Optical Conductivity of Superconductors

I. Kinetic theory for normal metal

Obtaining "Drude" conductivity

$$\vec{f} = m\vec{a}$$

$$\vec{f} = -e\vec{E} - \eta\vec{v}$$

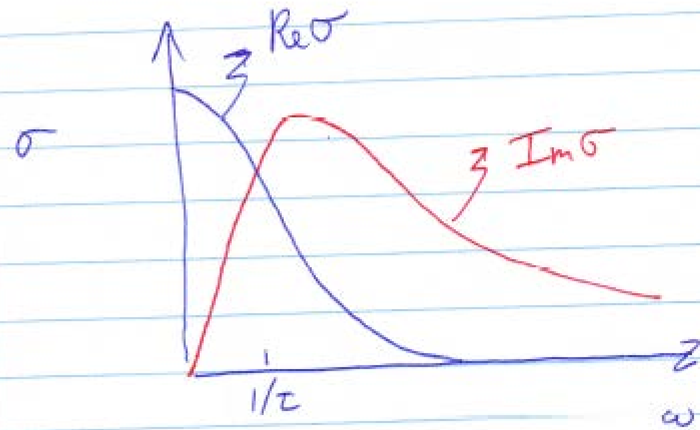
$$-e\vec{E}(\omega) - \eta\vec{v}(\omega) = -i\omega m\vec{v}(\omega)$$

$$\vec{v}(\omega) = \frac{-e\vec{E}(\omega)}{\eta - i\omega m}$$

$$\vec{J}(\omega) = -ne\vec{v}(\omega) = \frac{ne^2}{\eta - i\omega m}\vec{E}(\omega) = \frac{ne^2}{m}\frac{1}{\eta/m - i\omega}$$

Kinetic theory $\frac{\eta}{m} = \frac{1}{\tau} = \frac{\langle v \rangle}{l}$ where l is mfp.

Finally Drude theory $\sigma(\omega) = \frac{ne^2}{m} \frac{1}{1/\tau - i\omega}$

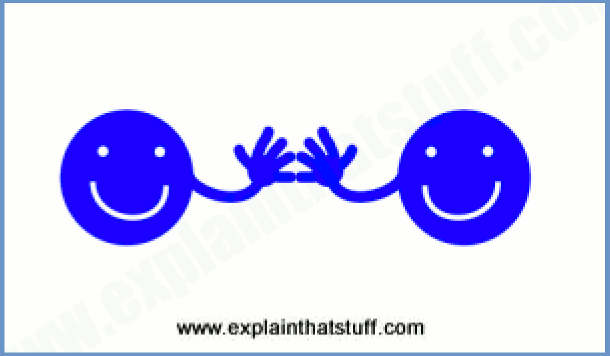


$\sigma = \sigma_1 + i\sigma_2$

$$\int d\omega \, \sigma_1(\omega) = \frac{\pi}{2} \frac{ne^2}{m}$$ Conductivity sum rule

These result are trivial to obtain by simple kinetic theory of or Boltzmann Eq. So why do more?

Answer: ∞-conductivity of SC is a purely QM effect! Cannot be understood by classical images of paired electrons somehow avoiding impurities!



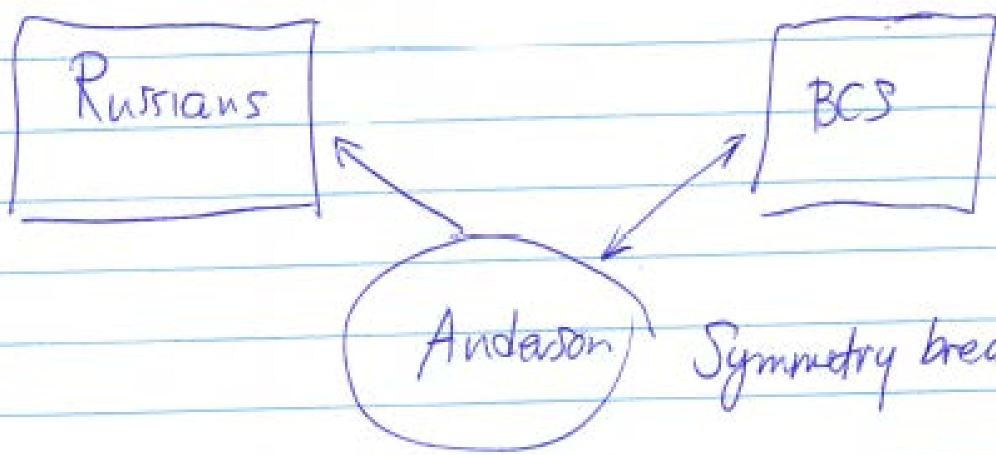
Think of Cooper pairing as a kind of marriage. Just as marriage can help two people sail through life's ups and downs by joining forces, so Cooper pairing allows electrons to travel through a conductor without getting bogged down in lots of troublesome little obstacles. [Chris Woodford, "How cool stuff works."

Quantum Mechanics approaches

Two historical approaches

Ginzburg - Landau - Gorkov : Macroscopic Quantum Field

BCS : exact knowledge of grnd + excited states
in mean-field theory



Symmetry breaking U(1)

[see Anderson remembers @ 50 yrs of BCS]

Some of the basics of QM approach

EM couples through potentials $\vec{A}, V$

$$\delta\hat{\mathcal{H}} \sim +e\int d^3r\, \vec{J}\cdot\delta\vec{A} - \rho\,\delta V$$

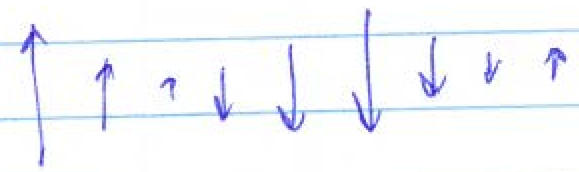
From linear response theory we can obtain

$$\vec{J}(\vec{q},\omega) = K(\vec{q},\omega)\,\vec{A}$$

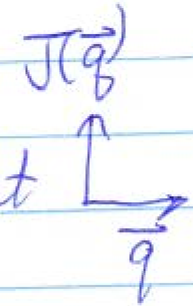
$$\rho(\vec{q},\omega) = \chi(\vec{q},\omega)\,V \quad [\text{screening}]$$

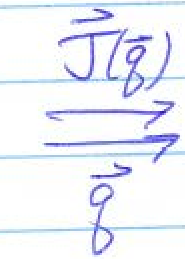
longitudinal and transverse responses

$$\vec{J}(\vec{r}) = \vec{J}(\vec{q})\, e^{i\vec{q}\cdot r} e^{-i\omega t}$$



transverse current





longitudinal current

generates charge density

$$\boxed{\sigma_T(\vec{q},\omega) = \frac{c}{i\omega} K(\vec{q},\omega)}$$

Optical conductivity and Meissner effect are two distinct limits of $K(\vec{q},\omega)$

Optical conductivity is the response to dc electric field that is uniform $(q=0)$

$$\boxed{\sigma(\omega) \equiv \frac{c}{i\omega} K(\vec{q}=0,\omega)}$$

$$\sigma_{dc} = \lim_{\omega\to 0} \frac{c}{i\omega} K(\vec{q}=0,\omega)$$

Meissner effect is the nonvanishing of

$$\boxed{K(\vec{q}) \text{ in the limit } q \to 0}$$

Summary

Optical conductivity

$$\sigma(\omega) \Longleftrightarrow K(\vec{q}=0, \omega)$$

Meissner $\quad K(\vec{q}, \omega=0)$

Calculating current in linear response

In second quantization we have

$$\vec{J}(\vec{r}) = \vec{J}_D(\vec{r}) + \vec{J}_p(\vec{r})$$

diamagnetic paramagnetic

$$\vec{J}_p(\vec{r}) = -\frac{e\hbar}{im}\left[\psi^\dagger(\vec{r})\nabla\psi(\vec{r}) - (\nabla\psi^\dagger(\vec{r}))\psi(\vec{r})\right]$$

$$\vec{J}_D(\vec{r}) = \frac{e^2}{mc}\psi^\dagger(\vec{r})\psi(\vec{r})\vec{A}(\vec{r})$$

Linear response theory

$$K(\vec{q},\omega) = R(\vec{q},\omega) + \frac{ne^2}{mc}$$

$$R(\vec{q},\omega) = \sum_n{}' \left| \langle n | J_p(\vec{q}) | 0 \rangle \right|^2 \times \left[\frac{1}{\hbar\omega - (E_n - E_0) + i\eta} - \frac{1}{\hbar\omega + (E_n - E_0) + i\eta} \right]$$

Kubo formula

$J_p(\vec{q})$ is obtained by expressing $J_p(\vec{r})$ in basis of plane waves.

$$\psi(\vec{r}) = \sum_k c_k e^{i\vec{k}\cdot\vec{r}}$$

Leading to

$$\boxed{\vec{J}_p(\vec{q}) = -\frac{e\hbar}{m}\sum_k \left(\vec{k}+\frac{\vec{q}}{2}\right) c^{\dagger}_{\vec{k}+\vec{q}}\, c_k}$$

[Also sum on spins $c^{\dagger}_{k+q,\uparrow}\, c_{k\uparrow}$ etc.]

Conductivity is a 2-particle Green fct

$|n\rangle$ are the exact many body states.

R is related to matrix elements

$$\langle n | c^{\dagger}_{k+q}\, c_k | 0 \rangle$$

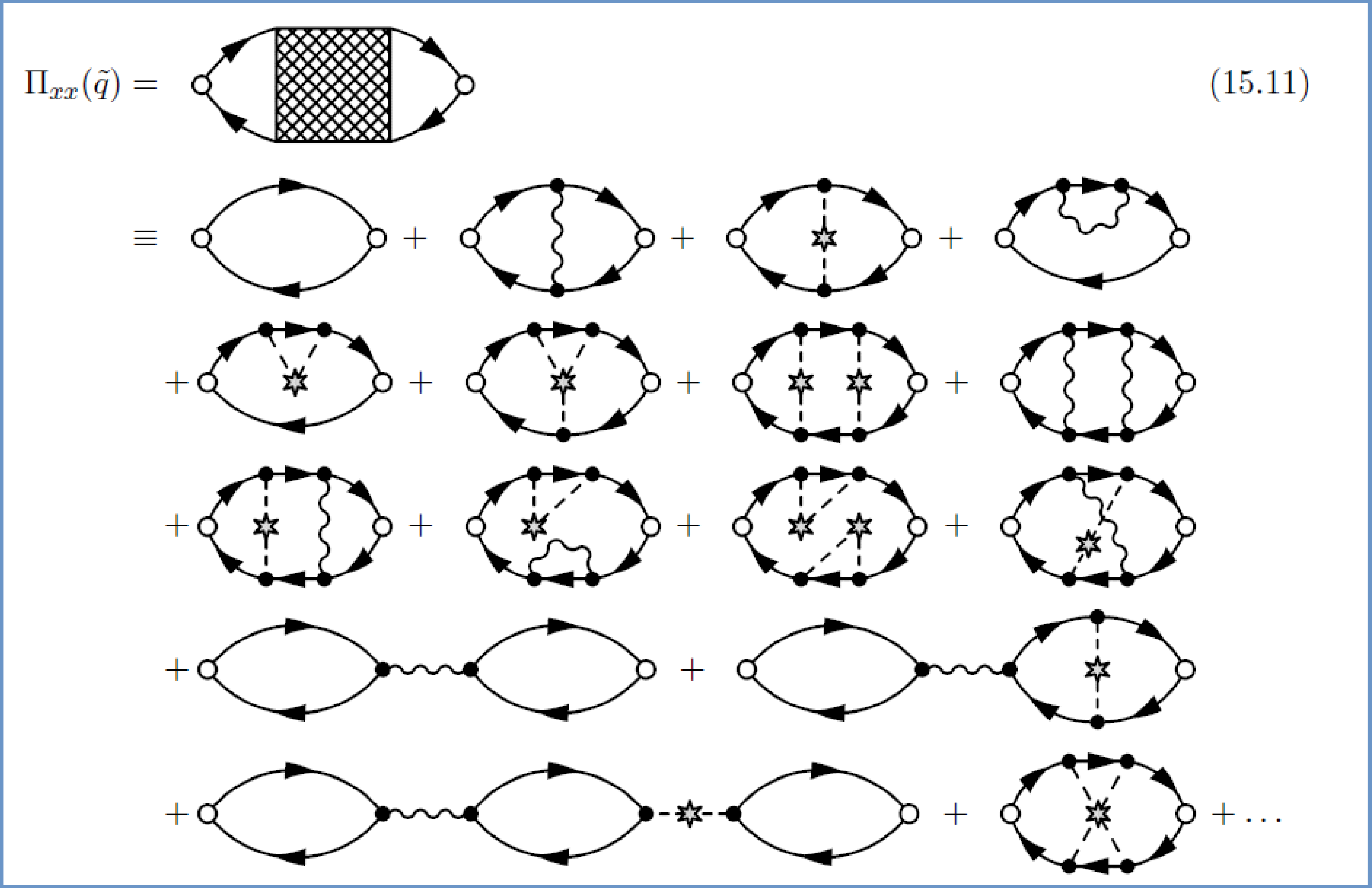
Which is essentially the 2-particle Green function.

It relates the overlap of the ground state with
2 electrons introduced in plane wave states with
the exact many body eigenstates. The
2 particle Green function is <u>not</u> simply the
convolution of two 1-particle Green functions.
Instead vertex corrections have to be included
otherwise big problems

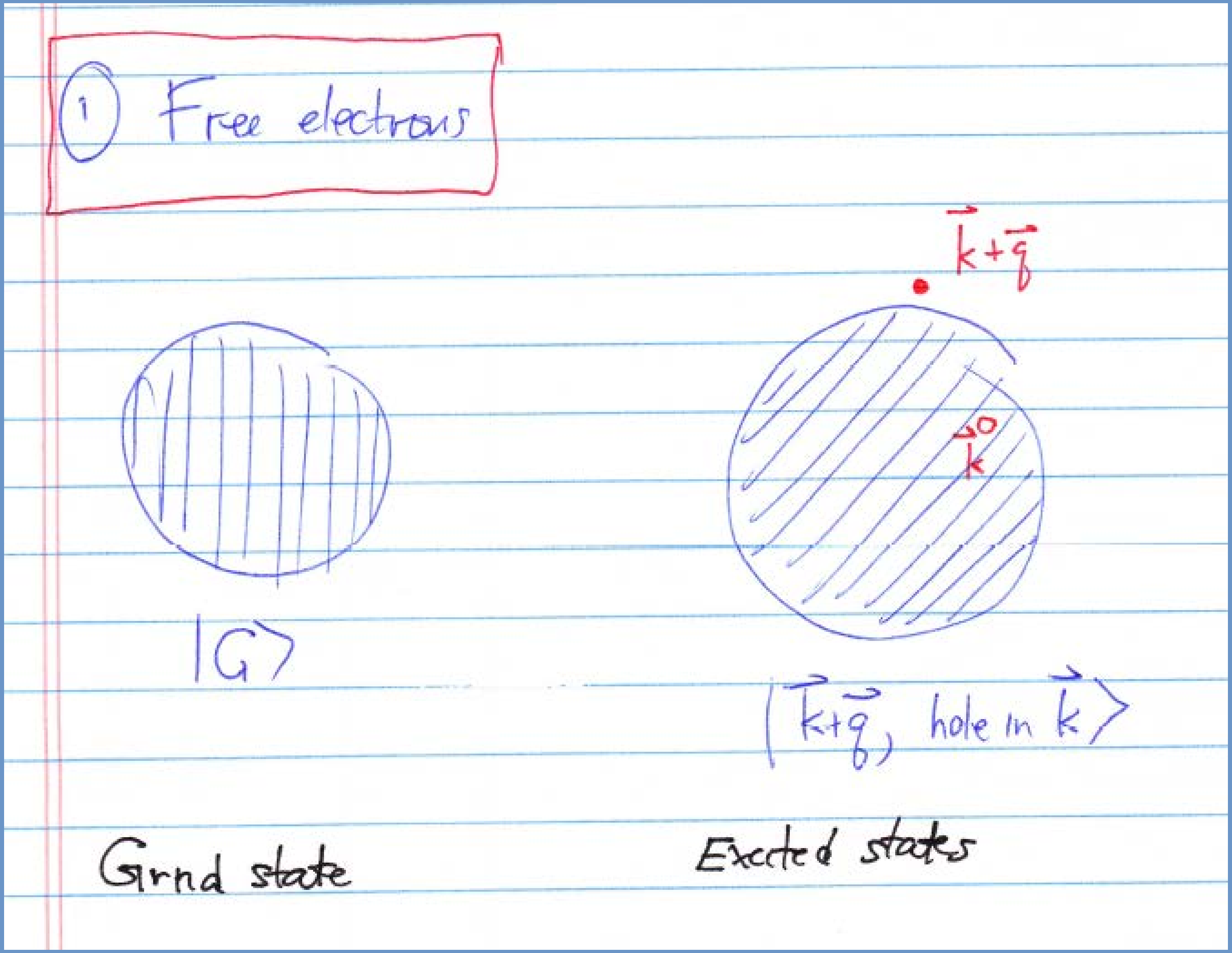
① Non conservation of charge

② Scattering rate not weighted by scattering
angle

Requires about 25 pages of this stuff



Instead we look at representative examples



We can calculate the imaginary part of R from the paramagnetic term by itself.

$$\boxed{\begin{array}{l} \mathrm{Im}\, R = \pi \sum_n \left| \langle n | J_p(\vec{q}) | 0 \rangle \right|^2 \delta\left[\hbar\omega - (E_n - E_0)\right] \\ \text{Fermi Golden Rule} \end{array}}$$

$$E_n - E_0 \cong \frac{\hbar^2 \vec{k}\cdot\vec{q}}{m} \quad \text{for } \vec{q} \ll \vec{k}_F$$

Optical conductivity $q \to 0$

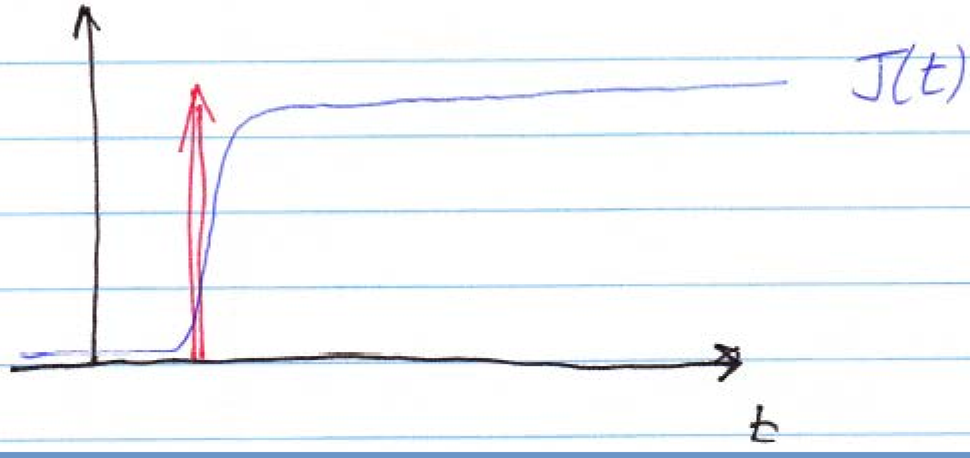
$$\mathrm{Im}\, R(\omega) = \pi \sum_n \langle n | \vec{J}_p(0) | 0 \rangle \, \delta\left[\hbar\omega - (E_n - E_0)\right]$$

$\equiv 0$ because cannot couple to e-h

pairs with net momentum $\vec{q}$.

Vanishing of dissipation at $\omega > 0$ is a consequence of perfect momentum conservation

Impulse response of free electrons



As $R(\omega) = 0$ we are left with

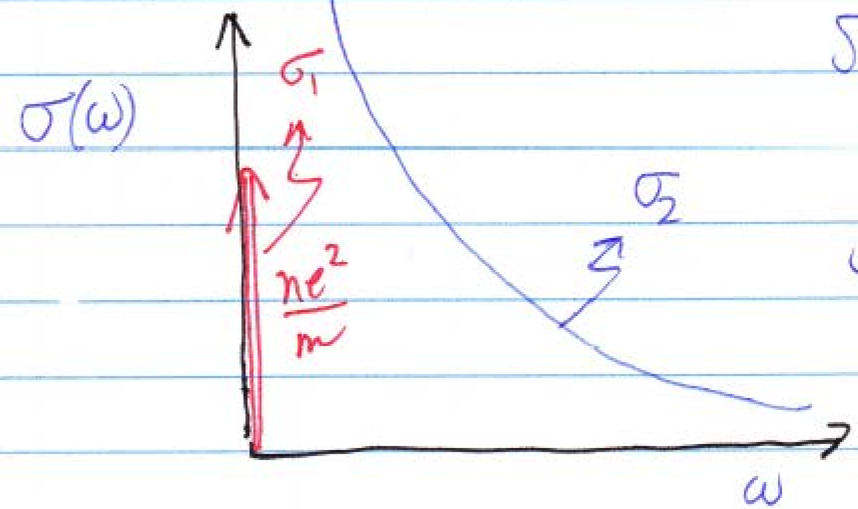
$$K(\omega) = \frac{ne^2}{mc}$$

$$\sigma(\omega) = -\frac{c}{i\omega} K(\omega) = \frac{i\,ne^2}{m\omega}$$

However, Kramers-Kronig shows that there must be a real part, which is a delta function

$$\sigma(\omega) = \frac{ne^2}{m}\left[\frac{\pi}{2}\,\delta(\omega) + \frac{i}{\omega}\right]$$

$\boxed{\text{Optical conductivity of free electrons}}$



Sum rule satisfied by δ-fct

$$\int d\omega\, \sigma_1(\omega) = \frac{ne^2}{m}$$

But is a perfect metal a superconductor?

Static q=0 response vanishes for normal metal

$$R(\vec{q}) = +\sum_n \frac{1}{\hbar^2 q^2}(E_n - E_0)^2 |\langle n|\rho_q|0\rangle|^2 \times \frac{2}{E_n - E_0}$$

$$= \cancel{\frac{2}{\hbar^2 q^2}} \sum_n \frac{2}{\hbar^2 q^2} |\langle n|\rho_q|0\rangle|^2 (E_n - E_0)$$

f-sum rule $\sum_n (E_n - E_0)|\langle n|\rho_q|0\rangle|^2 = \frac{Nq^2}{2m}$

Thus

$R(q) = \frac{Ne^2}{m}$ and this exactly cancels the diamagnetic term!

But is a perfect metal a superconductor? No!

Perfect metal
Order of limits matters

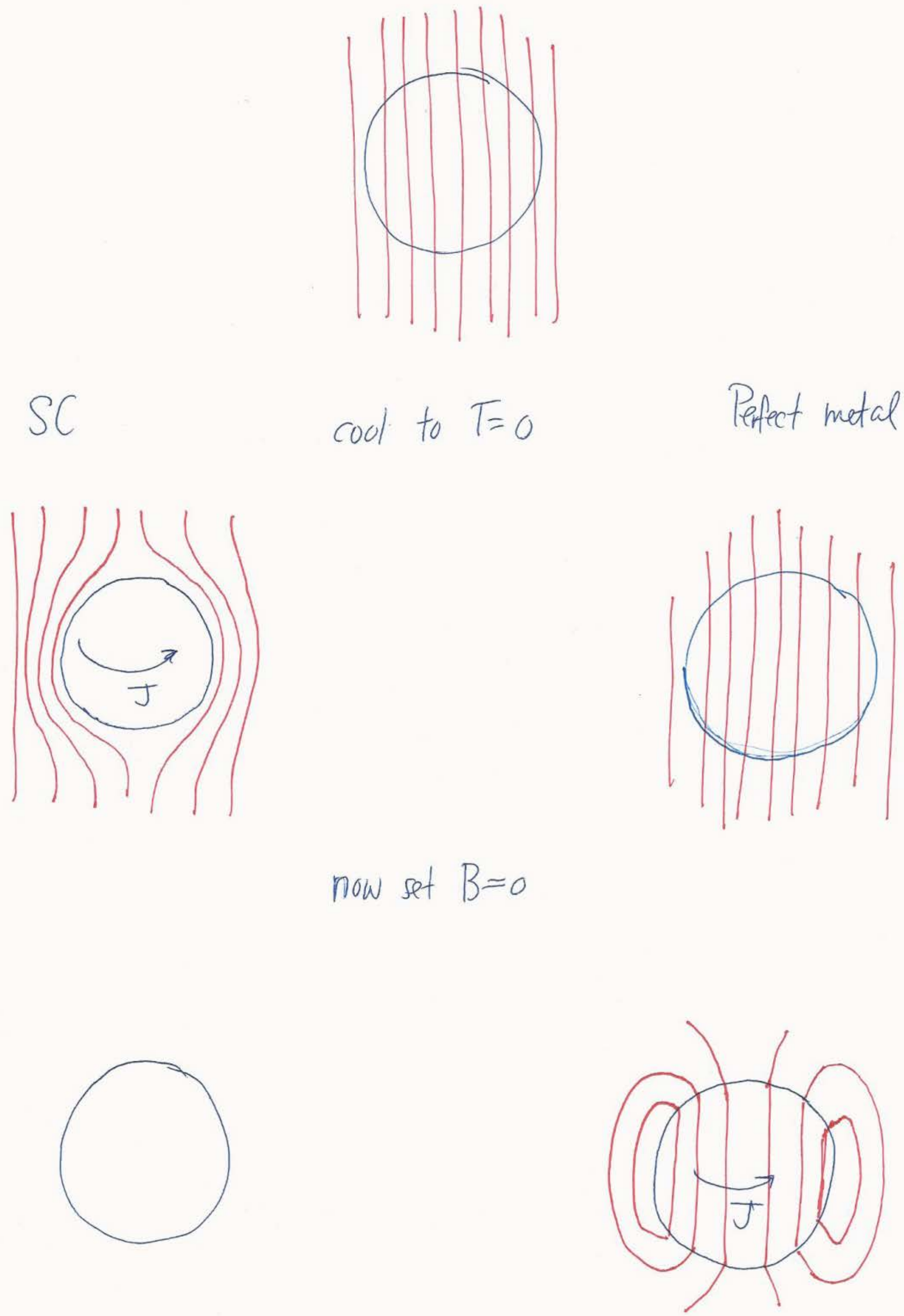
$$\lim_{\omega \to 0} \lim_{q \to 0} K(q,\omega) = -\frac{ne^2}{mc}$$

$$\lim_{q \to 0} \lim_{\omega \to 0} K(q,\omega) = 0$$

Superconductor

$$\lim_{\omega \to 0} \lim_{q \to 0} K(q,\omega) = -\frac{ne^2}{mc}$$

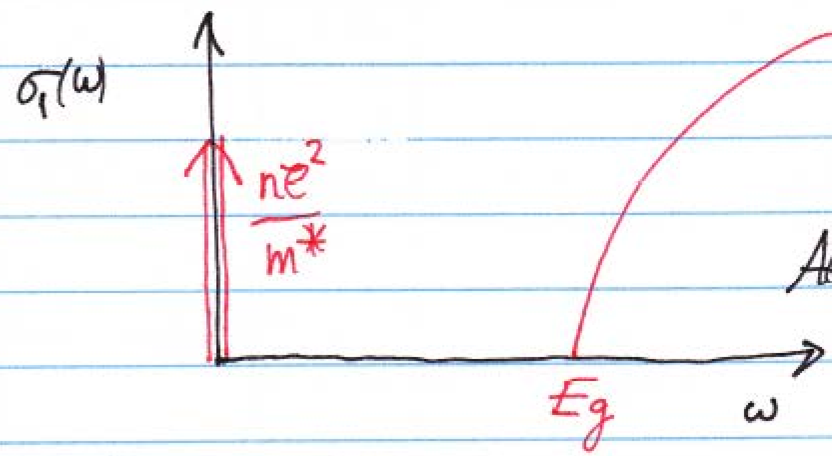
$$\lim_{q \to 0} \lim_{\omega \to 0} K(q,\omega) = -\frac{ne^2}{mc}$$


SC
cool to T=0
Perfect metal
J
now set B=0
J

What about ~~interacting~~ electrons?

Galilean invariance dictates the same result.

How about i~~nteracting~~ free electrons in a perfect lattice?



m^* is the effective bandstructure mass.

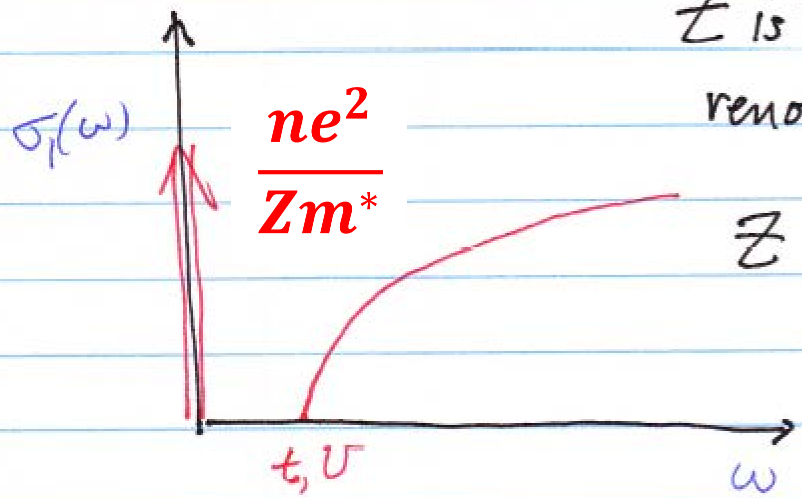
Also can show that

$\sigma_1(\omega) \propto \langle -T \rangle \delta(\omega)$

see White, et al.

What about interacting electrons on a perfect lattice?

[Hubbard model]



Z is the quasiparticle renormalization factor

$Z \sim$ mass enhancement

Disorder and optical conductivity

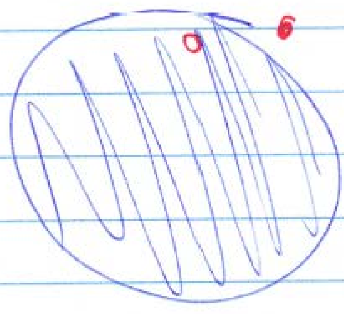
We have seen that the metal in the absence of disorder (and at $T=0$) has infinite conductivity. Indeed clean metals at low T exhibit exponentially small resistivity, as recently shown by Andy MacKenzie. The surprising (and non-trivial) conductivity property is the appearance of a conductivity in the disordered metal.

Drude conductivity of normal metal

The Drude conductivity is amazingly complicated to calculate by diagrammatic perturbation theory. see Bruus and Flensberg.

Takes 20+ dense pages in the standard many body text books. If we try a back-of-the-envelope approach

We can look at the coupling to states close to the Fermi energy



$$\Delta \mathcal{E} = \frac{\hbar^2}{m} \vec{k}_F \cdot \vec{q}$$

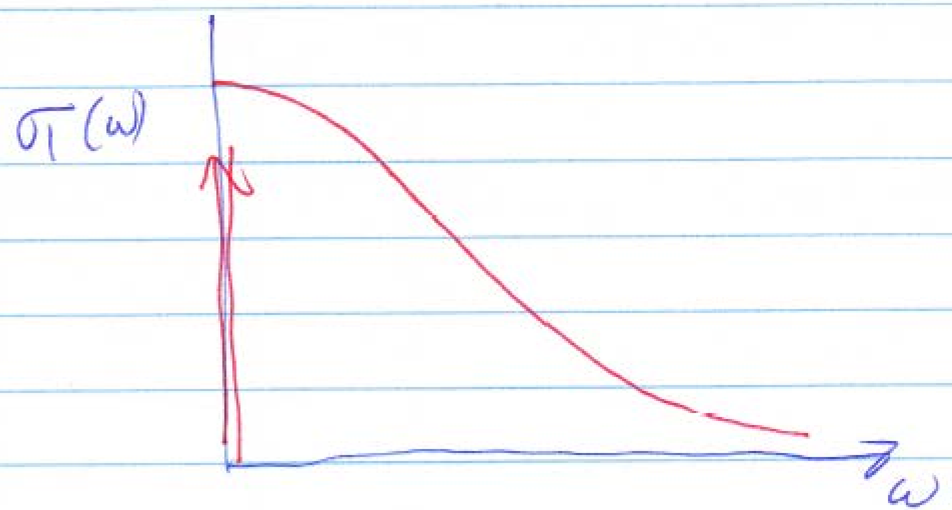
If momentum is conserved then we can't couple to there states with an infrared photon which has $q \approx 0$.

However in the presence of scattering with mean free path l, momentum will not be conserved on the scale $\Delta q \sim 1/l$

This allows us to couple to states with

$$\Delta \varepsilon = \frac{\hbar^2}{m} k_F / l \quad \text{or} \quad \Delta \omega = \frac{\hbar}{m} \frac{k_F}{l} = \frac{p_F}{ml} = \frac{v_F}{l} = \frac{1}{\tau}$$

Thus we recover the Drude peak with width v_F/l



Clean limit $\quad \sigma_1(\omega) = \frac{\pi}{2} \frac{ne^2}{m} \delta(\omega)$

Disorder $\quad \sigma_1(\omega) = \frac{ne^2}{m} \frac{v_F}{l}$

This result should be valid in weak scattering limit, $k_F l \gg 1$ when density of levels is not affected and weak localization effects are very small.

Now we can look at a superconductor in this regime.

Superconductor with weak disorder

This is the regime where "Anderson's Thm" applies. We choose for basis states the exact single particle states in the presence of disorder

$$\mathcal{H}_0 |\alpha\rangle = \varepsilon_\alpha |\alpha\rangle ; \quad \langle r|\alpha\rangle = \varphi_\alpha(\vec{r})$$

Anderson: pairing takes place between time-reversed states

Instead of pairing $k\uparrow$ and $-k\downarrow$, we pair

$\varphi_{\alpha\uparrow}(\vec{r})$ and $\varphi^*_{\alpha\downarrow}(\vec{r})$, which are degenerate

in the presence of time-reversal symmetry (we ignore

SO interaction which complicates matters but does not

change the essentials). Lead to BCS equation

$$\Delta(\vec{r}) = V_0 \sum_{\alpha,\beta} \phi_\alpha(\vec{r}) \varphi_\beta(\vec{r}) \langle c_{\alpha\downarrow} c_{\beta\uparrow} \rangle$$

assuming $\Delta(\vec{r})$ can be replaced by spatial average

$$\Delta = \frac{V_0}{\Omega} \sum_{\alpha} \langle c_{\alpha\downarrow} c_{\alpha\uparrow} \rangle$$

and effective $\mathcal{H}$

$$\mathcal{H} = \sum_{\alpha} \varepsilon_{\alpha} \; c^{\dagger}_{\alpha\uparrow} c_{\alpha\uparrow} + c^{\dagger}_{\alpha\downarrow} c_{\alpha\downarrow}$$

$$\cancel{+} - \Delta \, c^{\dagger}_{\alpha\uparrow} c^{\dagger}_{\alpha\downarrow} - \Delta^{*} c_{\alpha\downarrow} c_{\alpha\uparrow}$$

Diagonalized by BV transformation

$$\gamma_{\alpha\uparrow} = u_\alpha c_{\alpha\uparrow} + v_\alpha c^\dagger_{\alpha\downarrow}$$

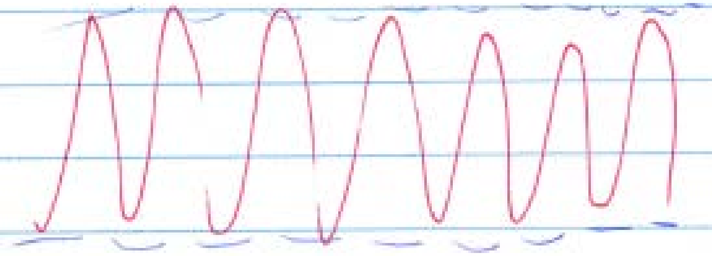
$$\gamma^\dagger_{\alpha\downarrow} = v^*_\alpha c_{\alpha\uparrow} + u_\alpha c^\dagger_{\alpha\downarrow}$$

$$E_\alpha = \left[(\varepsilon_\alpha - \mu)^2 + |\Delta|^2\right]^{1/2}$$

let $\xi_\alpha = \varepsilon_\alpha - \mu$

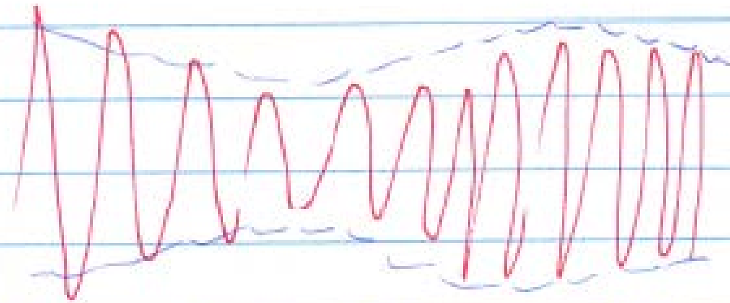
No disorder

e^{ikr}



Weak disorder

$e^{i[kr - \varphi(r)]}$



Amplitude relatively constant. Phase correlation lost on the scale of ℓ. In the superconductor the excited states accessed with infrared photons are a pair of quasiparticles $\cancel{\gamma^{*}_{\alpha}\gamma}$ $\gamma^{\dagger}_{\alpha\uparrow}\gamma^{\dagger}_{\beta\downarrow}$ for example.

We couple to these state via the perturbation term which is the paramagnetic current operator. In the basis $|\alpha\rangle$ this is written

$$\hat{J}_p = -\frac{ie\hbar}{m} \sum_{\alpha,\beta,\sigma} V_{\alpha\beta}\, c^{\dagger}_{\beta\sigma} c_{\alpha\sigma}$$

where $V_{\alpha\beta} = \int d^3r\, \varphi^*_\beta(\vec{r})\, \nabla \varphi_\alpha(\vec{r})$

Express $c^\dagger_{\beta\sigma} c_{\alpha\sigma}$ in terms of γ operators

The term in the current operator

$c^\dagger_{\beta\downarrow} c_{\alpha\downarrow}$ has a term $u_\beta v_\alpha \gamma^\dagger_{\beta\downarrow} \gamma^\dagger_{\alpha\uparrow}$

This creates two quasiparticles with energy E_α and E_β with opposite spin, and with amplitude proportional to $\boxed{V_{\alpha\beta}\, u_\beta v_\alpha}$. However there is another term that creates the same qp pair. ~~with~~

This is the time-reversed term

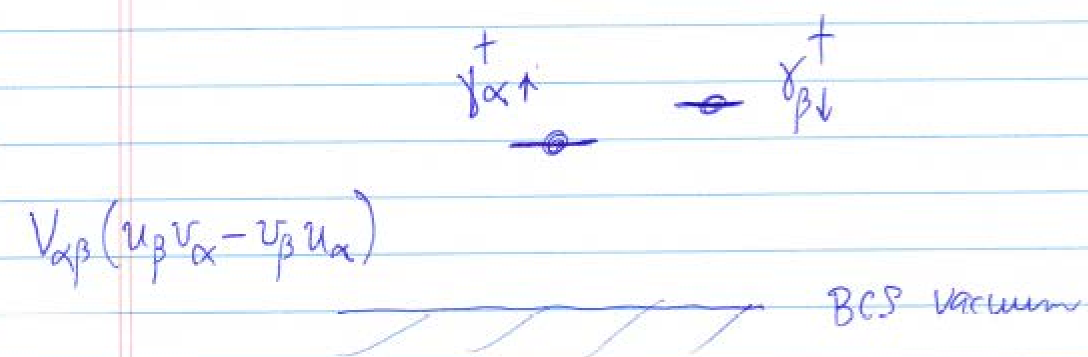
$$T\left\{c^\dagger_{\beta\downarrow} c_{\alpha\downarrow}\right\} = c^\dagger_{\alpha\uparrow} c_{\beta\uparrow}$$

which ~~so~~ has amplitude $\cancel{V_{\beta\alpha} v_\alpha u_\beta}$ $V_{\beta\alpha}\, u_\alpha v_\beta$

To find the overall matrix element we must take the sum

$$V_{\alpha\beta}\, u_\beta v_\alpha + V_{\beta\alpha}\, u_\alpha v_\beta$$

Because the current is odd under time-reversal we have $V_{\alpha\beta}\left(u_\beta v_\alpha - v_\beta u_\alpha\right)$ for the matrix element to generate the qp pair $\gamma^\dagger_{\alpha\uparrow}\gamma^\dagger_{\beta\downarrow}$ from the ground state



Sequence of steps beautifully described in PAL notes

leads to

$$\sigma(\omega) = \frac{e^2\pi}{\omega}\int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\xi' \left(u_\xi v_{\xi'} - v_\xi u_{\xi'}\right)^2 f(\xi, \xi')$$

$$\times\ \delta\left[\omega - \left(E_\xi + E_{\xi'}\right)\right]$$

Now what are these terms?

Recall ξ_α is normal state energy referred to μ.

u_ξ, v_ξ expresses the fact that the coherence factors depend on α only thru the normal state energy ξ_α and the gap Δ.

$f(\xi, \xi')$ is the squared matrix element connecting states with normal state energy ξ, ξ'

$\delta[\omega - (E_\xi + E_{\xi'})]$ is density of states factor

Conductivity in superconducting state

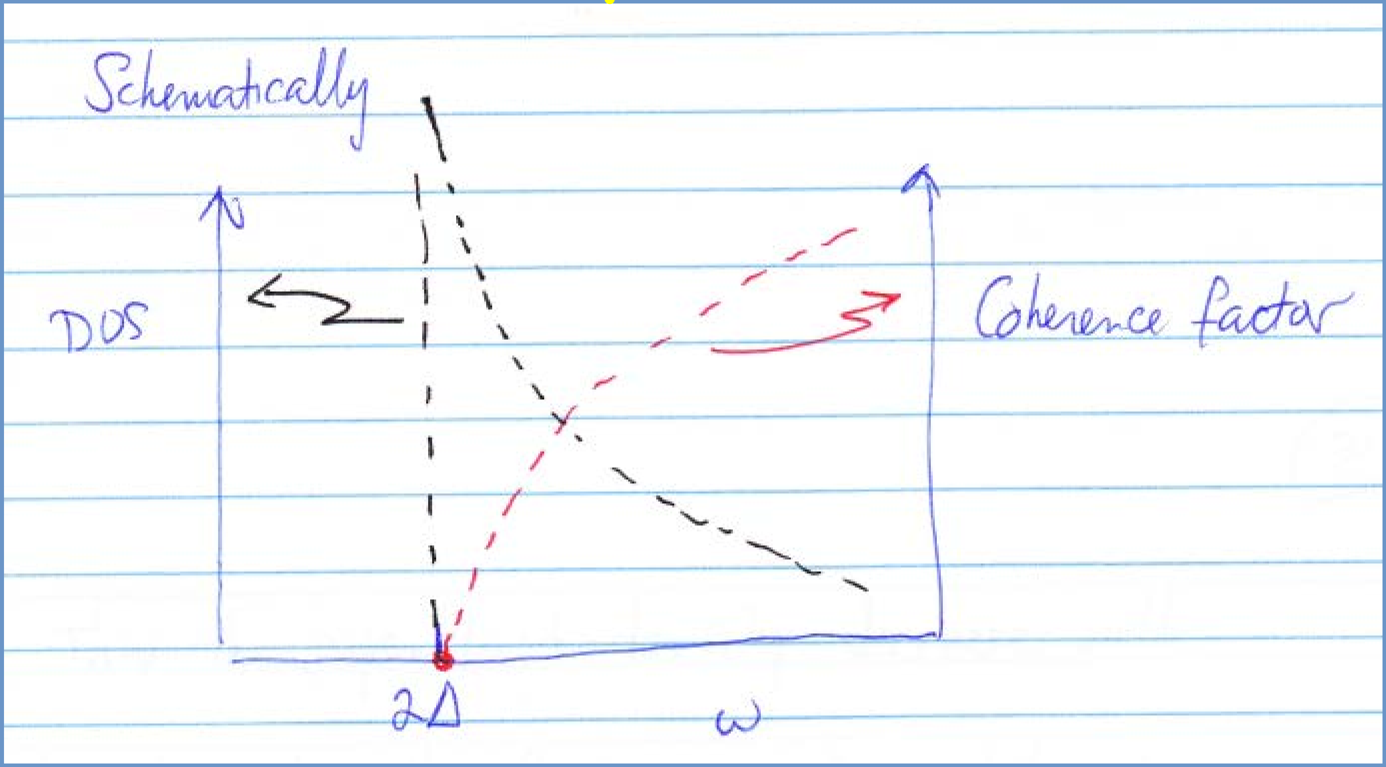
σ_n depends on $f(\xi, \xi')$

Also $(uv' - vu')^2 = \frac{1}{2}\left[1 - \frac{\xi\xi'}{EE'} - \frac{\Delta^2}{EE'}\right]$

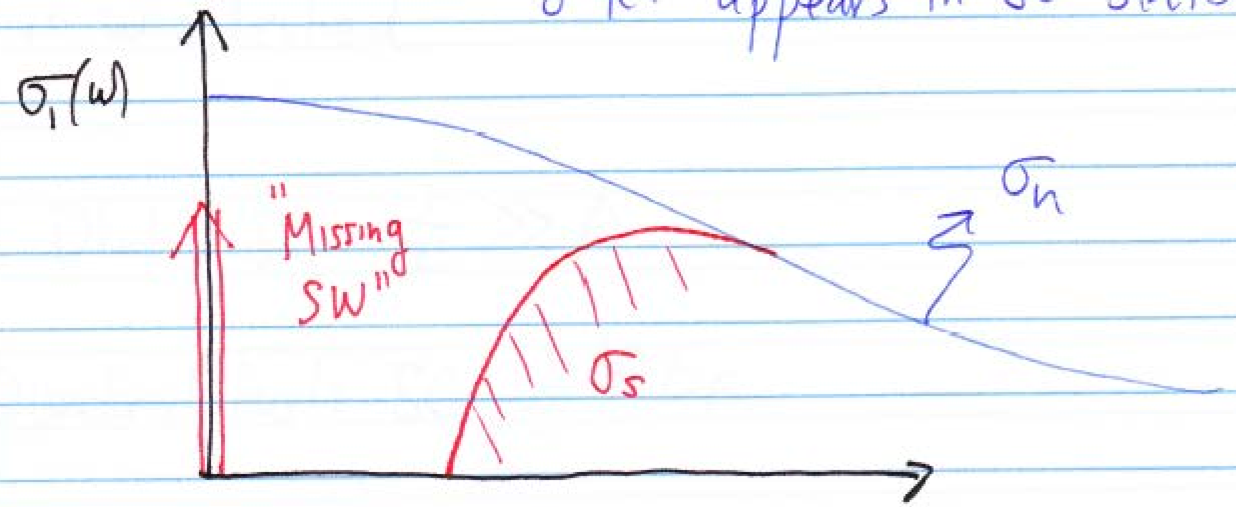
Finally

$$\sigma(\omega) = \frac{\sigma_n(\omega)}{\omega}\int d\xi \int d\xi' \left(1 - \frac{\Delta^2}{EE'}\right) \delta[\omega - (E+E')]$$

Mattis-Bardeen absorption is zero at threshold despite singular density of states



δ-fct appears in SC state!



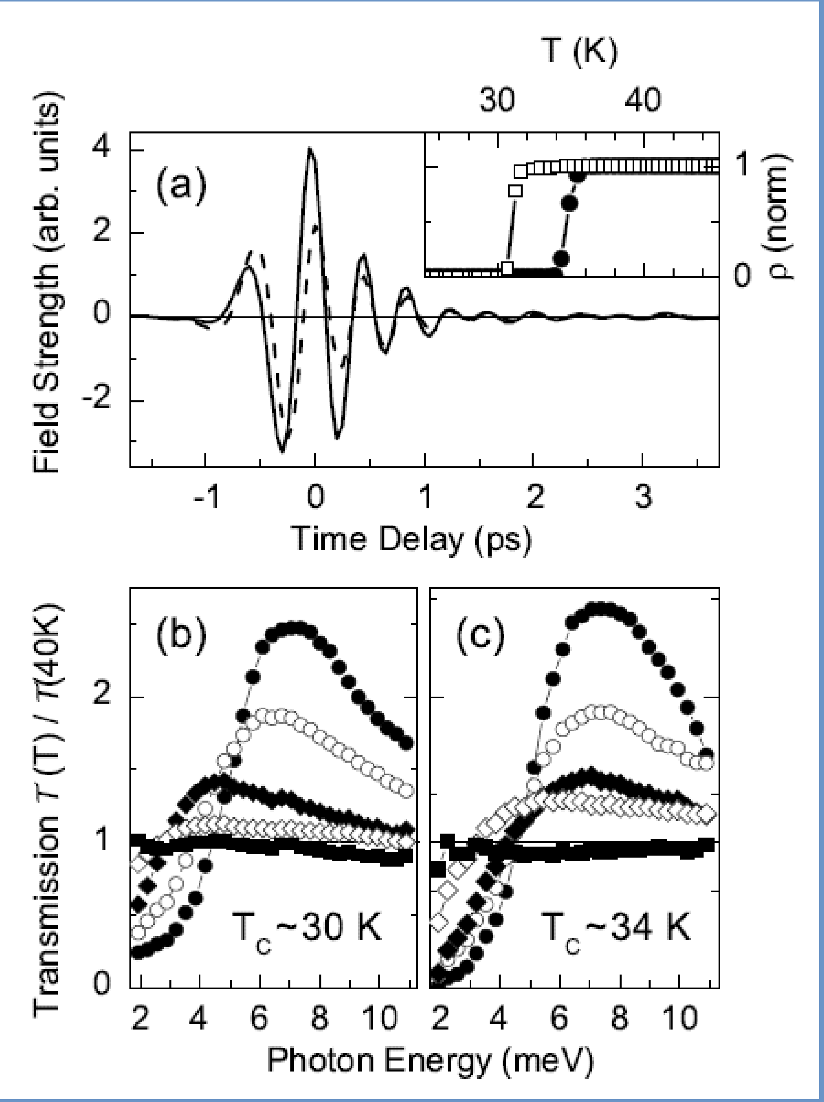
Spectral weight in the delta function is

$$\sim \frac{ne^2\tau}{m} \cdot 2\Delta \quad \text{in the limit that } \Delta \ll 1/\tau$$

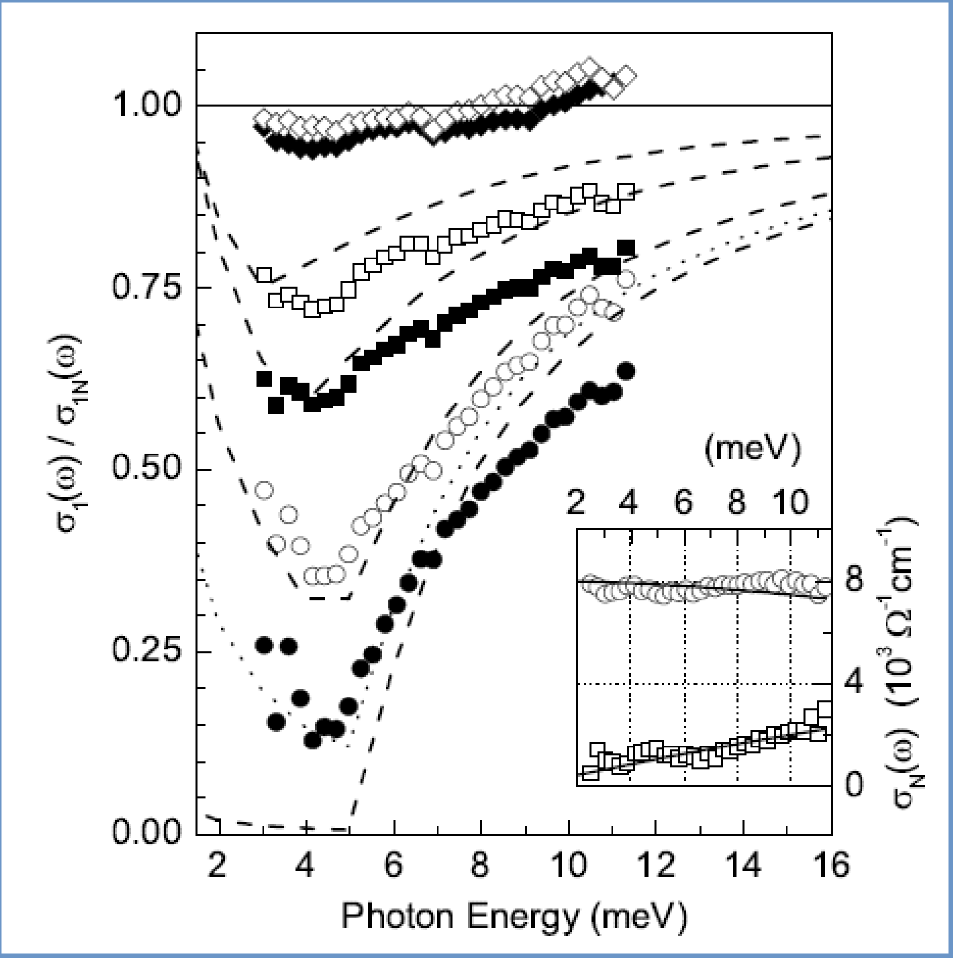
If coherence factor was unity then there would be no δ-fct.

Far-infrared optical conductivity gap in superconducting MgB_2 films

Kaindl et al. Phys. Rev. Lett. 88, 027003 (2002).



Mattis-Bardeen theory works in MgB_2

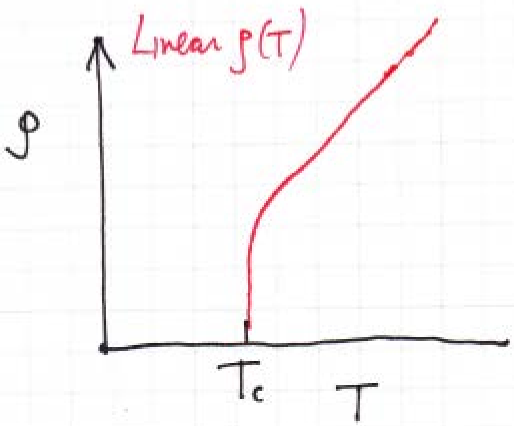


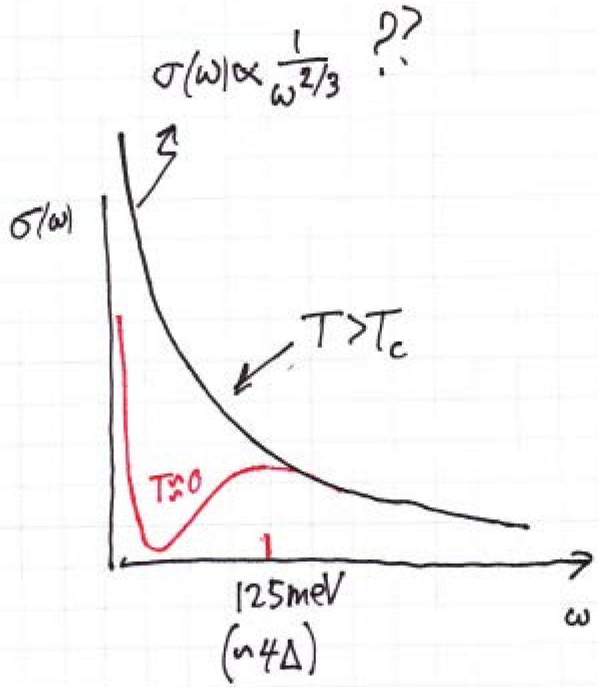
But not in cuprates

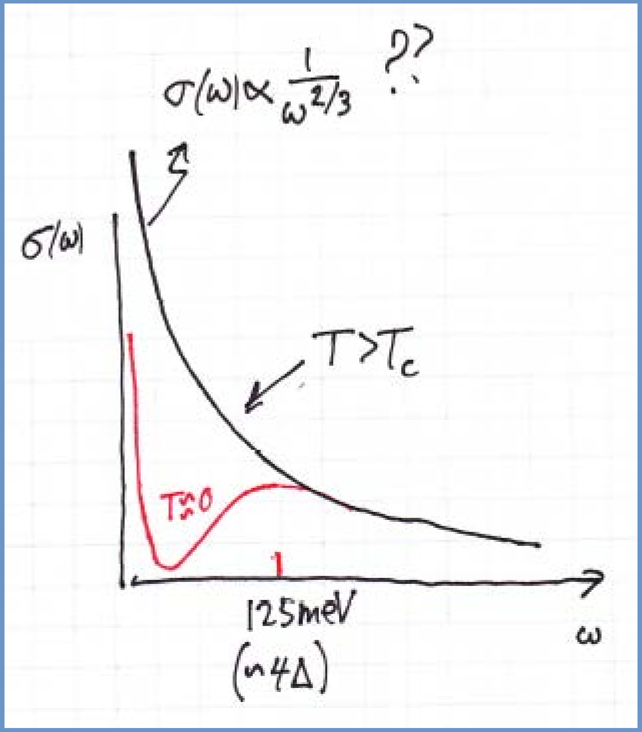
Mysteries of $\sigma(\omega)$ in cuprates.

Optical conductivity data obtained by KK inversion of reflectivity in IR. Consider side by side comparison of $\rho(T)$ and $\sigma(\omega)$.

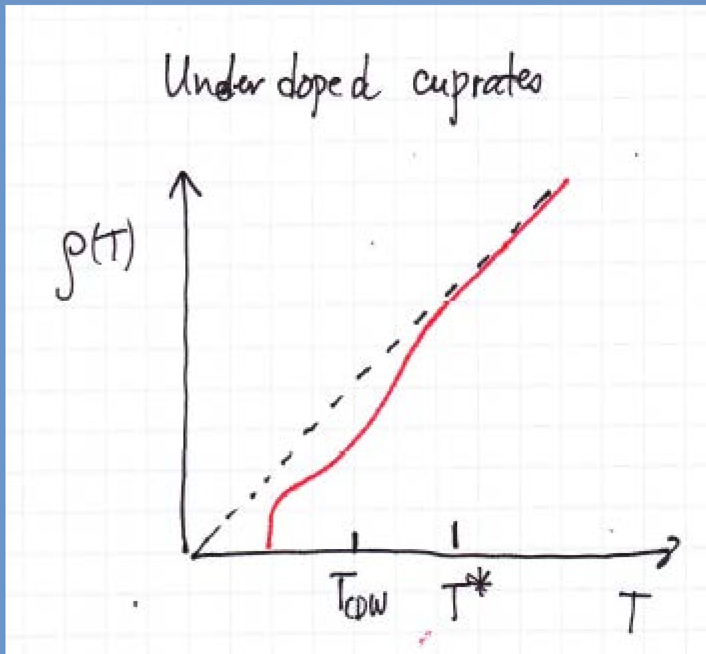
Optimal doping

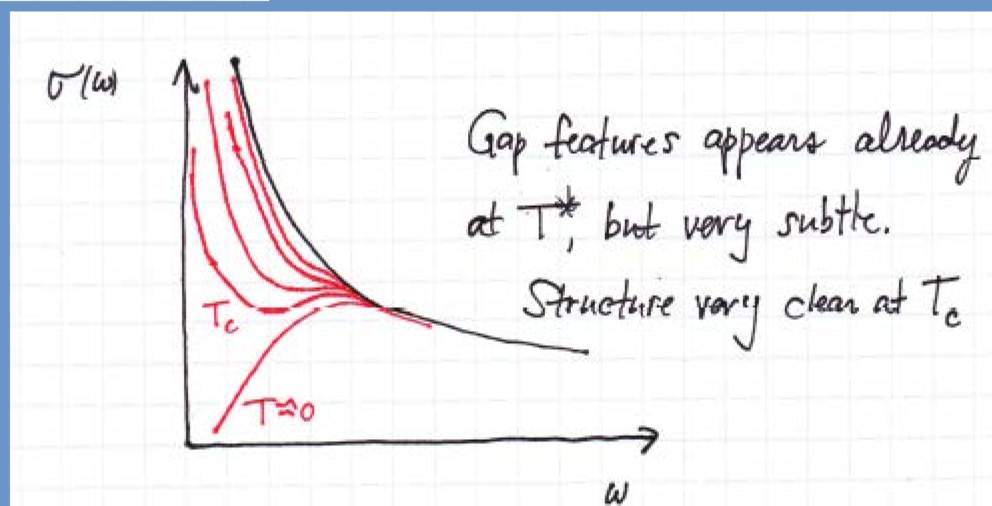


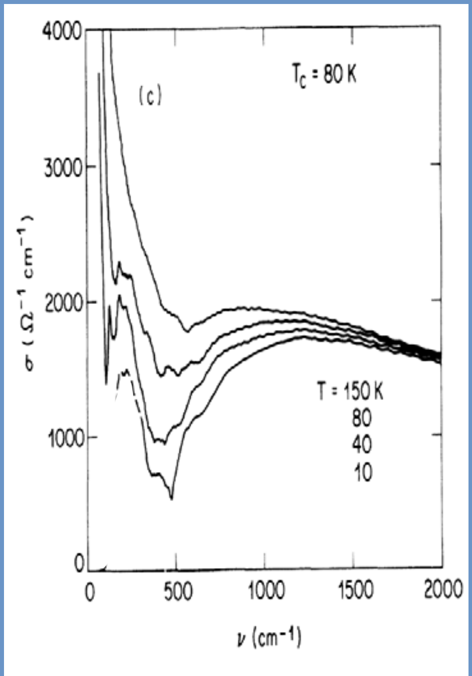




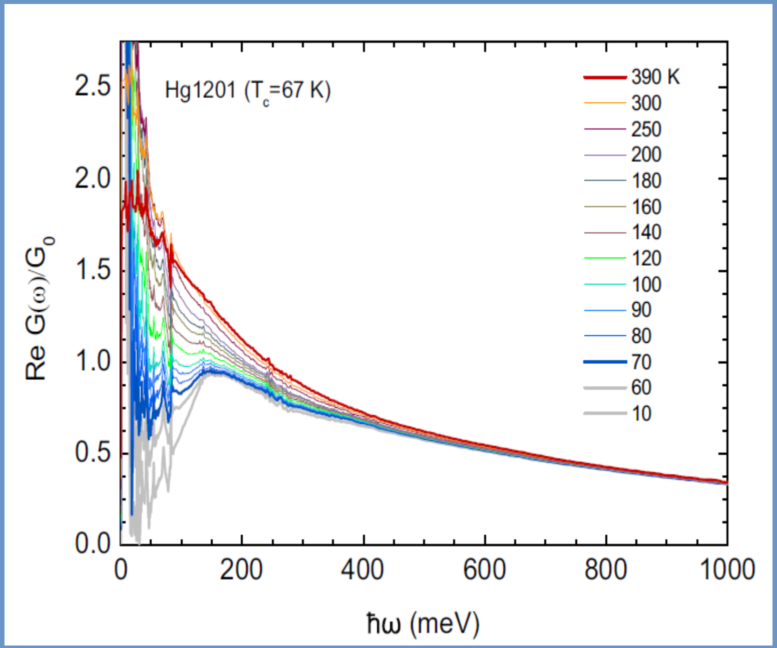
Gap appears at T_c in optimal cuprates. Originally interpreted as superconducting gap. However, it was soon clear that the absorption for $\hbar\omega > 4\Delta$ was independent of disorder and hence could not be the Mattis Bardeen absorption. The puzzle deepens in underdoped cuprates...


Underdoped cuprates
ρ(T)
T_CDW
T*
T


σ'(ω)
Gap features appears already at T*, but very subtle.
Structure very clear at T_c
T_c
T≈0
ω



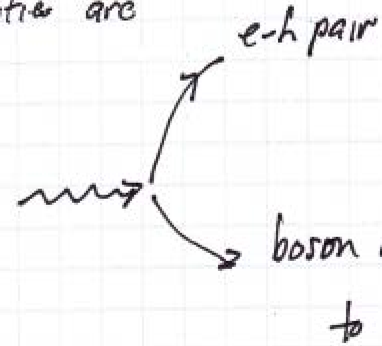
Bell Labs group
Thomas, Millis, JO (1990)

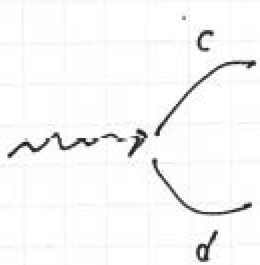


Greven, Barisic, van der Marel collaboration PNAS 2013

What is responsible for absorption edge at 4Δ?

We have seen that for clean metals the spectral weight is exhausted by the Drude peak. Finite frequency absorption is zero because of momentum conservation. So the possibilities are

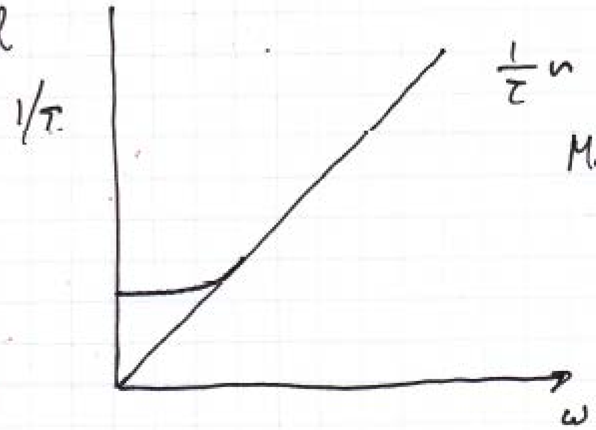




interband e-h pair such as CDW or $p \to d$ transition

Frequency dependent scattering rate picture

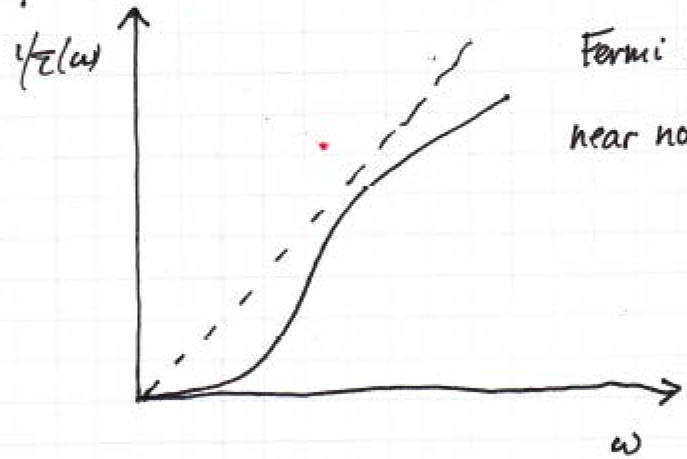
Optimal



$\frac{1}{\tau} \sim \max(\omega, T)$

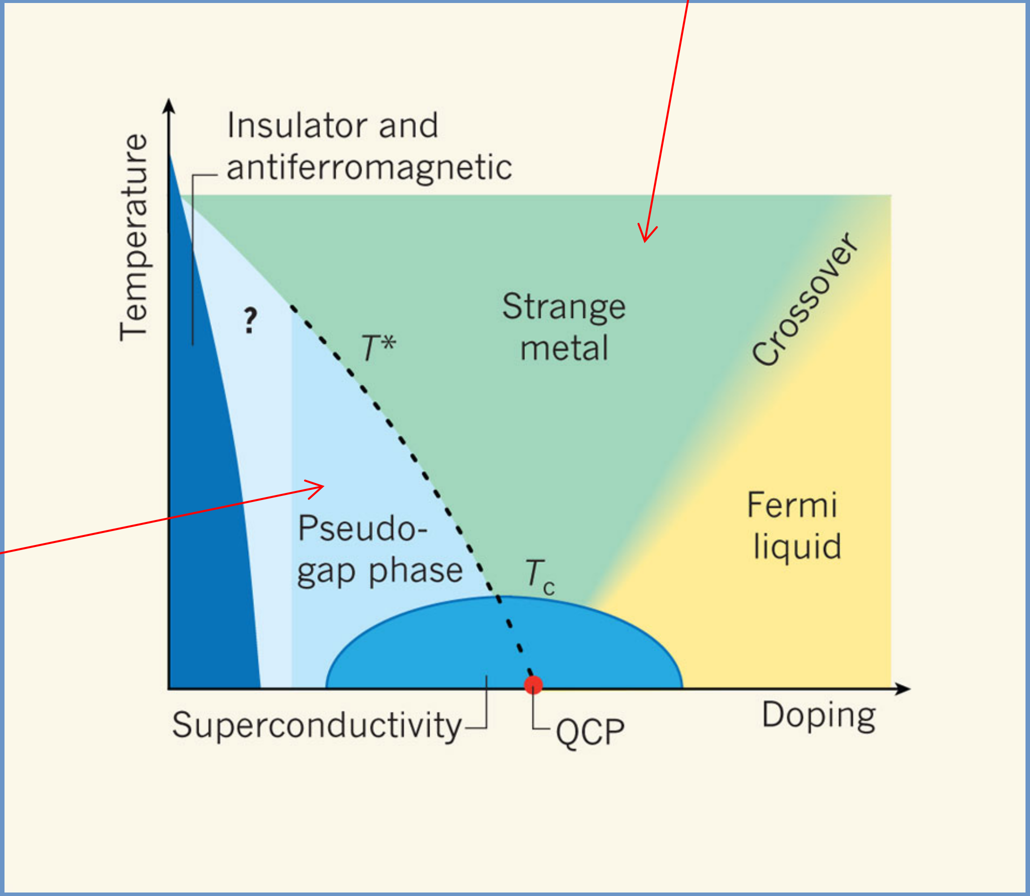
Marginal Fermi Liquid

Underdoped



Fermi liquid of near nodal quasiparticles

Z=0 everywhere ?



Pseudo-fermi liquid
living near nodes