Notes on correlation functions (ch 5)

1.- Summary:

- Static correlation fn: correlation between events at equal times

ex: density correlations → determine Energy & Thermodynamic potentials

- Dynamic: events at different times

ex: response functions → describe excitations of the system

→ Only 1 & 2 body correlations here

→ Note: Linear response because perturbations (light, scattering of particles) are very weak on the scale or microscopic forces

2.- Expectation Values & Correlation fns:

EV: $\langle \hat{O} \rangle = \sum_\alpha w_\alpha \langle \alpha | \hat{O} | \alpha \rangle$ $\hat{O}$ → operator

α → MB WF.

$T=0$ $\alpha = GS$ $\omega_\alpha = \delta_{\alpha,0}$

W_α → probability of α in the total α distribution.

Thermodynamic Eq:

$$\langle \hat{O} \rangle = \frac{1}{Z} \mathrm{Tr} \{ e^{-\beta(\hat{H} - \mu \hat{N})} \hat{O} \}$$

$$Z = \mathrm{Tr} \{ e^{-\beta(\hat{H} - \mu \hat{N})} \} \equiv e^{-\beta \Omega}$$

over all states

$E_\alpha = \langle \alpha | \hat{H} | \alpha \rangle$, $N_\alpha = \langle \alpha | \hat{N} | \alpha \rangle$ so

With $w_\alpha = \dfrac{e^{-\beta(E_\alpha - \mu N_\alpha)}}{Z}$ $\quad Z = \sum_\alpha e^{-\beta(E_\alpha - \mu N_\alpha)}$

→ Notation $(1) \rightarrow (\underbrace{\cancel{x}\, r_1, \sigma_1}_{x_1}, t_1)$

→ [redacted] correlated : $\langle \hat{A}(i)\, B(j) \rangle \neq \langle \hat{A}(i) \rangle \langle \hat{B}(j) \rangle$

$\cancel{C_{AB}(1,2) = \sum_\alpha w_\alpha \langle \alpha | A}$

→ Notation : (Heisenberg operator) $\hat{O}_H(1) = e^{i\hat{H}t_1}\, \hat{O}(x_1)\, e^{-i\hat{H}t_1}$
used in dynamic correlations

So :

$$C_{AB}(1,2) = \sum_\alpha \langle \alpha | \hat{A}_H(1)\, \hat{B}_H(2) | \alpha \rangle \equiv \langle \hat{A}_H(1)\, B_H(2) \rangle$$

→ Note that $\langle \hat{A}_H(1)\, \hat{B}_H(2) \rangle - \underbrace{\langle A_H(1) \rangle \langle B_H(2) \rangle}$ = fluctuations,

often is substracted

→ Notation : omit H for static correlation fns.

5.2 Static 1e^- properties : $(x = r, \sigma)$

• Density: $$n(x) = \langle \hat{n}(x) \rangle = N \sum_\alpha W_\alpha \int dx_2 \ldots dx_N \, |\psi_\alpha(x, x_2 \ldots x_N)|^2$$

→ integrate out all other e^- positions & spins.

Single slater ~~Ddeterminant~~ determinant $n(x) = \sum_i |\psi_i(x)|^2$

→ Density needs to be well described in our approximations

→ show figure

• 1 body Density Matrix (spin resolved)

$\rho(x, x')$: Correlation of ~~the MB WF~~ 1 particle correlation in the MB wave function at 2 different points of spin & space $(x, x' \to r, \sigma \to r'\sigma')$

$$\rho(r, r') = N \sum_\alpha W_\alpha \int dx_2 \ldots dx_N \, \psi_\alpha^*(x, x_2 \ldots x_N) \psi_{\alpha'}(x', x_2 \ldots x_N)$$

• $\rho(x, x') = n(x)$

. The eigenfunctions of $\rho(x, x')$ are the "Natural Orbitals" and the eigenvalues n_i are the occupation numbers:

$$\sum_{\sigma'} \int d^3r' \, \rho(x, x') \varphi_i(x') = n_i \underbrace{\varphi_i(x)}_{NO}$$

n_i and φ_i are the MB generalization of the KS orbitals and occupations

Note: in a SD wave function, $T=0$, for independent particles $n_i = 0$ or 1 (KS for example)

→ For a Full MB WF $0 \le n_i \le 1$ ⇒ interactions mix the independent particle states and result in non integer occupation # So $\rho(x,x')$ is not idempotent.

→ Fermions: always localized ($\rho(x,x') \to 0$ for $\delta r = r - r' \to \infty$) however the decay depends on the type of systems.

insulator → $e^{-\delta r}$

metal → $(\delta r)^{-3}$ (3D)

→ Bosons: off-diagonal long range order ($\delta r \to \infty$ $\rho(r,r') \to$ constant)

Momentum distribution

$P(\vec{k})$ → probability of finding a particle with momentum $\vec{k}_1$

→ integrate out all momenta of the 3N-dimensional momentum distribution.

all vectors

$$\rho(\vec{k}_1) = (2\pi)^{-3N} \sum_\alpha W_\alpha \int dk_2 \dots dk_N \left| \int dx_1 \dots dx_N \, \Psi_\alpha(x_1 \dots x_N) e^{-i\sum_j k_j r_j} \right|^2$$

$$\rho(k) = \frac{1}{(2\pi)^3 N} \int dr \int dr' e^{-ikr'} \rho(r, r-r')$$ → FT of the spin integrated 1B density matrix.

Normalized: $\int \rho(k)\, dk = 1$ (it's a probability distribution)

$\langle \hat{T} \rangle = \frac{N}{2} \int d\vec{k}\, k^2 \rho(k)$

In a real system (correlated) $0 \le \rho(k) \le 1$ even at $T=0$

in the HEG (Non interacting) the eigenstates are PW ($\psi_k = \frac{1}{\sqrt{V}} e^{ikr}$)

and $\rho_k = 1$ $k \le k_F$; $\rho_k = 0$ otherwise.

→ Interactions open a gap in the distribution (see fig 5.2) Correlations decrease the total energy ($V \downarrow$ but $K \uparrow$ mixing in higher momentum states) ⇒ discontinuity at k_F decreases : Z = ~~size~~ magnitude of the discontinuity ~ $\Sigma(\omega)$ self energy.

↓

QP strength. $Z \to 1$ for $U \to 0$ (at $r_s = 1$, weak correlation)

Z decreases with increasing correlation.

Connection to experiment: Compton scattering

measures spectra of X-ray scattering (high Energy)

$$J(q) = \frac{3}{8\pi k_F^3} \int_0^q dk\, k\, \rho(k)$$

⇒ invert experiment data and obtain $\rho(k)$

↓ exp ↓ e^-

in the impulse approximation (excited e^- = free e^-) see fig 11.7 for Na

→ Two particle correlations (still static)

$n(x,x')$ → Prob of finding 2 particles at x, 1 at x' (spin & position)

$$n(x,x') = \sum_{i\neq j} \langle \delta(x-x_i)\,\delta(x'-x_j)\rangle = N(N-1)\int dx_3 \ldots dx_N \,|\Psi_0(x,x',x_3 \ldots x_N)|^2$$

$$g(x,x') = \frac{n(x,x')}{n(x)\,n(x')}$$

See fig 5.3

$g(x,x') \to 1$ for $\delta r \xrightarrow{(|r-r'|)} \infty$, generally depends on the spin of e^-. It's unity for uncorrelated particles

$$g_{\sigma,\sigma'}(r) = \frac{\Omega}{N(N-1)}\int_\Omega dr' dr''\, n(\underbrace{r',r'',\sigma,\sigma'}_{\text{or } x' \; x''})\,\delta(r'-r''-r)$$

→ Probability of finding a particle of spin σ at distance r of particle of spin σ'.

$$g(\vec{r})_{Total} = \sum_{\sigma,\sigma'} g_{\sigma,\sigma'}(r)$$ See fig 5.3

e^- interaction energy/volume $\langle \hat{V}_{ee}\rangle = \frac{N(N-1)}{2\Omega}\int_\Omega dr\, \frac{(g(r)-1)}{r}$

The (-1) in the eq. comes from cancelling the ∞ of the e⁻-e⁻ interaction That is cancelled with The ∞ of the e⁻ ion interaction (Total system is neutral)

Structure factor : connected To The Fourier ~~Tr~~ Transform of The pair correlation fn. Measured by X-ray or neutron scattering

i.e. $\hat{\rho}^{\sigma}_{k}$ operator : The average value is The F.T of The spin resolved density : $\hat{\rho}^{\sigma}_{k} = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} e^{ikr_i} \delta_{\sigma,\sigma_i}$

→ static structure factor :

$$S^{\sigma\sigma'}_{kk'} = \langle \hat{\rho}^{\sigma}_{-k} \rho^{\sigma'}_{k} \rangle = \frac{1}{N} \int_{\Omega} dr\,dr'\, n(x,x')\, e^{i(kr-k'r')} + \frac{\delta_{\sigma\sigma'}}{N} \int dr\, n(x)\, e^{i(k-k')}$$

→ $S_{kk'}$ has The periodicity & symmetry of The crystal.

with Translational invariance $S_{kk'} = 0$ for $k \neq k'$

Diagonal part only, Total $S_k = \sum_{\sigma\sigma'} S^{\sigma,\sigma'}_{k,k}$

→ Non interacting HEG :

$$S_k = \begin{cases} N/2 & k=0 \\ \frac{k}{4k_F}\left(3-\left(\frac{k}{2k_F}\right)^2\right) & 0 \le k \le 2k_F \\ 1 & 2k_F \cancel{<} K \end{cases}$$

See fig 5.3 → S_k for N.I e^- should be quadratic for $k \to 0$ (right) but it is linear.

Why? $S_k \le \frac{k^2}{2\omega_p}\left(1-\frac{1}{\varepsilon_k}\right)^{1/2}$ S_k is bounded by the dielectric fn.

measures amplitude of density fluctuations

dielectric function.

→ Why is this? In a charged system the long-range Coulomb interaction suppresses density fluctuations much more strongly than in a free Fermi gas.

Long wave length (small k) fluctuations in ρ costs a lot of energy ⇒ system responds by screening this fluctuations. Their response is controlled by the dielectric fun ε_k.

So dielectric screening forces $S(k)$ to be smaller than what is predicted by the Pauli Principle alone.

So $S_k \to 0$ quadratically (or faster) and not linearly.

Crystalline solid → long range order in S_k (Bragg peaks) See fig 5.4

5.4 Dynamic correlation Functions

→ Notation : $(x_1, t_1) \to (\mathbf{r}_1, \sigma_1, t_1) \to (1)$

1 - Dynamic correlation in Time :

$C_{AB}(1,2) = \langle \hat{A}_H(1) \hat{B}_H(2) \rangle$ Note : $\hat{O}_H(t) \to$ Heisenberg operator

(Wave function is stationary and Time dependence is carried by operators).

• $\hat{H}$ is static (no phonons) for now.

Then Time dependence only as $t - t_0$

$$\hat{O}_H(t) = e^{i\hat{H}(t-t_0)} \hat{O} e^{-i\hat{H}(t-t_0)}$$ $t_0 \to$ reference Time, we can set To zero.

The correlation function can be expanded in Terms of

$|\alpha\rangle \to$ eigenstates of H

$$C_{AB}(x_1, x_2, t_1 - t_2) = \sum_\alpha W_\alpha e^{iE_\alpha(t_1-t_2)} \langle \alpha | \underbrace{\hat{A}(x_1)}_{\text{Time independent operator}} e^{-i\hat{H}(t_1-t_2)} \hat{B}(x_2) | \alpha \rangle$$

insert $\mathbb{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$

complete set of H eigenstates

$$C_{AB}(x_1, x_2, t_1 - t_2) = \sum_{\alpha,\lambda} W_\alpha A_{\alpha\lambda}(x_1) B_{\lambda\alpha}(x_2) e^{i(E_\alpha - E_\lambda)(t_1-t_2)}$$

$A_{\alpha\lambda} = \langle \alpha | \hat{A}(x_1) | \lambda \rangle$.

→ One subtract the uncorrelated term $C^0_{AB}(x_1 x_2) = \langle \hat{A}_H(1)\rangle \langle \hat{B}_H(2)\rangle$

$= \sum_\alpha W_\alpha A_{\alpha\alpha}(x_1) \sum_\lambda W_\lambda B_{\lambda\lambda}(x_2)$ (No time dependence).

For states with fixed particle number this term is non zero only if $\hat{A}$ and $\hat{B}$ conserve particle number.

Note : $\tilde{C}_{AB}(1,2) = -C_{BA}(2,1)$ (anticommutation of Fermionic operators.)

$\sim$, drop subscript AB or BA

Definition :

- Retarded Correlation Fn :

$$C^R(1,2) = \Theta(t_1 - t_2) \langle [\hat{A}(1), \hat{B}(2)] \rangle = \Theta(t_1 - t_2) \left[C(1,2) - \tilde{C}(1,2) \right]$$

- Advanced :

$$C^A(1,2) = \Theta(t_2 - t_1) \langle [\hat{A}(1), \hat{B}(2)] \rangle = \Theta(t_2 - t_1) \left(\tilde{C}(1,2) - C(1,2) \right)$$

- Time ordered :

Time ordering of operators

$$C^T(1,2) = \langle T[\hat{A}(1), \hat{B}(2)] \rangle = \Theta(t_1 - t_2) C(1,2) + \Theta(t_2 - t_1) \tilde{C}(1,2)$$

$$= C^R(1,2) + \tilde{C}(1,2) = C^A(1,2) + C(1,2)$$

Dynamic Correlation in frequency space:

→ fluctuation spectrum

$$C(x_1, x_2, \omega) = \int_{-\infty}^{\infty} dt \sum_{\alpha\lambda} W_\alpha A_{\alpha\lambda}(x_1) B_{\lambda\alpha}(x_2) e^{i(E_\alpha - E_\lambda)t} e^{i\omega t}$$

$$= 2\pi \sum_{\alpha,\lambda} W_\alpha A_{\alpha\lambda}(x_1) B_{\lambda\alpha}(x_2) \delta(E_\alpha - E_\lambda + \omega)$$

$$\tilde{C}(x_1 x_2 \omega) = -2\pi \sum_{\alpha\lambda} W_\alpha B_{\alpha\lambda}(x_2) A_{\lambda\omega}(x_1) \delta(E_\lambda - E_\alpha + \omega)$$

for a finite system the fluctuation spectrum is a set of δ-funcs.
in the thermodynamic limit → continuum, weighted density of transitions

→ Spectral Functions

Let's define the spectral function A:

$$2\pi A(x_1, x_2, \omega) = \left[C(x_1, x_2, \omega) - \tilde{C}(x_1, x_2, \omega)\right]$$

in thermal equilibrium where $\tilde{C}(x_1 x_2; \omega) = -e^{-\beta(\omega-\mu)} C(x_1, x_2; \omega)$
we have:

$$2\pi A(x_1, x_2, \omega) = C(x_1, x_2, \omega)\left[1 - e^{-\beta(\omega-\mu)}\right]$$

if $[\hat{A}(x_1), B(x_2)] = f(x_1, x_2)$ → scalar function,

sum rule for The spectral fn:

~~$\hat{A}(x_1$~~ $$\int d\omega\, A(x_1, x_2, \omega) = f(x_1, x_2)$$

The spectral function contains all The information about The dynamic correlation functions; (Drop x_1, x_2 but still There in The following)

→ Move To Complex ω plane

$$C^R(\omega) = i \lim_{\eta \to 0^+} \int d\omega' \frac{A(\omega')}{\omega - \omega' + i\eta}$$ → poles below real axis

$$C^A(\omega) = i \lim_{\eta \to 0^+} \int d\omega' \frac{A(\omega')}{\omega - \omega' - i\eta}$$ → poles above real axis.

See Fig 5.5

We can analitically continue These expressions into The full complex plane: $\omega \to z$ $\underset{\text{real } \omega}{C} \to \underset{\text{complex } \omega\ (z)}{\mathcal{C}}$

$$\mathcal{C}(z) = i \int_{-\infty}^{\infty} d\omega' \frac{A(\omega')}{z - \omega'}$$ → Lehman Representation

$\mathcal{C}$ is analytic everywhere except along The real axis where There are singularities & Branch cuts.

$$C^R(\omega) = \lim_{\eta \to 0^+} \mathcal{C}(\omega + i\eta)$$

$$C^A(\omega) = \lim_{\eta \to 0^+} \mathcal{C}(\omega - i\eta)$$

Finally can be shown:

$$2\pi A(\omega) = \lim_{\eta \to 0^+} \left[\mathcal{C}(\omega + i\eta) - \mathcal{C}(\omega - i\eta)\right] = C^R(\omega) - C^A(\omega)$$

spectral func

$$= 2\,\mathrm{Im}\left[i C^R(\omega)\right]$$

if $A(\omega)$ is real

Note (we will see that in terms of Greens Fns we have

$$A(\omega) = \frac{1}{\pi} \left| \mathrm{Im}\, G(\omega) \right|$$

Correlations at $T=0$ and N fixed

$$A(\omega) = \sum_\lambda \delta(\omega - \mathcal{E}_\lambda) \cdot \begin{cases} A_{0\lambda} B_{\lambda 0} & \text{for } \omega > \mu \\ -B_{0\lambda} A_{\lambda 0} & \text{for } \omega < \mu \end{cases}$$

$$\mathcal{E}_\lambda = \pm (E_\lambda - E_0) \quad \omega \gtrless \mu$$

GS

$$A(\omega) = \frac{1}{\pi} \begin{cases} +\mathrm{Im}\left[i C^T(\omega)\right] & \omega > \mu \\ -\mathrm{Im}\left[i C^T(\omega)\right] & \omega < \mu \end{cases}$$

Response Functions

→ Describes the response of a system to an external perturbation.

What is the change of $\langle \hat{A}_H(1) \rangle$ (expectation value of operator A at x_1 time t_1 when a perturbation a time $t_2 < t_1$ happened in x_2.

Perturbation: $\phi(2)$ a time dependent field that couples to operator $\hat{B}(2)$ acting on the system:

$$H \to \hat{H} + \int dx_2 \, \phi(x_2, t) \hat{B}(x_2)$$

$$\phi(x,t) = 0 \text{ for } t < t_0$$

includes effect of perturbation

$$\langle \hat{A}_H(1) \rangle^+ = \langle U^+(t_1, t_0) \hat{A}(x_1) U(t_1, t_0) \rangle$$

$$U(t_1, t_0) = e^{-i \int_{t_0}^{t_1} dt_2 \left[H + \int dx_2 \, \phi(2) \hat{B}(x_2) \right]}$$

Time evolution operator

This U can be expanded in powers of ϕ (not trivial cause $\hat{H}$ and $\int dx_2 \phi \hat{B}(x_2)$ do not necessarilly commute!

$$e^{-i \int_{t_0}^{t_1}} = 1 + i \int_{t_0}^{t_1}$$

The coefficients in the expansion of the full expectation value are called response functions.

Most experiments measure the 1st order $\langle \hat{A}_H(1) \rangle$

or so called linear response.

Second harmonic generation measures the second order

but we focus on linear response.

Linear Response

$$\delta \langle \hat{A}_H(1) \rangle = \langle A_H(1) \rangle^{+} - \langle A_H(1) \rangle = \int_{-\infty}^{\infty} dt_2 \int dx_2 \, \chi_{AB}(1,2) \phi_2$$

with $\chi_{AB}(1,2) = -i\,\Theta(t_1 - t_2) \langle [A_H(1), B_H(2)]_- \rangle$

Linear response function.

i.e. it is a correlation function of a commutator of Heisenberg operators $\rightarrow$ Corresponds to our definition of retarded correlation fn: $-i C^R_{AB}(1,2) \rightarrow \chi_{AB}(1,2)$

Using all we derived before we can see that $A(\omega) = -\frac{1}{\pi} \text{Im}\, \chi(\omega)$

real

χ is non zero for $t_1 > t_2$ and depends only on $t_1 - t_2$ because $\hat{H}$ is Time independent. (causality)

$\chi(z)$ (analytic continuation) has poles at $z = \epsilon_\lambda - \epsilon_\alpha - i\eta$ in the lower half of complex plane (characteristic of a causal response function).

~~Kramers~~ Kramers-Kronig Relations

$$\mathrm{Re}\,\chi(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}\,\chi(\omega')}{\omega - \omega'}$$

$$\mathrm{Im}\,\chi(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Re}\,\chi(\omega)}{\omega - \omega'}$$

(derived by closing The contour in The upper plane where $\chi(z)$ is analytic, assuming That $\chi(z)$ vanishes fast enough as $|z| \to \infty$, so as The integral on The half circle vanishes.

Fluctuation-dissipation Th

- Connects fluctuations in statistical equilibrium ~~to~~ to response of a system to a time-varying perturbation.

How? or Why? $\rightarrow$ an external (time dependent) perturbation induces excitations and power is dissipated.

The spectral fn gives the sum of all possible excitations.

In thermal eq. and for $B = A^+$ (autoadjoint operator)

$$\mathrm{Im}\,\chi(\omega) = \pi\left(1-e^{\beta\omega}\right)\sum_{\alpha\lambda} W_\alpha |A_{\lambda\alpha}|^2\,\delta\left(\omega + E_\lambda - E_\alpha\right)$$

$$= \frac{1-e^{\beta\omega}}{2}\int dt \langle \hat{A}^+(0)\hat{A}(t)\rangle e^{i\omega t}$$

$\Rightarrow$ This formula relates dissipation to fluctuations in time

ex: longitudinal conductivity in x direction is related to the current-current correlation fn χ_{jj} $\quad \mathrm{Re}\,\sigma_{xx}(q_x,\omega) = \dfrac{\mathrm{Im}\,\chi_{j_x j_x}(q_x,\omega)}{\omega}$

Useful response functions that connect to exp:

1.- Density-Density response

$\rightarrow$ Response to an external potential that couples to charge or spin here $\phi(2)\hat{B}(2) \to V_{ext}(2)\hat{n}(2)$

$A(1) \to \hat{n}(1)$

$\to \delta n(1) = n([V_{ext}], \vec{r}_1, \sigma_1, t_1) - n([V=0], \vec{r}_1, \sigma_1)$

$$\delta n(1) = \int_{-\infty}^{\infty} dt_2 \int dx_2\, \chi(1,2) V_{ext}(x_2, t_2) = \int d(2)\, \chi(1,2) V_{ext}(2)$$

with $\chi(1,2) = -i\,\theta(t_1 - t_2)\langle[\hat{n}(1), \hat{n}(2)]\rangle$

$$\delta V_{total}(1) = V_{ext}(1) + V_{ind}(1)$$

$$\delta V_{tot}(1) = V_{ext}(1) + \underbrace{\int d(3)\, v(1,3)\,\delta n(3)}_{\text{interaction due to the induced density}} = V_{ext}(1) + \int d(3)\int d(2)\, v(1,3)\,\chi(3,2)V_{ext}(2)$$

ext: response of the total charge density $n(r,t) = \sum_\sigma n_\sigma(r,t)$ to a spin independent external perturbation.

$$\delta V_{tot}(r_1, t_1) = \int dr_2 \int dt_2 \frac{V_{ext}(r_2, t_2)}{\epsilon(r_1, r_2, t_1 - t_2)}$$

with $$\epsilon^{-1}(r_1, r_2, t_1 - t_2) = \delta(r_1 - r_2)\,\delta(t_1 - t_2) + \int dr_3\, V_c(|r_1 - r_3|)\underbrace{\chi(r_3, r_2, t_1 - t_2)}_{\sum_{\sigma_1\sigma_2}\chi(1,2)}$$

in ω : $\delta V_{tot}(r_1,\omega) = \int dr_2\, \epsilon^{-1}(r_1,r_2;\omega)\, V_{ext}(r_2;\omega)$

$$= \delta(r_1-r_2) + \int dr_3\, V_c(|r_1-r_3|)\, \chi(r_3,r_2;\omega)$$

. For a periodic system :

$$\epsilon^{-1}_{GG'}(q,\omega) = \delta_{GG'} + V_c(q+G)\, \chi_{GG'}(q;\omega) \qquad (*)$$

$G \to RLV$; $\vec{q} \to$ in 1st Bz $\quad V_c = \dfrac{4\pi}{|q+G|^2}$

f sum rule $\Rightarrow \displaystyle\int_0^\infty d\omega\, \omega\, \mathrm{Im}\, \epsilon^{-1}_{GG'}(q,\omega) = -2\pi^2 n$

$n = \dfrac{N}{V}$

<u>Screened Coulomb interaction</u> :

$$W_{GG'}(q,\omega) = \frac{V_c(q+G')}{\epsilon_{GG'}(q,\omega)} \overset{(*)}{=} V_c(q+G) + V_c(q+G)\, \chi_{GG'}(q,\omega)\, V_c(q+G')$$

$$\equiv V_c(q+G) + \underbrace{W^P_{GG'}(q,\omega)}_{\text{Polarization}}$$

W^P has same analytical properties as χ

Connection to experiments:

1.- Loss function: imaginary part of χ is connected to dissipation: $\underbrace{-\mathrm{Im}\,\varepsilon^{-1}_{GG}(q,\omega)}_{\text{Loss fn.}} = -\frac{V}{c}(q+G)\,\mathrm{Im}\,\chi_{GG}(q,\omega)$

Loss fn. → measured in q-resolved e^- Energy Loss (eELS) with momentum Transfer $Q = q + G$

(off diagonal elements $\varepsilon^{-1}_{GG'}(q,\omega)$ are not accessed, but contribute to experimental results in spatially resolved e^-ELS.

2.- Dynamic structure factor:

Inelastic X-ray or Neutron scattering → gives spin resolved.

$S(k,\omega) = \sum_{\sigma\sigma'} S^{\sigma\sigma'}_{kk}(\omega)$

(diagonal part of the dynamic structure factor)

$Q = q + G$

$$S(Q,\omega) = -\frac{1}{\pi(1-e^{-\beta\omega})}\,\mathrm{Im}\,\chi_{GG}(q,\omega)$$

for $G \neq G'$ → off diagonal terms ⇒ coherent IXS

3.- Optical absorption spectrum

→ $\epsilon_M(q,\omega)$ = Macroscopic dielectric fn

→ inverse of the long-wavelength part of ϵ^{-1}

$\epsilon_M(q,\omega) = \left[\epsilon_{00}^{-1}(q,\omega)\right]^{-1}$ for $q \to 0$. The imaginary part is measured in the absorption spectra of light.

$$Q = q + G \; ; \; \epsilon_M(Q,\omega) = \frac{1}{\epsilon^{-1}_{G=G'}(q,\omega)} = \frac{1}{1 + V_c(Q)\,\chi_{G=G'}(q,\omega)}$$

→ Loss fn in terms of ϵ_M

$$-\mathrm{Im}\,\epsilon^{-1}(Q,\omega) = \frac{\mathrm{Im}\,\epsilon_M(Q,\omega)}{\left[\mathrm{Re}\,\epsilon_M(Q,\omega)\right]^2 + \left[\mathrm{Im}\{\epsilon_M(Q,\omega)\right]^2}$$

↓

Here ϵ_M is screened and zeros in $\mathrm{Re}\,\epsilon_M$ give the plasmon modes.

See fig 5.6

For $Q \to 0$ screening is large → see plasmon!

For larger Q effect is smaller → screening decreases with larger Q

smaller distances

We can rewrite :

$$\epsilon_M(Q,\omega) = 1 - \frac{V_c(Q)\chi_{G=G'}(q,\omega)}{1+V_c(Q)\chi_{G=G'}(q,\omega)} = 1 - V_c(Q)\bar{\chi}_{G=G'}(q,\omega)$$

with $\bar{\chi}_{G=G'}(q,\omega) = \chi_{G=G'}(q,\omega) - \chi(q,\omega)V_c(Q)\bar{\chi}(q,\omega)$

This is large for $Q \to 0$ because $V_c(Q \to 0)$ is large (long range Coulomb)