tau\to 0^- \\ \vec r_1 \to \vec r_2 = \vec r}} G(\vec r_1 \tau; \vec r_2 0) \equiv G(\vec r, \vec r; 0^-)$

from definition : $G(\vec r_1 \tau_1, \vec r_2 0) = -\langle T_\tau \psi(\vec r_1 \tau_1)\, \psi^+(\vec r_2 0)\rangle \Rightarrow \langle \psi^+(r_2, 0)\, \psi(r_1, 0)\rangle$

because $\tau_1 < 0$

2) Density matrix $\quad n(\vec r_1, \vec r_2) = \lim_{\tau\to 0^-} G(\vec r_1 \tau, r_2 0)$

3) Kinetic energy $\quad \langle \hat T\rangle = \lim_{\vec r' \to \vec r} \int \frac{\vec\nabla_{\vec r}^2}{2m} G(\vec r, \vec r'; 0^-)\, d^3r \equiv Tr(h^0 G)$

$$\lim_{\vec r' \to \vec r} \int \frac{\vec\nabla_{\vec r}^2}{2m} \langle \psi^+(\vec r')\, \psi(\vec r)\rangle = \langle \psi^+(\vec r) \frac{\nabla^2}{2m} \psi(\vec r)\rangle = \langle T\rangle \quad ✓$$

4) Potential energy $\quad \langle V_{ee}\rangle = \frac{1}{2} Tr(\Sigma G) \approx \frac{1}{2} Tr((i\omega - h^0) G)$

$\frac{1}{2} Tr((i\omega - h^0) G - 1)$

It should depend on two body density matrix :

$$\langle V_{ee}\rangle = \frac{1}{2} \iint V_c(\vec r - \vec r')\, \langle \psi^+(\vec r)\, \psi^+(\vec r')\, \psi(\vec r')\, \psi(\vec r)\rangle\, d^3r\, d^3r'$$

$$\approx \langle \underbrace{n(\vec r)\, n(\vec r')}\rangle \neq \langle n(\vec r)\rangle \langle n(\vec r')\rangle$$

needs single particle G.

$n(\vec r)\, n(\vec r')$ needs charge response function χ_c

Trick : Use equation of motion :

$$\frac{\partial}{\partial \tau_1} \hat\psi(\tau_1) = \frac{\partial}{\partial \tau_1}\left(e^{iH\tau_1} \hat\psi\, e^{-iH\tau_1}\right) = [H, \psi(\tau_1)] = -h_0(1)\, \hat\psi(1) - \int d2\, V(2,1)\, \hat\psi^+_{(2)}\, \hat\psi(2)\, \hat\psi(1)$$

evaluation of commutator :

$\boxed{\text{Note here we use } \int 1 \equiv \int d^3r_1 \text{ but not } \int 1 = \int d^3r_1 \int d\tau_1}$

$$H = \int d1\, \psi_1^+ h_0(1) \psi_1 + \frac{1}{2} \int \psi_1^+ \psi_2^+\, V(2-1)\, \psi_2\, \psi_1\, d1\, d2$$

$$[H, \psi(1)] = \int d2\, h_0(2) [\psi^+(2)\psi(2), \psi(1)] + \frac{1}{2} \int d2 d3\, V(2,3) [\psi^+(2)\psi^+(3)\psi(3)\psi(2), \psi(1)]$$

$$= -h_0(1)\psi(1) - \int d2\, V(2,1)\, \psi^+(2)\, \psi(2)\, \psi(1)$$

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$$\psi^\dagger(1)\frac{\partial}{\partial\tau_1}\psi(1) = -\psi^\dagger(1)h_0(1)\psi(1) - \int d2\, V(2,1)\psi^\dagger(1)\psi^\dagger(2)\psi(2)\psi(1)$$

$$\int d1 \langle \psi^\dagger(1)\left[\frac{\partial}{\partial\tau_1} + h_0(1)\right]\psi(1)\rangle = -2\langle V_{ee}\rangle$$

$$G(1) = -\langle T_\tau \psi(1)\psi^\dagger(0)\rangle$$

$$\lim_{\tau_1\to 0^-}\frac{\partial}{\partial\tau_1}G(1) = \langle \psi^\dagger(0^-)\frac{\partial}{\partial\tau_1}\psi(0)\rangle$$

$$\lim_{\tau_1\to 0^-} G(1) = \langle \psi^\dagger(0^-)\psi(0)\rangle$$

$$\langle V_{ee}\rangle = -\frac{1}{2}\lim_{\tau\to 0^-}\int d1 \left(\frac{\partial}{\partial\tau} + h_0\right)G(1) = -\frac{1}{2}\frac{1}{\beta}\sum_{i\omega}\int(-i\omega + h_0)G(\vec{r}_1, i\omega)\, d^3r_1$$

$$G(\vec{r}_1\tau) = \frac{1}{\beta}\sum_{i\omega} e^{-i\omega\tau}G(\vec{r}_1 i\omega)$$

$$\frac{\partial}{\partial\tau}G(\vec{r}_1\tau) = \frac{1}{\beta}\sum_{i\omega}\left[(-i\omega)e^{-i\omega\tau}G(\vec{r}_1 i\omega) + 1\right]$$

need to add proper constant to make it converge at $\tau\to 0$

$$\langle V_{ee}\rangle = \frac{1}{2}\frac{1}{\beta}\sum_{i\omega}\left[\int d^3r\,(i\omega - h_0)G(\vec{r}_1 i\omega) - 1\right]$$

Definition: $\mathrm{Tr}(\hat{O}G) \equiv \frac{1}{\beta}\sum_{i\omega}\int d^3r\, \hat{O}\, G(\vec{r}_1 i\omega)$

We can use Dyson : $G^{-1} = i\omega - h_0 - \Sigma$

$$\langle V_{ee}\rangle = \frac{1}{2}\mathrm{Tr}\left((G^{-1}+\Sigma)G - 1\right) = \frac{1}{2}\mathrm{Tr}(\Sigma G)$$

← this converges $G\sim\frac{1}{\omega_n}$, $\Sigma\sim\frac{1}{\omega_n}$

5) Total energy : $\langle T\rangle + \langle V_{ee}\rangle = \mathrm{Tr}\left((h_0 + \frac{1}{2}\Sigma)G\right)$

$\frac{1}{2}$ comes from two body interaction

6) Grand canonical partition function

But only if willing to integrate over coupling constant strength.

It contains entropy $S = -k_B T\,\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$ which measures "disorder"

When density matrix has eigenvalues 1 and 0, there is no entropy. When all eigenvalues are equal (and not 0 or 1) the entropy is maximal.

Can be directly computed by Luttinger-Ward approach (will see later).

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$\hat{H}_\lambda = \hat{H}_0 + \lambda \hat{V}_{ee}$ and λ will be set to unity at the end.

Then $\frac{\partial}{\partial\lambda} \ln Z = \frac{\partial}{\partial\lambda} Tr\left(e^{-\beta(H_0+\lambda V_{ee}-\mu N)}\right) = -\frac{\beta}{\lambda}\langle \lambda V_{ee}\rangle_\lambda$

where $\langle \lambda V_{ee}\rangle = \dfrac{Tr\left(e^{-\beta(H_0+\lambda V_{ee}-\mu N)}\cdot \lambda V_{ee}\right)}{Tr\left(e^{-\beta(H_0+\lambda V_{ee}-\mu N)}\right)}$

$\Omega = -\frac{1}{\beta}\ln Z$

$\frac{\partial}{\partial\lambda}\Omega = -\frac{1}{\beta}\frac{\partial}{\partial\lambda}\ln Z = \frac{1}{\lambda}\langle \lambda V_{ee}\rangle_\lambda$

hence

$$\underset{\substack{\uparrow\\ \text{interacting}\\ \text{system}}}{\Omega} = \underset{\substack{\uparrow\\ \text{non-interacting}\\ \text{system}}}{\Omega_0} + \int_0^1 \frac{d\lambda}{\lambda}\langle \lambda V_{ee}\rangle_\lambda = \Omega_0 + \frac{1}{2}\int_0^1 \frac{d\lambda}{\lambda} Tr_\lambda(\Sigma_\lambda G_\lambda)$$

like slowing turning on interactions. Should work in the absence of phase transitions.

Link to Experiment

$A_k(\omega) = -\frac{1}{\pi}\,Im\,G_k(\omega)$ is the spectra, which usually assumed to be measured by ARPES.

Conservation of momentum

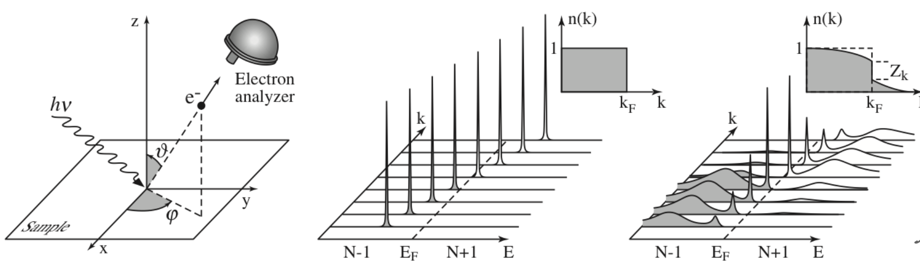
$\frac{h\vec{\nu}}{c_{light}} \approx 0 = -\vec{k}_i + (\vec{k}_d + \vec{K})$

$\vec{k}_i$: initial in material; $\vec{k}_d$: detected; $\vec{K}$: reciprocal

Conservation of energy

$h\nu + E_k = \frac{k_d^2}{2m} - \phi$, with $E_k = -|\omega|$

photon energy; detected by detector; work function



Photoemission geometry — Non-interacting electron system — Fermi liquid system

But this is really based on sudden approximation. In reality one needs to add matrix elements because the outgoing electron is plane wave, not just a hole in the solid

$$\underset{\substack{\uparrow\\ \text{measures negative energies}}}{G^R_k(-\omega)} = \iint d t\; i\,\underset{\substack{\uparrow\\ \text{create a hole in the material, and see}\\ \text{how it propagates.}}}{\langle[\psi^+_k(\vec{r},t), \psi(0,0)]\rangle}\, e^{+i\omega t - i\vec{k}\vec{r}}$$

$$G^R_k(-\omega) = \iint dt\, i\,\langle[\underset{\substack{\uparrow\\ \text{into which }(k,\omega)\text{ will hole relax}}}{\psi^+_k(t)}, \psi(0,0)]\rangle\, e^{i\omega t}$$

But here we do not care about outgoing electron

propagating hole, described by G; e^- goes to detector

Need to add matrix elements; basis for electrons in the solid: $|\langle \psi_{ik}(\vec{r})|e^{i\vec{k}\vec{r}}\rangle|^2$ — plane waves

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The two particle Green's function

$$G_2(\vec{r}_1\tau_1, \vec{r}_2\tau_2, \vec{r}_2{}'\tau_2{}', \vec{r}_1{}'\tau_1{}') = -\langle T_\tau\, \psi(\vec{r}_1\tau_1)\, \psi(\vec{r}_2\tau_2)\, \psi^+(\vec{r}_2{}'\tau_2{}')\, \psi^+(\vec{r}_1{}'\tau_1{}') \rangle$$

Short:

$$G_2(1,2,2',1') = -\langle T_\tau\, \psi(1)\psi(2)\psi^+(2')\psi^+(1')\rangle$$

Can express all other susceptibilities with G_2:

$$\chi_{charge}(1,2) = -\langle T_\tau\, n(1)\, n(2)\rangle = G_2(1,2,2^+,1^+)$$

$$\chi_{spin}(1,2) = -\langle T_\tau\, \vec{S}(1)\, \vec{S}(2)\rangle = -\langle T_\tau\, \psi^+_{s_1}(1)\, \sigma_{s_1 s_1'}\, \psi_{s_1'}(1)\, \psi^+_{s_2}(2)\, \sigma_{s_2 s_2'}\, \psi_{s_2'}(2)\rangle$$

$$= \sigma_{11'}\,\sigma_{22'}\, G_2(1,2,2^+,1^+)$$

Retarded Equivalent

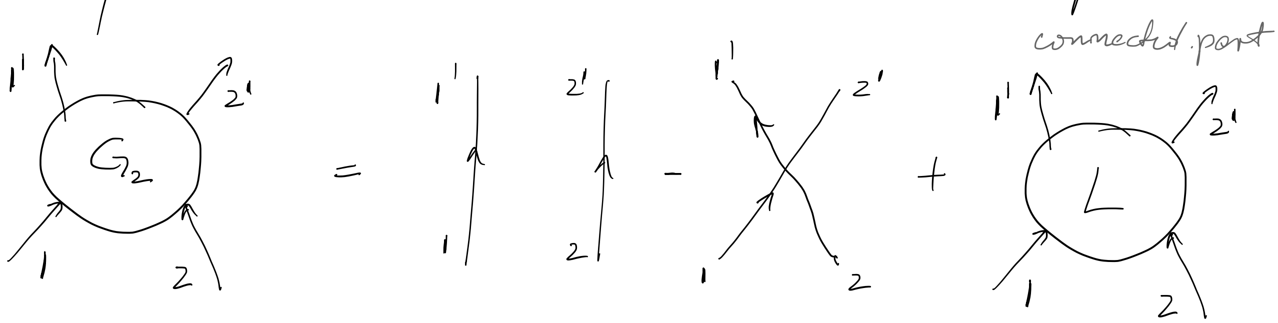
$$G_2^R(\vec{r}_1 t_1, \vec{r}_2 t_2, \vec{r}_2{}' t_2{}', \vec{r}_1{}' t_1{}')\Big|_{\substack{t_1'=t_1^+ \\ t_2'=t_2^+}} = -\,\theta(t_1-t_2)\langle \psi^+(\vec{r}_1{}'\tau_1^+)\psi(\vec{r}_1\tau_1)\psi^+(\vec{r}_2{}'\tau_2^+)\psi(\vec{r}_2\tau_2) - \psi^+(\vec{r}_2{}'\tau_2^+)\psi(\vec{r}_2\tau_2)\psi^+(\vec{r}_1{}'\tau_1^+)\psi(\vec{r}_1\tau_1)\rangle + 1 \leftrightarrow 2$$

The general case is a mess with 12 terms!

Homework:

Using Lehman representation show that G_2^R is analytically continued equivalent of G_2

Usually we calculate so-called connected part:



$$G_2(1,2,2',1') = G(1,1')G(2,2') - G(1,2')G(2,1') + L(1,2,2',1')$$

Note: every book seems to define the signs and orders of simple slightly differently.