Optical Conductivity of Superconductors

I. Kinetic theory for normal metal

\[ f = m \frac{\dot{a}}{a} \]

\[ \dot{f} = -e \dot{E} - \eta \dot{v} \]

\[ -e \dot{E}(\omega) - \eta \dot{v}(\omega) = -i \omega m \dot{v}(\omega) \]

\[ \dot{v}(\omega) = -\frac{e \dot{E}(\omega)}{\eta - i \omega m} \]

\[ \dot{J}(\omega) = me \dot{v}(\omega) = \frac{ne^2}{\eta - i \omega m} \overline{E}(\omega) = \frac{ne^2}{m} \frac{1}{\eta - i \omega m - i \omega} \]
Kinetic theory \( \frac{e}{m} = \frac{1}{\tau} = \frac{1}{l} \) where \( l \) is mfp.

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

\[ \sigma = \sigma_1 + i\sigma_2 \]

\[ \int d\omega \sigma_1(\omega) = \frac{\pi}{2} \frac{ne^2}{m} \]

These results are trivial to obtain by simple kinetic theory of or Boltzmann Eq. So why do more?
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 - Gor'kov: Macroscopic Quantum Field

BCS: exact knowledge of ground and excited states in mean-field theory

[see Anderson remembers @ 50 yrs of BCS]
Some of the basics of QM approach

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

$$\delta H = e \int d^3 r \vec{J} \cdot \vec{A} - \rho SV$$

From linear response theory we can obtain:

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

$$\rho(\vec{q}, \omega) = X(\vec{q}, \omega) V \ [\text{screening}]$$
longitudinal and transverse responses

\[ \mathbf{\tau}(\mathbf{r}) = \mathbf{\tau}_L(\mathbf{q}) e^{i \mathbf{q} \cdot \mathbf{e}} e^{-i \omega t} \]

\[ \mathbf{\tau}_L(\mathbf{q}) \]

\[ \mathbf{\tau} \]

\[ \mathbf{\tau}_L(\mathbf{q}) \]

longitudinal current generates charge density
Optical conductivity and Meissner effect are two distinct limits of $K(q, \omega)$.

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

$$\sigma(\omega) = \frac{C}{i\omega} K(q = 0, \omega)$$

$$\sigma_{dc} = \lim_{\omega \to 0} \frac{C}{i\omega} K(q = 0, \omega)$$
Meissner effect is the nonvanishing of
\[ K(\bar{q}) \text{ in the limit } q \to 0. \]

Summary

Optical conductivity
\[ \sigma(\omega) \iff K(\bar{q} = 0, \omega) \]

Meissner \[ K(\bar{q}, \omega = 0) \]
Calculating current in linear response

In second quantization we have

\[ \mathbf{J}(\mathbf{r}) = \mathbf{J}_D(\mathbf{r}) + \mathbf{J}_p(\mathbf{r}) \]

\[ \mathbf{J}_D(\mathbf{r}) = \frac{e^2}{mc} \mathbf{\nabla} \mathbf{\nabla} + \mathbf{A}(\mathbf{r}) \]

\[ \mathbf{J}_p(\mathbf{r}) = -\frac{e}{2m} \left[ \mathbf{\nabla}^2 \mathbf{\nabla} \mathbf{\nabla} \right] \psi^*(\mathbf{r}) \psi(\mathbf{r}) - (\mathbf{\nabla} \psi^*(\mathbf{r})) \psi(\mathbf{r}) \]

\( \theta \) dia magnetic \( \gamma \) paramagnetic
Linear response theory

\[ K(\vec{q}, \omega) = R(\vec{q}, \omega) + \frac{n e^2}{m c} \]

\[ R(\vec{q}, \omega) = \sum_n \left| \langle n | J_p(\vec{q}) | 0 \rangle \right|^2 \times \]

\[ \left[ \frac{1}{\hbar \omega - (E_n - E_0) + i \eta} - \frac{1}{\hbar \omega + (E_n - E_0) + i \eta} \right] \]

\[ \xi \text{ Kubo formula} \]
$J_p(\vec{q})$ 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

$$\overrightarrow{J_p}(\vec{q}) = -\frac{e\hbar}{m} \sum_k (\vec{k} + \vec{q}) \frac{c_k^+ c_{k+q}}{2}$$

Also sum over spins $c_k^+ c_{k+q} \uparrow \uparrow \text{ etc.}$
Conductivity is a 2-particle Green fct.

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

$R$ is related to matrix elements

$\langle n | c_{k+q}^{\dagger} c_k^{\dagger}(0) \rangle$

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 not simply the convolution of two 1-particle Green functions. Instead vertex corrections have to be included otherwise big problems.

- Non-conservation of charge
- Scattering rate not weighted by scattering angle
Requires about 25 pages of this stuff

\[ \Pi_{xx}(\bar{q}) = \begin{array}{c}
\text{Diagram 15.11} \\
\end{array} \]
Instead we look at representative examples

1. Free electrons

- Ground state: $|G\rangle$
- Excited states: $|k + q\rangle$, hole in $k\rangle$
We can calculate the imaginary part of $R$ from the paramagnetic term by itself.

$$\text{Im} \ R = \sum_n \left| \langle n | J_p(\mathbf{q}) | 0 \rangle \right|^2 \delta \left[ \hbar \omega - (E_n - E_0) \right]$$

Fermi Golden Rule

$$E_n - E_0 \approx \frac{\hbar^2 k \cdot \mathbf{q}}{m} \quad \text{for} \quad \mathbf{q} \ll k_F$$
Optical conductivity $g \to 0$

$$\text{Im } R(\omega) = \pi \sum_n <n| \vec{j}_p(0|0) > \delta [\hbar \omega - (E_n - E_0)]$$

$= 0$ because cannot couple to e-h pairs with net momentum $\vec{g}$. 
Vanishing of dissipation at \( \omega \to \infty \) is a consequence of perfect momentum conservation.

Impulse response of free electrons.

\[ J(t) \]
As $R(\omega) = 0$ we are left with

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

$$\sigma(\omega) = -\frac{C}{i\omega} K(\omega) = i \frac{ne^2}{mcw}$$

However, Kramers-Kronig shows that there must be a real part, which is a delta function.
\[ \sigma(\omega) = \frac{ne^2}{m} \left[ \frac{\omega}{\hbar} \delta(\omega) + \frac{i}{\omega} \right] \]

Optical conductivity of free electrons

Sum rule satisfied by \( \delta \)-fct

\[ \frac{1}{2} \int d\omega \sigma(\omega) = \frac{1}{4} \frac{ne^2}{m} \]
But is a perfect metal a superconductor?
Static $q=0$ response vanishes for normal metal

\[
R(q) = \sum_n \frac{1}{\hbar^2 q^2} \left( \frac{E_n - E_0}{E_n - E_0} \right)^2 \left| \langle n | \rho | 0 \rangle \right|^2 \times \frac{2}{E_n - E_0}
\]

\[
= \frac{2}{\hbar^2 q^2} \sum_n \frac{2}{\hbar^2 q^2} \left| \langle n | \rho | 0 \rangle \right|^2 (E_n - E_0)
\]

\[
\text{f-sum rule } \sum_n (E_n - E_0) \left| \langle n | \rho | 0 \rangle \right|^2 = \frac{Nq^2}{2m}
\]

Thus

\[
R(q) = \frac{Ne^2}{m^2} \quad \text{and this exactly cancels the diamagnetic term!}
\]
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 $T=0$

now set $B=0$
What about interacting electrons?

Galilean invariance dictates the same result.

How about interacting electrons in a perfect lattice?

\[ \sigma(w) \propto \frac{ne^2}{m^*} \]

\[ Eg \quad \omega \]

\[ m^* \text{ is the effective bandstructure mass.} \]

Also can show that \( \sigma(w) \propto \langle -T \rangle S(w) \)

see White, et al.
What about interacting electrons on a perfect lattice?

[Hubbard model]

\[ \frac{ne^2}{Zm^*} \]

\( Z \) is the quasiparticle renormalization factor

\( Z \sim \text{mass enhancement} \)
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 reactivity, as recently shown by Andy Mackenzie.

The surprising (and non-trivial) conductivity property is the appearance of no conductivity in the disordered metal.
Drude conductivity of normal metal

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

Take 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

$$\Delta \varepsilon = \frac{e^2}{m} k_F \vec{q}$$
If momentum is conserved then we can't couple to these states with an infrared photon which has $q \ll 0$.

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

This allows us to couple to states with

\[ \Delta E = \frac{\hbar^2}{2m} \frac{K F}{l} \quad \text{or} \quad \Delta \omega = \frac{\hbar}{m} \frac{K F}{l} = \frac{P F}{m l} = \frac{V E}{l} = \frac{1}{2} \]
Thus we recover the Drude peak with width $\nu F/\hbar$

\[ \sigma_T(w) \]

Clean limit \( \sigma_T(w) = \frac{\pi e^2}{m} \frac{\hbar}{2} \delta(w) \)

Disorder \( \sigma_T(w) = \frac{ne^2}{m} \frac{\nu F}{\lambda} \)
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

\[ H_0 |\alpha\rangle = \Delta_\alpha |\alpha\rangle; \quad <r |\alpha\rangle = \phi_{\alpha}(r) \]
Anderson: pairing takes place between time-reversed states

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

$$\phi_{\alpha \uparrow}(\vec{r})$$ and $$\phi_{\alpha \downarrow}^*(\vec{r})$$, 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

$$\Delta(\vec{r}) = V_0 \sum_{\alpha, \beta} \phi_{\alpha \uparrow}(\vec{r}) \phi_{\beta \downarrow}(\vec{r}) \langle c_{\alpha \uparrow} c_{\beta \downarrow} \rangle$$
assuming $\Delta(r)$ can be replaced by spatial average

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

and effective $\mathcal{H}$

$$\mathcal{H} = \sum_{\alpha} \mathcal{E}_{\alpha} \left( c_{\alpha \uparrow}^+ c_{\alpha \downarrow} + c_{\alpha \downarrow}^+ c_{\alpha \uparrow} \right)$$

$$\mathcal{H} - \Delta C_{\alpha \uparrow}^+ C_{\alpha \downarrow} - \Delta^* C_{\alpha \downarrow}^+ C_{\alpha \uparrow}$$
Diagonalized by BV transformation

\[ \gamma_{\alpha \uparrow} = u_{\alpha} c_{\alpha \uparrow} + \nu_{\alpha} c_{\alpha \downarrow}^+ \]

\[ \gamma_{\alpha v}^+ = u_{\alpha}^* c_{\alpha \uparrow} + u_{\alpha} c_{\alpha \downarrow}^+ \]

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

let \( \xi_\alpha = \varepsilon_\alpha - \mu \)
No disorder

\[ e^{ikr} \]

Weak disorder

\[ e^{ikr - \gamma(x)} \]

Amplitude relatively constant. Phase correlation lost on the scale of \( \ell \). In the superconductor the excited states accessed with infrared photons are a pair of quasiparticles \( \alpha^+ \beta \) or \( \beta^+ \alpha \) for example.
We couple to these states via the perturbation term which is the paramagnetic current operator. In the basis $|\alpha\rangle$ this is written

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

where $V_{\alpha\beta} = \int d^3r \, \phi_\beta^*(\vec{r}) \nabla \phi_\alpha(\vec{r})$
Express $C^\dagger_{\beta\sigma} C_{\alpha\sigma}$ in terms of $\gamma$ operators

The term in the current operator

$C_{\beta\sigma} C_{\alpha\sigma}$ has a term $u_\beta \gamma^\dagger_{\alpha\sigma} \gamma^\dagger_{\beta\sigma}$

This creates two quasiparticles with energy $E_\alpha$ and $E_\beta$ with opposite spin, and with amplitude proportional to $V_{\alpha\beta} u_\beta V_{\alpha\sigma}$. However, there is another term that creates the same $\gamma$ pair. With

This is the time-reversed term

$T \{ C^\dagger_{\beta\sigma} C_{\alpha\sigma} \} = C^\dagger_{\alpha\sigma} C^\dagger_{\beta\sigma}$

which has amplitude $V_{\beta\sigma} V_{\alpha\sigma} u_\beta V_{\alpha\sigma} u_\sigma$. 

To find the overall matrix element we must take the sum:

\[ V_{\alpha \beta} u_\beta u_\alpha + V_{\alpha \alpha} u_\alpha u_\beta \]

Because the current is odd under time-reversal we have \( V_{\alpha \beta} (u_\beta u_\alpha - u_\alpha u_\beta) \) for the matrix element to generate the \( g \) pair \( \gamma^+_{\alpha} \gamma^+_{\beta} \) from the ground state

\[ V_{\alpha \beta} (u_\beta u_\alpha - u_\alpha u_\beta) \]

BCS vacuum
Sequence of steps beautifully described in PAL notes leads to

\[ \sigma(\omega) = \frac{e^2 \pi}{\omega} \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\xi' \left( \frac{\varepsilon_{5}}{\varepsilon_{5}} - \frac{\varepsilon_{5}}{\varepsilon_{5}} \right)^{2} f(\xi, \xi') \]

\[ \times 8 \left( \omega - (\varepsilon_{5} + \varepsilon_{5}) \right) \]
Now what are these terms?

Recall $\tilde{\Sigma}$ is normal state energy referred to $\mu$.

$\Sigma, \Sigma'$ expresses the fact that the coherence factor depends on $\Delta$ only thru the normal state energy $\tilde{\Sigma}$ and the gap $\Delta$.

$f(\tilde{\Sigma}, \tilde{\Sigma}')$ is the squared matrix element connecting states with normal state energy $\tilde{\Sigma}, \tilde{\Sigma}'$.

$\delta \left[ \omega - (E_{\tilde{\Sigma}} + E_{\tilde{\Sigma}'}) \right]$ is density of states factor.
Conductivity in superconducting state

\[ \sigma_0 \text{ depends on } f(\xi, \xi') \]

Also

\[ (\nu\nu' - \nu'\nu)^2 = \frac{1}{2} \left[ 1 - \frac{\xi\xi'}{EE'} - \frac{\Delta^2}{EE'} \right] \]

Finally

\[ \sigma(\omega) = \frac{\sigma_0}{\omega} \int d\xi \int d\xi' \left( 1 - \frac{\Delta^2}{EE'} \right) \delta[\omega - (E + E')] \]
Mattis-Bardeen absorption is zero at threshold despite singular density of states.
Spectral weight in the delta function is

\[ \nu \frac{ne^2 \tau}{m} \cdot 2\Delta \]  

in the limit that \( \Delta \ll \frac{1}{\tau} \)

If coherence factor was unity then there would be no S-fct.
Far-infrared optical conductivity gap in superconducting MgB$_2$ films

Mattis-Bardeen theory works in MgB$_2$
But not in cuprates

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

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

Optimal depining

$\sigma(w) \propto \frac{1}{\omega^{2/3}}$ ?

Optical conductivity $\sigma(w)

Linear $\rho(T)$

$T_c \ T$

$T > T_c$

$125 \text{ meV} (\hbar 4 \Delta)$
Gap appears at $T_c$ in optimal cuprates. Originally interpreted as superconducting gap. However, it was soon clear that the absorption for $h\omega > 4\Delta$ was independent of disorder and hence could not be the Mattis-Bardeen absorption. The puzzle deepens in underdoped cuprates...
Under doped cuprates

\[ \rho(T) \]

\[ T_{CDW} \quad T^* \quad T \]

Gap features appear already at \( T^* \), but very subtle. Structure very clear at \( T_c \).
Bell Labs group
Thomas, Millis, JO (1990)

Greven, Barisic, van der Marel collaboration PNAS 2013
What is responsible for absorption edge at $4\Delta$?

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:

- e-h pair
- boson or another e-h pair
- to conserve momentum

interband e-h pair such as CDW or $p\rightarrow d$ transition
Frequency dependent scattering rate picture

Optimal

\[ \frac{1}{T} \]

Marginal Fermi Liquid

\[ \frac{1}{2} n \max (\omega, T) \]

Underdoped

\[ \mu(T) \]

Fermi liquid of near nodal quasiparticles
Pseudo-fermi liquid living near nodes

Z=0 everywhere?