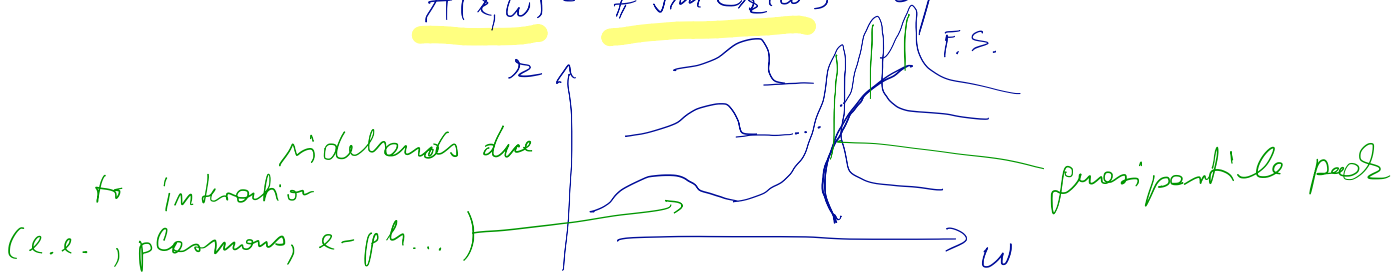
Correlation Functions (R.M. Chapter 5)

1) Provide a way to characterize the system theoretically, and many of C.F. are directly measured in experiment:

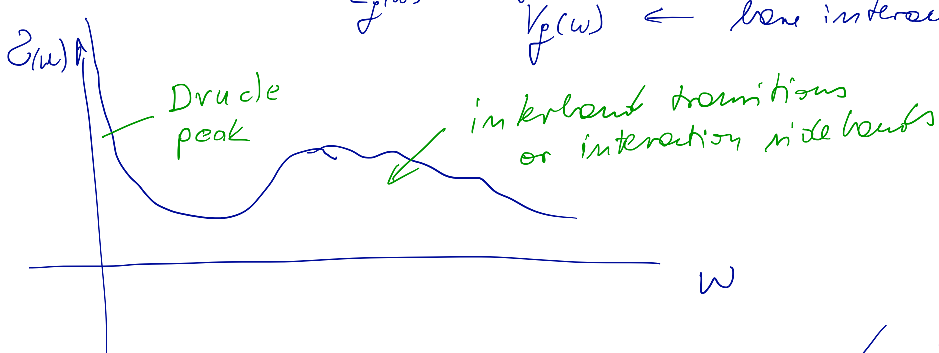
a) $A(k,\omega) = -\frac{1}{\pi} \operatorname{Im} G_k(\omega)$ by ARPES



b) optical conductivity $\sigma_{q=0}(\omega) = \omega \operatorname{Im}\left(\varepsilon_q(\omega)\right)$ where ε is dielectric function

and $\frac{1}{\varepsilon_q(\omega)} = \frac{W_q(\omega)}{V_q(\omega)}$ ← screened interaction
← bare interaction

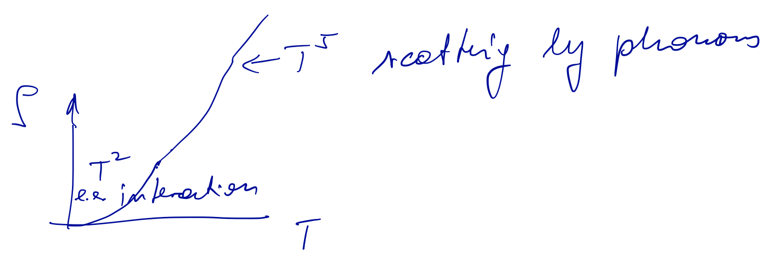
$\frac{1}{\varepsilon_q(\omega)} = 1 - V_q \chi_q(\omega)$



$\chi_c(\vec{r}_1\tau_1, \vec{r}_2\tau_2) = \langle \psi_1^+ \psi_2^+ \psi_2 \psi_1 \rangle$

$1 \equiv (\vec{r}_1, \tau_1)$
$2 \equiv (\vec{r}_2, \tau_2)$

c) resistivity: $\rho = \frac{1}{\sigma_{q=0}(\omega=0)}$

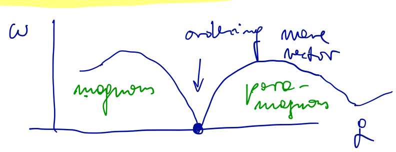


d) spin susceptibility

Inelastic neutron scattering measures $S(q,\omega) = \frac{\chi_s''(q,\omega)}{1-e^{-\beta\omega}}$

where $\chi_s(\vec{r}_1\tau_1, \vec{r}_2\tau_2) = \langle \psi_{s_1}^+(\vec{r}_1\tau_1)\vec{\sigma}_{s_1s_2}\psi_{s_2}(\vec{r}_1\tau_1)\,\psi_{s_3}^+(\vec{r}_2\tau_2)\vec{\sigma}_{s_3s_4}\psi_{s_4}(\vec{r}_2\tau_2)\rangle$

$= \langle \vec{S}(\tau_1)\cdot\vec{S}(\tau_2)\rangle$



e) Single particle correlation function (main building block of many body)

b...d) Two particle correlation function (harder to compute, but clearly very important)

(2)

Short note on the grand canonical ensemble

At constant particle number use

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = e^{-\beta F} \qquad dF(V,T,N) = -p\,dV - S\,dT + \mu\,dN$$

When the number of particles is not constant, we use Legendre transform

$$Z = \mathrm{Tr}\left(e^{-\beta(H-\mu\hat{N})}\right) = e^{-\beta\Omega} \qquad \text{where } \Omega = F - \mu N$$

$$d\Omega(V,T,\mu) = -p\,dV - S\,dT - N\,d\mu$$

In these lectures we will use

$\mathrm{Tr}(e^{-\beta H} \dots)$ instead of $\mathrm{Tr}(e^{-\beta(H-\mu N)} \dots)$ for short notation, hence H in such trace stands for $\hat{H} \to \hat{H} - \mu\hat{N}$.

③ # Dynamic Correlation Function

Imaginary time & time ordered

$$\langle\langle A; B\rangle\rangle \equiv -\langle T_\tau A(\vec r_1,\tau_1)\, B(\vec r_2,\tau_2)\rangle = -\frac{1}{Z}\mathrm{Tr}\left(T_\tau\, e^{-\beta H}\, \underbrace{e^{H\tau_1}A(\vec r_1)\,e^{-H\tau_1}}_{\text{Heissenberg, in imaginary time}}\; e^{H\tau_2}B(\vec r_2)\,e^{-H\tau_2}\right)$$

here $H \equiv \hat H - \mu \hat N$ if working with grand canonical ensemble.

where $\langle T_\tau A(\tau_1)\, B(\tau_2)\rangle = \Theta(\tau_1>\tau_2)\langle A(\tau_1)\, B(\tau_2)\rangle \overset{\text{fermions}}{\underset{\text{bosons}}{\mp}} \Theta(\tau_2>\tau_1)\langle B(\tau_2)\, A(\tau_1)\rangle$

most useful for calculation

Real time & time ordered

$$\langle\langle A; B\rangle\rangle^T = -i\frac{1}{Z}\mathrm{Tr}\left(T_t\, e^{-\beta H}\, e^{iHt_1} A(\vec r_1)\, e^{-iHt_1}\, e^{iHt_2} B(\vec r_2)\, e^{-iHt_2}\right)$$

useful for $T=0$ calculations

Retarded C.F.

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

fermionic ($+$)

bosonic ($-$)

meassured in experiment

Can be obtained from Matsubara by analitic continuation

Fourier transform

$$\langle\langle A; B\rangle\rangle(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\langle\langle A(t); B(0)\rangle\rangle\, dt \qquad \text{real time}$$

$$\langle\langle A; B\rangle\rangle(i\omega) = \int_{0}^{\beta} e^{i\omega \tau}\langle\langle A(\tau); B(0)\rangle\rangle\, d\tau \qquad \text{imaginary time \& imaginary frequency}$$

What is relation between them?

$$\langle\langle A; B\rangle\rangle^R = -i\,\Theta(t_1-t_2)\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H}\left\{e^{iHt_1} A\, e^{-iH(t_1-t_2)} B\, e^{-iHt_2} \pm e^{iHt_2} B\, e^{-iH(t_2-t_1)} A\, e^{-iHt_1}\right\}\right)$$

$$= -i\,\Theta(t_1-t_2)\frac{1}{Z}\sum_{m,n} e^{E_m(-\beta+it_1)}\langle m|A|n\rangle\, e^{-iE_n(t_1-t_2)}\langle n|B|m\rangle\, e^{-iE_m t_2} \pm e^{E_m(-\beta-it_2)}\langle m|B|n\rangle\, e^{-iE_n(t_2-t_1)}\langle n|A|m\rangle\, e^{-iE_m t_1} =$$

many body eigenstates

$$= -i\,\Theta(t_1-t_2)\sum_{m,n}\langle m|A|n\rangle\langle n|B|m\rangle\, e^{i(E_m-E_n)(t_1-t_2)}\left(\frac{e^{-\beta E_m}}{Z} \pm \frac{e^{-\beta E_n}}{Z}\right)$$

$$\langle\langle A; B\rangle\rangle^R(\omega) = -i\int_0^\infty dt\, e^{i(\omega+i\delta)t}\sum_{m,n}\langle m|A|n\rangle\langle n|B|m\rangle\, e^{i(E_m-E_n)t}\left(\frac{e^{-\beta E_m}}{Z} \pm \frac{e^{-\beta E_n}}{Z}\right) =$$

to make it converge

$$= \sum_{mn}\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{(\omega+E_m-E_n+i\delta)}\left(\frac{e^{-\beta E_m} \pm e^{-\beta E_n}}{Z}\right)$$

(Lehmann representation)

Define $A(\omega) \equiv \sum_{mn}\delta(\omega+E_m-E_n)\langle m|A|n\rangle\langle n|B|m\rangle \times \left(\frac{e^{-\beta E_m}}{Z} \pm \frac{e^{-\beta E_n}}{Z}\right)$

$$\langle\langle A; B\rangle\rangle^R(\omega) = \int \frac{A(x)}{\omega - x + i\delta}\, dx$$

(spectral representation)

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Now for Matsubara equivalent:

$$\langle\langle A; B\rangle\rangle(i\omega) = -\int_0^\beta d\tau\, e^{i\omega\tau}\left\{\Theta(\tau>0)\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H} e^{H\tau} A\, e^{-H\tau} B\right) \mp \Theta(\tau<0)\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H} B\, e^{H\tau} A\, e^{-H\tau}\right)\right\}$$

$A(\tau)$ $B(0)$

$$= -\sum_{mn}\int_0^\beta d\tau\, e^{i\omega\tau}\langle m|A|n\rangle\langle n|B|m\rangle\left\{\Theta(\tau>0)\frac{1}{Z}e^{E_m(-\beta+\tau)-E_n\tau} \mp \Theta(\tau<0)\frac{1}{Z}e^{E_n(-\beta-\tau)+E_m\tau}\right\}$$

$$= -\sum_{m,n}\langle m|A|n\rangle\langle n|B|m\rangle\frac{e^{-\beta E_m}}{Z}\int_0^\beta e^{\tau((E_m-E_n)+i\omega)}d\tau = \sum_{m,n} -\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}\frac{e^{-\beta E_m}}{Z}\left(e^{\beta i\omega+\beta(E_m-E_n)}-1\right)$$

$$= \sum_{m,n}\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}\frac{e^{-\beta E_m}}{Z}\left(\pm e^{\beta(E_m-E_n)}+1\right) =$$

$$\beta i\omega = \begin{cases}\text{fermion} & (2n+1)\pi\\ \text{boson} & 2n\pi\end{cases} \qquad e^{\beta i\omega} = \begin{cases}-1\\ +1\end{cases}$$

$$= \sum_{m,n}\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}\left(\frac{e^{-\beta E_m}\pm e^{-\beta E_n}}{Z}\right)$$

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we can also integrate $\int_{-\beta}^0 d\tau\left(\pm\frac{1}{Z}\right)e^{-\beta E_n+\tau(E_m-E_n+i\omega)}\langle m|A|n\rangle\langle n|B|m\rangle = \pm\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}e^{-\beta E_n}\left(1-e^{-\beta(i\omega+E_m-E_n)}\right)$

$$= \pm\left(e^{-\beta E_n}\pm e^{-\beta E_m}\right)\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}$$

equal

Conclusion: $\langle\langle A;B\rangle\rangle^R(\omega) = \langle\langle A;B\rangle\rangle\underbrace{(i\omega\to\omega+i\delta)}_{\text{Analytic continuation}}$

It is much easier to work with Matsubara $i\omega$ than real time/frequency. No need to take care of convergence, poles, (limit $\beta\to\infty$, $V\to\infty$).

It turns out $T=0$ calculation can be wrong because the correct order of limits is $(\beta\to\infty, V\to\infty)$, which is done in Matsubara, while $T=0$ calculation corresponds to $(V\to\infty, \beta\to\infty)$, which can be different.

Conclusion: Matsubara method is "safer" and easier.

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Properties of correlation functions

back to Lehmann representation

$$\langle\langle A;B\rangle\rangle^R_{(\omega)} = \sum_{mM} \frac{\langle m|A|M\rangle\langle M|B|m\rangle}{(\omega+E_m-E_M+i\delta)}\left(\frac{e^{-\beta E_m}\pm e^{-\beta E_M}}{Z}\right)$$

if $B=A^+$ like $G^R=-\langle T_\tau\, \psi(\tau)\, \psi^+(0)\rangle$

or $\chi_s = -\langle T_\tau\, \vec S(\tau)\cdot\vec S(0)\rangle$

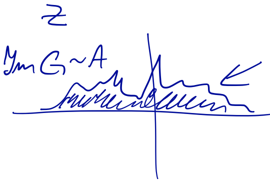
or $\chi_c = -\langle T_\tau\, \rho(\tau)\, \rho(0)\rangle$

then $\langle m|A|M\rangle\langle M|A^+|m\rangle = |\langle m|A|M\rangle|^2>0$

$$\mathrm{Im}\left(\langle\langle A;A^+\rangle\rangle^R(\omega)\right) = \sum_{m,M} -\pi\,\delta(\omega+E_m-E_M)\,|\langle m|A|M\rangle|^2\,\frac{e^{-\beta E_m}\pm e^{-\beta E_M}}{Z}$$

for fermions $\mathrm{Im}\left(\langle\langle A;A^+\rangle\rangle^R(\omega)\right)<0$

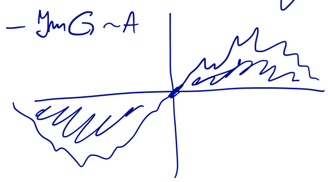
$-\mathrm{Im}\,G\sim A$



causality requires positive spectral function

for bosons $\mathrm{Im}\left(\langle\langle A;A^+\rangle\rangle^R(\omega)\right) = -\mathrm{sign}(\omega)$;

$-\mathrm{Im}\,G\sim A$



$E_M>E_m \Rightarrow \omega>0 \Rightarrow -\pi\cdot$ positive

$E_M<E_m \Rightarrow \omega<0 \Rightarrow$

What about real part? From spectral representation

$$\langle\langle A;B\rangle\rangle^R(\omega) = \int \frac{A(x)}{\omega-x+i\delta}\,dx$$

$$G(\omega) = \int_{-\infty}^{\infty} \frac{-\frac{1}{\pi}\mathrm{Im}\,G(x)}{\omega-x+i\delta}\,dx$$

$$\mathrm{Re}\,G(\omega) = \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{\mathrm{Im}\,G(x)}{x-\omega}\,dx$$

Kramers-Kronig relations

Sum Rules for spectra.

Back to its definition $A(\omega) \equiv \sum_{mM}\delta(\omega+E_m-E_M)\langle m|A|M\rangle\langle M|B|m\rangle\left(\frac{e^{-\beta E_m}}{Z}\pm\frac{e^{-\beta E_M}}{Z}\right)$

$$\int_{-\infty}^{\infty} A(\omega)\,d\omega = \sum_{m,M}\langle m|A|M\rangle\langle M|B|m\rangle\frac{e^{-\beta E_m}}{Z} \pm \langle M|B|m\rangle\langle m|A|M\rangle\frac{e^{-\beta E_M}}{Z} = \langle AB\pm BA\rangle = \langle [A,B]_\pm\rangle$$

For fermionic $G=-\langle T_\tau\,\psi(\tau)\psi^+(0)\rangle \Rightarrow [\psi,\psi^+]_+=1 \Rightarrow \int A(\omega)\,d\omega=1$

For bosons $\Rightarrow [\psi,\psi^+]_-=1 \Rightarrow \int A(\omega)\,d\omega=1$

For susceptibility $A=B=\begin{cases} S \\ \rho\end{cases} \Rightarrow \begin{array}{l}[S,S]_-=0\\ [\rho,\rho]_-=0\end{array} \Rightarrow \int \chi''(\omega)\,d\omega=0$

⑥ For bosons it is convenient to rewrite:

$$A(\omega) \equiv \sum_{nm} \delta(\omega+E_m-E_n)\langle n|A|m\rangle\langle m|B|n\rangle \left(\frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z}\right) = \sum_{nm} \delta(\omega+E_m-E_n)\langle n|A|m\rangle\langle m|B|n\rangle \frac{e^{-\beta E_n}}{Z}\left(1-e^{-\beta(E_m-E_n)}\right)$$

$$A(\omega) = \left(1-e^{-\beta\omega}\right) \underbrace{\sum_{n,m} \delta(\omega+E_m-E_n)\langle n|A|m\rangle\langle m|B|n\rangle \frac{e^{-\beta E_n}}{Z}}_{\text{positive}}$$

Complex representation

Back to spectral representation: $\langle\langle A;B\rangle\rangle^R(\omega) = \int \frac{A(x)}{\omega - x + i\delta}\,dx$

Matsubara: $\langle\langle A;B\rangle\rangle(i\omega) = \int \frac{A(x)}{i\omega - x}\,dx$

Complex quantity defined in the entire plane for convenient integration: $\langle\langle A;B\rangle\rangle(z) = G(z) = \int \frac{A(x)}{z-x}\,dx$

has poles when z is on real axis

if $z = \omega + i\delta \Rightarrow$ retarded G

$z = \omega - i\delta \Rightarrow$ advanced G