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Optical properties of correlated electron systems: basic theoretical aspects and optical sum rule - Part I

Lara BENFATTO

ISC CNR, Department of Physics
University of Rome "La Sapienza"
Rome
ITALY

Optical properties of correlated electron systems: basic theoretical aspects and optical sum rule. Lecture I

Lara Benfatto

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Outline

Outline

Basic definitions

Vertex corrections

Two paradigmatic examples
- Impurity scattering
- Superconductivity

Sum rule

Definition of the current

- Coupling to the gauge field $\mathbf{A}$: in a continuum system we use the minimal substitution

$$\mathbf{p} + \frac{e}{c}\mathbf{A} \Rightarrow \frac{\hbar}{i}\nabla + \frac{e}{c}\mathbf{A}$$

- As a consequence the kinetic term becomes:

$$H_0 = \frac{1}{2m}\int d\mathbf{x} c^+(\mathbf{x}) \left[-i\hbar\nabla + \frac{e}{c}\mathbf{A}\right]^2 c(\mathbf{x})$$

- The current operator is then given by

$$\begin{aligned} \mathbf{j} &= -\frac{\partial H}{\partial \mathbf{A}} = -\frac{e}{m} c^+(x)\left(-i\hbar\overleftrightarrow{\nabla} + e\mathbf{A}\right) c(x) = \\ &= -e\mathbf{j}^P(x) - \frac{e^2}{m}\hat{n}(x)\mathbf{A} \end{aligned}$$

- In practice, the Hamiltonian up to quadratic order is

$$H(A_i) = H(0) + \int d\mathbf{x} \left[eA_i(\mathbf{x}) j_i^P(\mathbf{x}) + \frac{e^2}{2} A_i^2(\mathbf{x}) n(\mathbf{x}) \right]$$

- In the lattice one would like an equivalent expansion. This is provided by the Peierls ansatz

$$c_i \rightarrow c_i e^{ie \int^{\mathbf{r}_i} \mathbf{A}\cdot d\mathbf{r}} \quad \Rightarrow c_{i\sigma}^\dagger c_{i+\delta\sigma} \rightarrow c_{i\sigma}^\dagger c_{i+\delta\sigma} e^{ie\mathbf{A}(\mathbf{r}_i)\cdot\delta}$$

- Notice that this modifies only the kinetic term: the interaction term is supposed to be Gauge invariant (i.e. density-density interactions)

$$H_0(\mathbf{A}) \quad = \quad -t \sum_{i\delta} \left(c_{i\sigma}^\dagger c_{i+\delta\sigma} e^{ie\mathbf{A}(\mathbf{r}_i)\cdot\delta} + h.c. \right)$$

$$H_0(\mathbf{A}) \quad = \quad -t\sum_{i\delta}\left(c^\dagger_{i\sigma}c_{i+\delta\sigma}e^{ie\mathbf{A}(\mathbf{r}_i)\cdot\delta} + h.c.\right)$$

- By expanding in powers of $\mathbf{A}$ we get

$$H(A_i) \approx H(0) + \sum_j\left[eA_i(\mathbf{r_j})j_i^P(\mathbf{r_j}) + \frac{e^2}{2}A_i^2(\mathbf{r_j})\tau_{ii}(\mathbf{r_j})\right],$$

so that

$$j_i(\mathbf{r}) = -\frac{\partial H}{\partial A_i(\mathbf{r})} = -ej_i^P(\mathbf{r}) - e^2\tau_{ii}(\mathbf{r})A_i(\mathbf{r})$$

where ($\varepsilon_\mathbf{k} = -2t(\cos k_x + \cos k_y)$)

$$j_x^P \quad = \quad it\sum_\sigma(c^\dagger_{i\sigma}c_{i+x\sigma} - c^\dagger_{i+x\sigma}c_{i\sigma}) \Rightarrow j_x^P(\mathbf{q}=0) = \frac{1}{N}\sum_{\mathbf{k}\sigma}\frac{\partial\varepsilon_\mathbf{k}}{\partial k_x}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$$

$$\tau_{xx} \quad = \quad t\sum_\sigma(c^\dagger_{i\sigma}c_{i+x\sigma} + c^\dagger_{i+x\sigma}c_{i\sigma}) \Rightarrow \tau_{ii} = \frac{1}{N}\sum_{\mathbf{k},\sigma}\frac{\partial^2\varepsilon_\mathbf{k}}{\partial k_i^2}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$$

The electromagnetic kernel

$$j_i(\mathbf{r}) = -e j_i^P(\mathbf{r}) - e^2 \tau_{ii}(\mathbf{r}) A_i(\mathbf{r}) \Rightarrow H = H(0) + \mathbf{j}\cdot\mathbf{A}$$

- In linear response theory we then have ($\mu \sim$ space and time)

$$j_\mu(q) = e^2 K_{\mu\nu}(q) A_\nu(q)$$

where the electromagnetic kernel $K_{\mu\nu}$ is defined as:

$$K_{\mu\nu}(\mathbf{q}, i\Omega_m) = -\langle \tau_{\mu\mu} \rangle \delta_{\mu\nu}(1-\delta_{\nu 0}) + \Pi_{\mu\nu}(\mathbf{q}, i\Omega_m).$$

The diamagnetic tensor

$$\langle \tau_{ii} \rangle = \frac{1}{N}\sum_{\mathbf{k},\sigma} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_i^2} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle = \frac{1}{N}\sum_{\mathbf{k},\sigma} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_i^2} n_{\mathbf{k},\sigma}$$

generalizes to a lattice system the term n/m while $\Pi_{\mu\nu}(\mathbf{q}, i\Omega_m) \sim \langle j^P j^P \rangle$ is the current-current correlation function, with $j_P \sim \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}}$, $\mathbf{v}_{\mathbf{k}} = \partial \varepsilon_{\mathbf{k}} / \partial \mathbf{k}$

Optical conductivity

$$j_\mu(q) = e^2 K_{\mu\nu}(q) A_\nu(q)$$

- By using the relation between $\mathbf{A}$ and the electric field $\mathbf{E}$

$$\mathbf{A}(\omega) = \frac{\mathbf{E}(\omega)}{i(\omega + i0)} \quad \mathbf{J} = \sigma \mathbf{E}$$

one arrives at the famous Kubo formula

$$\sigma(\omega) = -ie^2 \frac{K_{ii}(\mathbf{q}=0,\omega)}{V(\omega+i0)} = ie^2 \frac{< \tau_{ii} > - \Pi_{ii}(\mathbf{q}=0,\omega)}{V(\omega+i0)},$$

- The real part of the optical conductivity is

$$\mathrm{Re}\sigma(\omega) = \frac{\pi e^2}{V}\delta(\omega)[< \tau > - \mathrm{Re}\Pi(\mathbf{0},\omega)] + \frac{\pi e^2}{V}\frac{\mathrm{Im}\Pi(\mathbf{0},\omega)}{\omega}$$

Do we really have a delta-like contribution??

Charge conservation and Gauge Invariance

- Charge conservation

$$\dot{\rho} + \nabla \cdot \mathbf{j} = 0 \quad \Rightarrow q_\mu j_\mu(q) = 0 \quad q = (\mathbf{q}, \omega)$$

- Gauge invariance

$$A_\mu \to A_\mu + \partial_\mu \chi \qquad A_\mu(q) \to A_\mu(q) + i q_\mu \chi(q)$$

- Since $j_\mu = K_{\mu\nu} A_\nu$ one must have

$$q_\mu K_{\mu\nu}(q) = K_{\mu\nu}(q) q_\nu = 0 \Rightarrow \Pi_{ii}(\mathbf{q} \to 0, \omega = 0) = \langle \tau_{ii} \rangle$$

$$\boxed{\mathrm{Re}\Pi(\mathbf{0}, 0) = < \tau >}$$

$$\begin{aligned} \mathrm{Re}\sigma(\omega) &= \frac{\pi e^2}{V} \delta(\omega) [< \tau > - \mathrm{Re}\Pi(\mathbf{0}, \omega)] + \frac{\pi e^2}{V} \frac{\mathrm{Im}\Pi(\mathbf{0}, \omega)}{\omega} = \\ &= \frac{e^2}{V} \frac{\mathrm{Im}\Pi(\mathbf{q} = \mathbf{0}, \omega)}{\omega} \end{aligned}$$

Gauge invariance and Optical sum rule

$$\mathrm{Re}\Pi(\mathbf{0},0) = <\tau> \qquad \mathrm{Re}\sigma(\omega) = \frac{e^2}{V}\frac{\mathrm{Im}\Pi(\mathbf{q}=\mathbf{0},\omega)}{\omega}$$

- By using the Kramers-Kronig (KK) relations for $\Pi(\mathbf{q}=0,\omega)$ one can derive the well-know sum rule:

$$W(T) = \int_0^\infty \mathrm{Re}\sigma(\omega)d\omega = \frac{e^2}{2V}\int_{-\infty}^\infty \frac{\mathrm{Im}\Pi(\mathbf{q}=\mathbf{0},\omega)}{\omega}d\omega =$$

$$= \frac{\pi e^2}{2V}\mathrm{Re}\Pi(\mathbf{q}=\mathbf{0},\omega=0) = \frac{\pi e^2}{2V} <\tau> = \frac{\pi e^2}{VN}\sum_{\mathbf{k},\sigma}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_i^2}n_{\mathbf{k},\sigma}$$

The optical sum rule is a consequence of charge conservation. The approximations used to compute $K_{\mu\nu}$ must satisfy the above relations, i.e. one must choose a **conserving approximation**. This is not at all an easy task..

Outline

- Let us imagine to have a given interacting model

$$H = H_0 + H_{int}$$

The bare Green's function is $G_0^{-1} = i\omega_n - \xi_{\mathbf{k}}$. We treat the interaction term in some approximation in order to obtain the new Greens' function from the Dyson equation:

$$G^{-1}(p) = G_0^{-1}(p) - \Sigma(p)$$

- The current-current correlation function will be

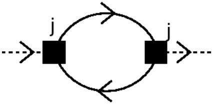
$$\Pi_{\mu\nu}(\mathbf{q}, i\Omega_m) = \frac{1}{N}\int_0^\beta d\tau e^{i\Omega_m\tau}\langle T_\tau j_\mu^P(\mathbf{q},\tau) j_\nu^P(-\mathbf{q},0)\rangle$$

with $\mathbf{j}^P(\mathbf{q},t) = \frac{1}{N}\sum_{\mathbf{k},\sigma}\mathbf{v}(\mathbf{k}) c^\dagger_{\mathbf{k}-\mathbf{q}/2\sigma} c_{\mathbf{k}+\mathbf{q}/2\sigma}$, and $\mathbf{v}(\mathbf{k}) = \frac{\partial\varepsilon_{\mathbf{k}}}{\partial\mathbf{k}}$.

$$\Pi \sim \langle e^{H\tau} c^\dagger c e^{-H\tau} c^\dagger c\rangle$$

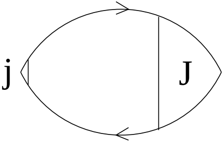
This is a very complicated function!

- The zero-th order is the so-called *bare bubble*



$$\Pi^0_{\mu\nu}(\mathbf{q}, i\Omega_m) = -2\sum_k [G(\mathbf{k}-\mathbf{q}/2, i\omega_n + i\Omega_m) v_\mu(\mathbf{k}) G(\mathbf{k}+\mathbf{q}/2, i\omega_n) v_\nu(\mathbf{k})]$$

- To guarantee a conserving approximation one has to replace one velocity with a 'dressed' current J



$$\Pi_{\mu\nu}(\mathbf{q}, i\Omega_m) = -2\sum_k [G(k_-) v_\mu(\mathbf{k}) G(k_+) J_\nu(k_+, k_-)]$$

The dressed current is found as the solution of an integral equation, that depends on the approximation used for the self-energy

Outline

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Vertex corrections

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Sum rule

The bare bubble

- Let us start from the bare bubble and let us compute it by introducing the spectral representation of the Green's function

$$G(i\omega,\mathbf{k})=\int dz\frac{A(z,\mathbf{k})}{i\omega-z}\quad A(z,\mathbf{k})=-\frac{1}{\pi}\mathrm{Im}G^R(\omega,\mathbf{k})$$

- We can then perform easily the sum over Matsubara frequencies

$$\Pi_{\mu\nu}(\mathbf{q},i\Omega)=-2\sum_{\mathbf{k}}\int dz_1dz_2[A(z_1,\mathbf{k}_+)v_\mu A(z_2,\mathbf{k}_-)v_\nu]\frac{f(z_1)-f(z_2)}{z_1-z_2-i\Omega}$$

so that $\mathrm{Im}\Pi(\Omega)\to-\pi\delta(z_1-z_2-\Omega)$ and

$$\mathrm{Re}\sigma(\omega)=\frac{e^2}{V}\frac{\mathrm{Im}\Pi(\mathbf{q}=\mathbf{0},\omega)}{\omega}=$$

$$=-2\pi\sum_{\mathbf{k}}\mathbf{v}_x(\mathbf{k})^2\int dz\frac{f(z+\omega)-f(z)}{\omega}A(z+\omega,\mathbf{k})A(z,\mathbf{k})$$

Scattering by impurities

- Scattering by impurities leads to a finite lifetime of quasiparticles

$$A(z, \mathbf{k}) = M(z - \xi_{\mathbf{k}}) = \frac{1}{\pi} \frac{\Gamma}{(z - \xi_{\mathbf{k}})^2 + \Gamma^2}$$

- By using $v_x(\mathbf{k}) \sim v_F^2$ the conductivity is

$$\sigma(\omega) \sim v_F^2 \int dz d\xi \frac{f(z+\omega) - f(z)}{\omega} \left[M(z + \omega - \xi) M(z - \xi) \right]$$

$f(z+\omega) - f(z) \Rightarrow$ particle-hole excitations between occupied and unoccupied states

- At low temperature this reduces to

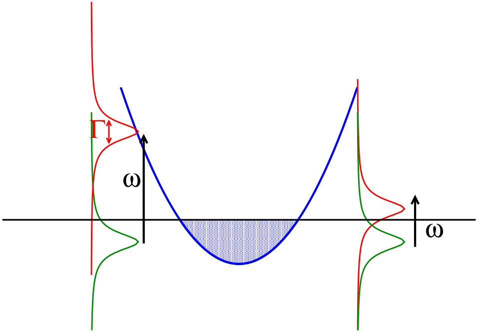
$$\sigma(\omega) \sim \int_{-\omega}^{0} dz \frac{1}{\omega} \int_{-\infty}^{\infty} d\xi \, M(z+\omega, \xi) M(z, \xi) = \frac{2\Gamma}{\omega^2 + (2\Gamma)^2}$$

- We then obtain the well-known Drude formula

$$\sigma_D(\omega) = \frac{ne^2}{m} \frac{\tau}{1+(\omega\tau)^2}$$

with

$$1/\tau_{tr} \equiv \Gamma_{tr} = 2\Gamma$$

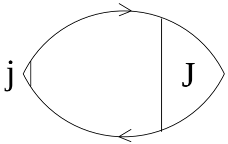


However, Boltzmann theory tells us that the transport scattering rate does not coincide with the quasiparticle one

$$\Gamma = \frac{1}{\tau} \sim \int \frac{d\mathbf{k}'}{(2\pi)^3} |T_{\mathbf{kk}'}|^2, \quad \Gamma_{tr} = \frac{1}{\tau_{tr}} \sim \int \frac{d\mathbf{k}'}{(2\pi)^3} |T_{\mathbf{kk}'}|^2 (1-\cos\theta')$$

What is missing? **Vertex corrections!**

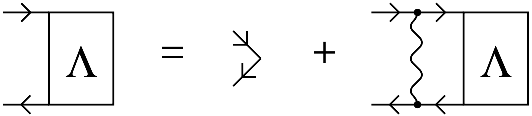
- The 'correct' dc conductivity contains both the bare velocity $\mathbf{v}$ and the dressed current $\mathbf{J}$:



$$\sigma_{dc} = e^2 \sum_{\mathbf{k}} \left(-\frac{\partial f}{\partial \xi_{\mathbf{k}}} \right) v_x J_x \frac{1}{\Gamma_{\mathbf{k}}} \approx \frac{e^2}{4\pi} \frac{k_F J_F}{\Gamma_F}$$

- The current is the solution of the equation

$$J_\alpha(p_+, p_-) = v_\alpha + \sum_{\mathbf{p}'} J(p'_+, p'_-) W_{\mathbf{p}\mathbf{p}'}(i\omega_n, i\omega_n + i\Omega_m) G(p'_+) G(p'_-)$$



- At zero frequency and in the Fermi-liquid approximation this can be solved. One finds that

$$J_\alpha = v_\alpha \Lambda, \quad \Lambda = \frac{\tau_{tr}}{\tau} = \frac{\Gamma}{\Gamma_{tr}}$$

so that

$$\sigma_{dc} = \frac{e^2}{4\pi}\frac{k_F J_F}{\Gamma_F} = \frac{e^2 k_F v_F}{\Gamma_{tr}} = \frac{ne^2\tau_{tr}}{m}$$

In practice, vertex correction can be recast
in a redefinition of the transport scattering rate,
that gives back the Boltzmann result.
This is somehow general for single-band systems,
but *not* so general for **multiband** ones

Superfluid density

- What is a superconductor? It is a perfect diamagnet. The London equation tells us that in the London gauge $\nabla \cdot \mathbf{A} = 0$ ($\mathbf{A}$ purely travserse) for $q_y \to 0$ one has

$$\mathbf{j}_x(q_y) = -\frac{1}{4\pi^2\lambda^2}\mathbf{A}_x(q_y) = -\frac{n_s e^2}{mc}\mathbf{A}_x(q_y) \quad q_y \to 0$$

- Since $j_x = K_{xx} A_x$ for $\mathbf{q} \to 0$ the superfluid density $D_s = n_s/m$ is given by the static limit of the *transverse* correlation function

$$\frac{D_s}{\pi e^2} = \tau_{xx} - \Pi_{xx}(i\Omega_m = 0, q_x = 0, q_y \to 0)$$

- How do we compute D_s within the BCS approximation?

The bare bubble

- The bare-bubble current-current correlation function within the BCS approximation is given by

$$\Pi^0_{xx}(\mathbf{q}, i\Omega) = \frac{2}{N}\sum_{\mathbf{k}} v_x^2(1-f-f')(vu'-uv')\left[\frac{uv'}{i\Omega_m - E - E'} + \frac{u'v}{i\Omega_m + E + E'}\right] +$$
$$+ \frac{2}{N}\sum_{\mathbf{k}} v_x^2(f'-f)(vv'+uu')\left[\frac{vv'}{i\Omega_m + E - E'} - \frac{uu'}{i\Omega_m - E + E'}\right]$$

Here $E' = E_{\mathbf{k}+\mathbf{q}/2}, E = E_{\mathbf{k}-\mathbf{q}/2}$, u, v are the usual BCS coherence factors.

- The superfluid density is then $(\tau_{xx} - \Pi_{xx}(i\Omega_m = 0, q_x = 0, q_y \to 0))$

$$\frac{D_s}{\pi e^2} = \tau_{xx} - \sum_{\mathbf{k}} v_x^2(\mathbf{k})\frac{\partial f}{\partial E_{\mathbf{k}}} = \sum_{\mathbf{k}} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_i^2} n_{\mathbf{k},\sigma} - \sum_{\mathbf{k}} \left(\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_i}\right)^2 \frac{\partial f}{\partial E_{\mathbf{k}}}$$

and it seems to work well....

$$\frac{D_s}{\pi e^2} = \tau_{xx} - \sum_{\mathbf{k}} v_x^2(\mathbf{k}) \frac{\partial f}{\partial E_{\mathbf{k}}} = \sum_{\mathbf{k}} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_i^2} n_{\mathbf{k},\sigma} - \sum_{\mathbf{k}} \left(\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_i} \right)^2 \frac{\partial f}{\partial E_{\mathbf{k}}}$$

- As $T \to 0$ $\partial f / \partial E_{\mathbf{k}} = \delta(E_{\mathbf{k}}) \sim e^{-\Delta/T}$ accounts for quasiparticle excitations
- At $T = T_c$ $E_{\mathbf{k}} = \xi_{\mathbf{k}}$, $n_{\mathbf{k}} = f(\xi_{\mathbf{k}})$ and the second term, integrated per part, cancels out the first term
- However, we have seen that GI would require also for the *longitudinal* limit:

$$\tau_{xx} - \Pi_{xx}(i\Omega_m = 0, q_x \to 0, q_y = 0) = 0$$

and this is clearly violated (the two limits are identical)

What is missing? Vertex corrections! How to include them?
Very elegant and efficient way: integrate out phase fluctuations

- Effective action for phase fluctuations:

$$S = \frac{1}{8}\sum_{\mathbf{q}} K_{ab}^{BCS}(\mathbf{q}) q_a q_b |\theta(\mathbf{q})|^2 \sim \frac{1}{8\pi}\int d\mathbf{r} D_s (\nabla\theta)^2$$

- Minimal-coupling substitution:

$$\nabla\theta \to \nabla\theta - 2e\mathbf{A} \quad \Rightarrow q_a\theta(\mathbf{q}) - 2eA_a(\mathbf{q})$$

- After integrating out the phase fluctuations one obtains an RPA-like resummation

$$K_{ab}(\mathbf{q},0) = K_{ab}^{BCS} - \frac{q_c q_d K_{ac}^{BCS} K_{bd}^{BCS}}{q_c q_d K_{cd}^{BCS}}$$

$$K_{xx}(\mathbf{q}\to 0,0) = K_{xx}^{BCS} - \frac{q_x^2 (K_{xx}^{BCS})^2}{q_x^2 K_{xx}^{BCS} + q_y^2 K_{yy}^{BCS}}$$

This correction is purely *longitudinal*: this is way the superfluid density obtained in the bare-bubble approximation is correct!

Disordered systems

- Vertex corrections contain the physics of phase fluctuations, missing in BCS. For a clean system these couple only to the longitudinal component of $\mathbf{A}$ since

$$S_g = \frac{1}{8\pi}\int d\mathbf{r} D_s(\nabla\theta - 2e\mathbf{A})^2 \Rightarrow \int D_s \nabla\theta \cdot \mathbf{A} = -\int D_s \theta(\nabla \cdot \mathbf{A})$$

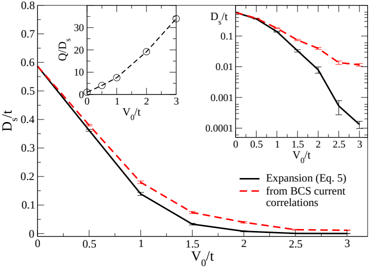
- However, for a dirty system

$$S_g \sim \frac{1}{8\pi}\int d\mathbf{r} D_s(\mathbf{r})(\nabla\theta - 2e\mathbf{A})^2$$

In this case phase fluctuations couple also to the *transverse* component of the gauge field
$\Rightarrow$ the BCS expression for D_s is no more correct

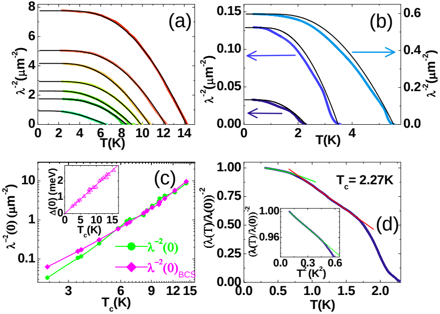
Disordered systems

THEORY



Disordered Hubbard model
G.Seibold, L.Benfatto, C. Castellani and J.Lorenzana, Phys. Rev. Lett. **108**, 207004 (2012)

EXPERIMENTS



Films of NbN
M. Mondal, A. Kamlapure, M. Chand, G. Saraswat, S. Kumar, J. Jesudasan, L. Benfatto, V. Tripathi, P. Raychaudhuri, Phys. Rev. Lett. **106**, 047001 (2011)

The way out to vertex corrections

- As long as the interaction is momentum-independent vertex corrections vanish, and the bare-bubble approximation is gauge invariant
- Eliashberg theory for electron-boson interactions

$$\Sigma(i\omega_n) = -TV \sum_m D(\omega_n - \omega_m) G(i\omega_m), \quad D(\omega_l) = \int d\Omega \frac{2\Omega B(\Omega)}{(\Omega^2 + \omega_l^2)}$$

- Dynamical Mean Field Theory (DMFT), self-consistent solution for $\Sigma(\omega)$

Outline

$$W = \int_0^\infty \mathrm{Re}\,\sigma_{ii}(\omega,T)d\omega = \frac{\pi e^2}{2VN}\sum_{\mathbf{k},\sigma}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_i^2}n_{\mathbf{k},\sigma}$$

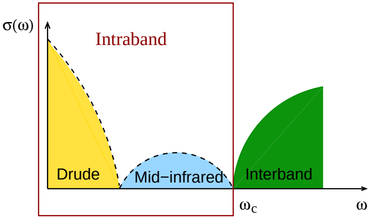
- If we could really account for **all** frequencies we would recover the free-electron dispersion $\varepsilon_{\mathbf{k}} = \mathbf{k}^2/2m$ (the so-called f-sum rule)

$$W = \frac{\pi n e^2}{2m}$$

- However, in real systems we integrate up to a finite cut-off ω_c

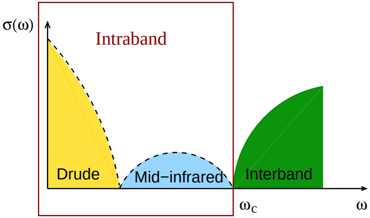
$$W(\omega_c,T) = \int_0^{\omega_c} \mathrm{Re}\,\sigma_{ii}(\omega,T)d\omega$$

where $\varepsilon_{\mathbf{k}}$ refers only to the band(s) near the Fermi level



Restricted optical sum rule

$$W(\omega_c, T) = \int_0^{\omega_c} \mathrm{Re}\, \sigma_{ii}(\omega, T) d\omega = \frac{\pi e^2}{2VN} \sum_{\mathbf{k},\sigma} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_i^2} n_{\mathbf{k},\sigma}$$



where $\varepsilon_{\mathbf{k}}$ refers only to the band(s) near the Fermi level with effective mass m_b

- Roughly speaking we can say that the sum rule scales then with

$$W(\omega_c) \simeq \frac{\pi e^2 n}{2 m_b}$$

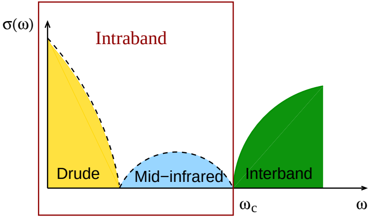
where the band mass m_b can be compared to its DFT estimate

The absolute value of the sum rule gives information on the correlations on the energy scales of the full bandwidth

Restricted optical sum rule

$$W(\omega_c,T)=\int_0^{\omega_c}\mathrm{Re}\,\sigma_{ii}(\omega,T)d\omega=$$

$$\frac{\pi e^2}{2VN}\sum_{\mathbf{k},\sigma}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_i^2}n_{\mathbf{k},\sigma}$$



where $\varepsilon_{\mathbf{k}}$ refers only to the band(s) near the Fermi level

- Systems near half-filling (as e.g. cuprates): $\varepsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)\Rightarrow\partial^2\varepsilon_{\mathbf{k}}/\partial k_x^2=2t\cos k_x$

$$W(\omega_c,T)\simeq\langle K\rangle$$

The temperature dependence of the sum rule gives information on the role of interactions on the occupation number, i.e. on the transfer of spectral weight from the Drude-like part to something else

Sommerfeld expansion

- The case of a 'standard' metal: we can use the Sommerfeld expansion to get

$$\tilde{W}(T) = \frac{W(T)}{(\pi e^2 a^2/2V)} = -\frac{1}{N}\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} f(\xi_{\mathbf{k}}) =$$
$$= -\int d\varepsilon N(\varepsilon)\varepsilon f(\varepsilon-\mu) = \int_0^\mu d\varepsilon N(\varepsilon)\varepsilon - c(\mu)T^2,$$

  where $c(\varepsilon) = (\pi^2/6)[\varepsilon N'(\varepsilon) + N(\varepsilon)]$
- For a flat DOS $N = 1/2D$ where D is the semi-bandwidth

$$\tilde{W}(T) = \tilde{W}(0) - \frac{\pi^2}{12D}T^2 = \tilde{W}(0) - BT^2$$

So spectral weight is expected
to *decrease* at temperature *increases*
How much? Let's try to make an estimate..

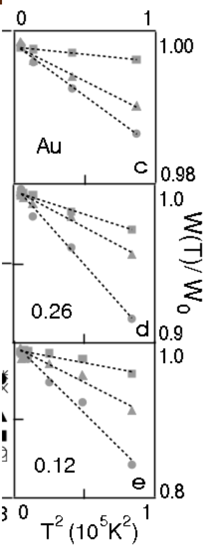
Conventional...

$$\tilde{W}(T) = \tilde{W}(0) - \frac{\pi^2}{12D}T^2 \quad B \sim \frac{1}{D}$$

- Let us put numbers:
  $\tilde{W}(0) \sim N \int_0^{\varepsilon_F} d\varepsilon\varepsilon \sim \varepsilon_F^2/D \sim 1$eV for $D \sim 1$ eV. The relative variation up to room temperature $T \sim 300$ K~ 30 meV are

$$\frac{\Delta\tilde{W}(300K)}{\tilde{W}(0)} \simeq \frac{T^2}{D\tilde{W}(0)} \sim (30\times 10^{-3})^2 \sim 10^{-3}$$

i.e. relative spectral-weight variarions are expected to be of order of few per-mille.



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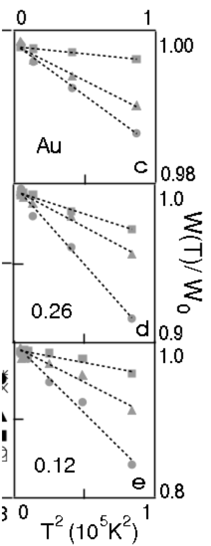
...and beyond

$$\tilde{W}(T) = \tilde{W}(0) - \frac{\pi^2}{12D} T^2 \quad B \sim \frac{1}{D}$$

- Cuprates: the spectral-weight variations are one order of magnitude **larger** than expected
- Pnictides: almost empty bands $\varepsilon_{\mathbf{k}} \approx \mathbf{k}^2/2m_b$ so

$$W \simeq \frac{\pi e^2 n}{2m_b}$$

and one would expect almost no temperature dependence. One finds instead strong **increase** of the sum rule with increasing temperature.



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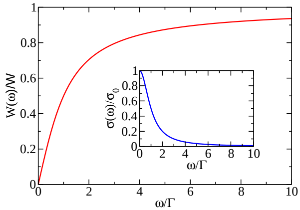
The issue of the cut-off

- Let us consider a Drude model

$$\sigma_{Drude}(\omega, T) = \frac{\Omega_P^2}{8\pi}\frac{\Gamma}{\Gamma^2+\omega^2}$$

$$\Omega_P^2 = \frac{4\pi n}{m}$$

$$W(\omega) = 2\int_0^{\omega} \sigma_{Drude}(\omega')d\omega'$$



- If one integrates up to a finite cut-off

$$W(\omega_c) = \frac{\Omega_P}{8} f(\omega_c), \quad f(\omega_c) = \left(1 - \frac{\Gamma(T)}{\pi\omega_c\tau}\right)$$

The presence of the cut-off itself can introduce a temperature dependence of the spectral weight

Take-home messages

- Gauge invariance, conserving approximation and optical sum rule: different ways to state charge conservation
- The optical sum rule in conventional systems does not look so interesting: as we shall see, in correlated ones it is instead a great source of information
- Few useful references

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