Eliashberg's Theory of Superconductivity with

Antonio Sanna

Max Planck Institute
Halle Germany

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Superconductivity beyond BCS

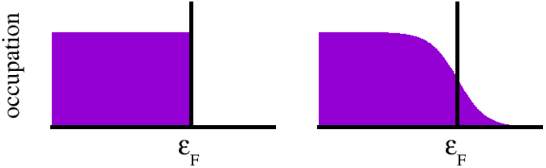
– The BCS theory has a relatively simple mathematical structure. And allows to describe in detail the phenomenology of superconductivity.

– However its predictive power is poor. It is used mostly as a model theory. And, when it is applied to real materials, couplings and T_c are fitted to the experimental value.

– What is missing in BCS? mainly to account for the intrinsic time scale of the superconducting interactions (in particular phonons).

a 2x2 Hamiltonian ...

The essential kind of correlation in superconductivity is the one between electrons and holes. This creates the phase space in which the pairing interaction can scatter the cooper pairs.



To describe such an interaction is convenient to define a 2x2 matrix Hamiltonian:

$$\bar{H}_0(\mathbf{k}) = \begin{pmatrix} H_0(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & -H_0(\mathbf{k}) \end{pmatrix} \quad (1)$$

where the off-diagonal terms Δ couple the electron and hole parts. And can be thought as an external pairing field or as an infinitesimal symmetry breaking one.

... and a 2x2 Green's function

To account, at the same time, for the effect of temperature and of the dynamical interactions, we need to work with Matsubara Green's functions (Fetter).

$$\bar{G}(\mathbf{k}, i\omega_n) = \begin{pmatrix} G(\mathbf{k}, i\omega_n) & -F(\mathbf{k}, i\omega_n) \\ -F^*(\mathbf{k}, i\omega_n) & G(\mathbf{k}, -i\omega_n) \end{pmatrix}, \tag{2}$$

where G is the normal state Green's functions. And F is called anomalous Green's function, and is the Fourier transform of the anomalous average $< \psi_{\mathbf{k}\uparrow}(t)\psi_{\mathbf{k}\downarrow}(t') >$

perturbation theory : $\bar{G}_0$

Our reference non interacting systems is the solution of[1] :

$$\left[i\omega_n \bar{I} + \bar{H}_0(\mathbf{k})\right] \bar{G}_0(\mathbf{k}, i\omega_n) = \bar{I} \tag{3}$$

Before to start with perturbation theory we put all that we know

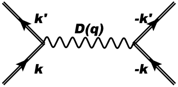
into $\bar{H}_0$. We choose $\bar{H}_0$ as the Kohn Sham system that already includes some Coulomb correlation effects.

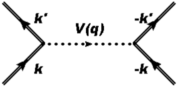
$$H_0(\mathbf{k}) := H_{KS}(\mathbf{k}) = \xi_{KS}(\mathbf{k}) \tag{4}$$

[1] $\bar{I}$, $\bar{\sigma}_i$ are the Pauli matrices

perturbation theory : $\bar{H}_{int}$

A perturbation Hamiltonian is the added to $\bar{H}_0$. The perturbation is given by the phonon field and by a Coulomb interaction between electrons[2]:

$\bar{H}_{int} =$ 

$+$ 

(5)

$D(\mathbf{q})$ and $V(\mathbf{q})$ being the phononic propagator and an electronic interaction.

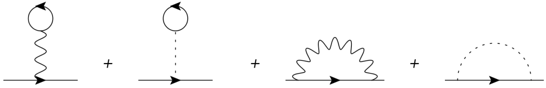
[2] In part this term is already included in the Kohn Sham Hamiltonian $\bar{H}_{KS}$; that means that we must keep one eye on avoiding to double count some effect

perturbation theory : $\bar{\Sigma}$ 1/3

The interacting Green's function corresponding to $\bar{H}_{int}$ may be expressed in terms of the total irreducible Self energy $\bar{\Sigma}$

$$\left[\bar{G}(\mathbf{k}, i\omega_n)\right]^{-1} = \left[\bar{G}_0(\mathbf{k}, i\omega_n)\right]^{-1} - \bar{\Sigma}(\mathbf{k}, i\omega_n), \quad (6)$$

An approximated $\bar{\Sigma}$ can be obtained by perturbation theory: the first order terms are:



– The first two give only diagonal contributions, in part already accounted for in the Kohn Sham Hamiltonian, and can be ignored.

– Then we boost to an higher order the two exchange-like diagrams by dressing all propagators lines

So we consider the following approximation for Σ :

$\bar{\Sigma} =$ 

- The double phonon lines just means that we put in the propagator dressed phonons ('s phonons)
- Within Migdal's theorem corrections to this diagram would be of order m/M (electronic / ionic mass)
- The double Coulomb line means that we use a screened Coulomb interaction (i.e. rpa)
- Superconducting corrections to the phonon/Coulomb propagator will be ignored
- Vertex corrections on the Coulomb part have been ignored (without any serious reason)
- Diagonal contributions from the Coulomb part will be ignored to avoid double counting of KS xc-effects

So we are left with the following approximation for the Self Energy:

$$\bar{\Sigma}(\mathbf{k}, i\omega_n) = -k_B T \sum_{\mathbf{k}',n'} \bar{\sigma}_3 \bar{G}(\mathbf{k}', i\omega_{n'}) \bar{\sigma}_3 \times \left[\sum_\nu \left| g_{\mathbf{k},\mathbf{k}',\nu} \right|^2 D_\nu(\mathbf{k}-\mathbf{k}', i\omega_n - i\omega_{n'}) + \bar{\sigma}_1 W(\mathbf{k}-\mathbf{k}') \right] \tag{7}$$

Eliashberg's equations 1/3

Now having a Self energy we can come back to the Dyson equation6 and look for a solution

$$\left[\bar{G}(\mathbf{k}, i\omega_n)\right]^{-1} = \left[\bar{G}_0(\mathbf{k}, i\omega_n)\right]^{-1} - \bar{\Sigma}(\mathbf{k}, i\omega_n), \tag{8}$$

This is a self-consistent equations because $\bar{\Sigma}$ depends on $\bar{G}$. To solve it we expand $\bar{\Sigma}$ in Pauli matrices:

$$\begin{aligned} \bar{\Sigma}(\mathbf{k}, i\omega_n) &= i\omega_n \left[1 - Z(\mathbf{k}, i\omega_n)\right] \bar{I} + \chi(\mathbf{k}, i\omega_n)\bar{\sigma}_3 \\ &+ \phi_1(\mathbf{k}, i\omega_n)\sigma_1 + \phi_2(\mathbf{k}, i\omega_n)\bar{\sigma}_2, \end{aligned} \tag{9}$$

and we get a formal solution:

$$\bar{G}(\mathbf{k}, i\omega_n)^{-1} = i\omega_n Z\bar{I} - (\epsilon_{\mathbf{k}} + \chi)\bar{\sigma}_3 - \phi_1\bar{\sigma}_1 - \phi_2\bar{\sigma}_2. \tag{10}$$

reinserting $\bar{G}$ into the Dyson equation we are left with a set of coupled self-consistent equations, named after Eliashberg:

$$\begin{aligned}
\left[1 - Z(\mathbf{k}, i\omega_n)\right] i\omega_n &= \frac{1}{\beta} \sum_{\mathbf{k}', n', \nu} \left| g_{\mathbf{k},\mathbf{k}',\nu} \right|^2 \frac{i\omega_{n'} Z(\mathbf{k}', i\omega_{n'}) D_\nu(\mathbf{k}-\mathbf{k}', i\omega_n - i\omega_{n'})}{\Theta(\mathbf{k}', i\omega_{n'})} \\
\chi(\mathbf{k}, i\omega_n) &= \frac{1}{\beta} \sum_{\mathbf{k}', n', \nu} \left| g_{\mathbf{k},\mathbf{k}',\nu} \right|^2 \frac{\chi(\mathbf{k}', i\omega_{n'}) + \xi_{\mathbf{k}'}}{\Theta(\mathbf{k}', i\omega_{n'})} D_\nu(\mathbf{k}-\mathbf{k}', i\omega_n - i\omega_{n'}) \\
\phi^{ph}_{1(2)}(\mathbf{k}, i\omega_n) &= -\frac{1}{\beta} \sum_{\mathbf{k}', n', \nu} \left| g_{\mathbf{k},\mathbf{k}',\nu} \right|^2 \frac{\phi_{1(2)}(\mathbf{k}', i\omega_{n'}) D_\nu(\mathbf{k}-\mathbf{k}', i\omega_n - i\omega_{n'})}{\Theta(\mathbf{k}', i\omega_{n'})} \\
\phi^{C}_{1(2)}(\mathbf{k}, i\omega_n) &= -\frac{1}{\beta} \sum_{\mathbf{k}', n'} W_{\mathbf{k},\mathbf{k}'} \frac{\phi_{1(2)}(\mathbf{k}', i\omega_{n'})}{\Theta(\mathbf{k}', i\omega_{n'})} \\
\phi_{1(2)}(\mathbf{k}, i\omega_n) &= \phi^{ph}_{1(2)}(\mathbf{k}, i\omega_n) + \phi^{C}_{1(2)}(\mathbf{k}, i\omega_n) \qquad (11) \\
\Theta(\mathbf{k}, i\omega_n) &= \left[Z(\mathbf{k}, i\omega_n)\omega_n\right]^2 + \left[\epsilon_{\mathbf{k}} + \chi(\mathbf{k}, i\omega_n)\right]^2 + \phi_1(\mathbf{k}, i\omega_n)^2 + \phi_2(\mathbf{k}, i\omega_n)^2
\end{aligned}$$

Eliashberg's equations 3/3

- We can set $\phi_2 = 0$, and work with a single off diagonal contribution $\phi = \phi_1$, that is real on the Matsubara axis.
- χ acts on the diagonal part of $\bar{G}$. It generates a shift in the Fermi energy that can be neglected assuming electron/hole symmetry.
- The Coulomb part of these equations has some convergency problems, an high energy cut-off needs to be enforced.

The fully anisotropic $\mathbf{k}$-dependent Eliashberg's equations are difficult to tackle. Here we assume that the phononic coupling is constant near the Fermi energy:

$$\begin{aligned} Z(\mathbf{k}, i\omega_n) &\rightarrow \langle Z(\mathbf{k}, i\omega_n)\rangle_{\epsilon_{\mathbf{k}}=E_F} = Z(i\omega_n) \\ \phi(\mathbf{k}, i\omega_n) &\rightarrow \phi(i\omega_n) \\ \Delta(\mathbf{k}, i\omega_n) &\rightarrow \Delta(i\omega_n) \\ \Theta(\mathbf{k}, i\omega_n) &\rightarrow \Theta(\epsilon_{\mathbf{k}}, i\omega_n) \end{aligned} \tag{12}$$

we define an average electron phonon coupling (task 250)

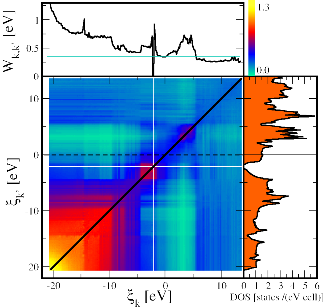
$$\alpha^2F(\omega) = \frac{1}{N_{E_F}} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\nu} |g_{\mathbf{k},\mathbf{k}',\nu}|^2 \delta(\epsilon_{\mathbf{k}'}) \delta(\epsilon_{\mathbf{k}}) \delta(\omega - \omega_{\mathbf{q}\nu}) \tag{13}$$

Isotropic Eliashberg's equations 2/3

The Coulomb coupling has a large energy scale. For example it can be calculated at the rpa level (soon available in):

For the time being we assume $W_{\mathbf{k},\mathbf{k}'}$ to be constant within an energy range of $\sim$ 10eV. Then the integration of the Coulomb part of the Eliashberg's equations becomes analytic (Scalapino). And will depend on a single parameter μ^*.

$$\mu^* = \frac{N_{E_F} W_{E_F}}{1 - N_{E_F} W_{E_F} ln\left(E_F/\omega_c\right)} \qquad (14)$$



Isotropic Eliashberg's equations 3/3

And we are left with the final form:

$$
\begin{aligned}
[1 - Z(i\omega_n)]i\omega_n &= -\frac{\pi}{\beta}\sum_{\omega_{n'}} \frac{Z(i\omega_{n'})i\omega_{n'}}{\Xi(i\omega_{n'})} \int \frac{2\omega\alpha^2F(\omega)}{(\omega_n - \omega_{n'})^2 + \omega^2} d\omega \\
\phi^{ph}(i\omega_n) &= \frac{\pi}{\beta}\sum_{\omega_{n'}} \frac{\phi(i\omega_{n'})}{\Xi(i\omega_{n'})} \int \frac{2\omega\alpha^2F(\omega)}{(\omega_n - \omega_{n'})^2 + \omega^2} d\omega \\
\phi^{C}(i\omega_n) &= -\mu^*\frac{\pi}{\beta}\sum_{\omega_{n'}} \frac{\phi(i\omega_{n'})}{\Xi(i\omega_{n'})}\theta(\omega_c - |\omega_{n'}|) \qquad (15) \\
\Xi(i\omega_n) &= \sqrt{[Z(i\omega_n)\omega_n]^2 + \phi^2(i\omega_n)},
\end{aligned}
$$

Now ... run with task 260 !!

Evaluating the output

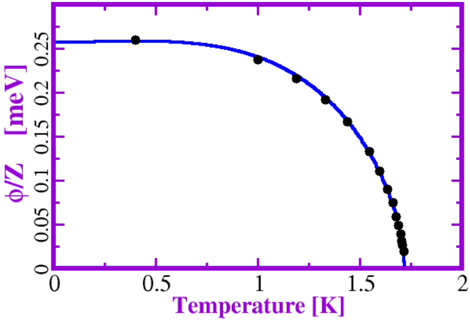
Solving the equations give us the Matsubara Green's function:

$$\bar{G}(\mathbf{k}, i\omega_n) = -\frac{\begin{pmatrix} i\omega_n Z(i\omega_n) + \xi_{\mathbf{k}} & \phi(i\omega_n) \\ \phi(i\omega_n) & i\omega_n Z(i\omega_n) - \xi_{\mathbf{k}} \end{pmatrix}}{\left[Z(i\omega_n)\omega_n\right]^2 + \xi_{\mathbf{k}}^2 + \phi^2(i\omega_n)}. \quad (16)$$

and now we are going to extract some physics out of it

T_c

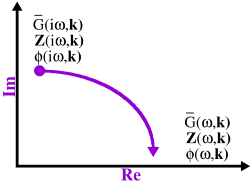
T_c is defined as the temperature at which the anomalous density becomes zero
so we just need to look at ϕ :



we have T_c

Real Axis

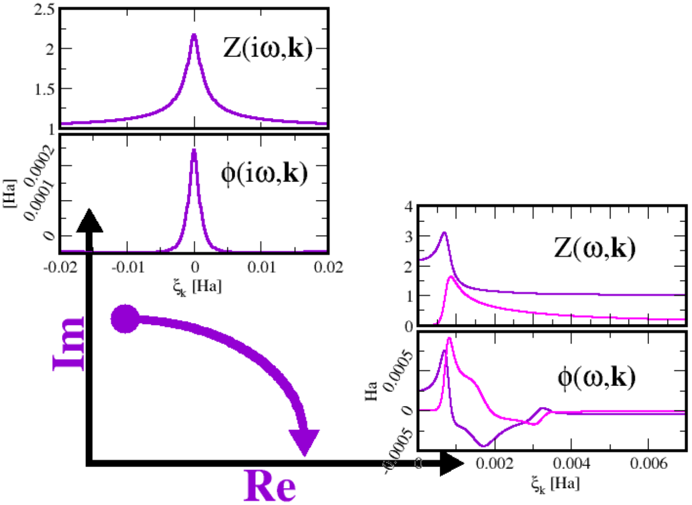
Beyond T_c, $\bar{G}$ contains information about the single particle excitation spectrum of the superconductor. To extract it we need the retarded (physical) Green's Function. The way to get it is to perform an analytic continuation from the imaginary to the real axis of our $\bar{G}$.



$$\bar{G}(\mathbf{k},\omega) = -\frac{\begin{pmatrix} \omega Z(\omega) + \xi_{\mathbf{k}} & \phi(\omega) \\ \phi(\omega) & \omega Z(\omega) - \xi_{\mathbf{k}} \end{pmatrix}}{\left[Z(\omega)\omega\right]^2 + \xi_{\mathbf{k}}^2 + \phi^2(\omega)}. \quad (17)$$

The analytic continuation of ϕ and Z is done directly by with the Padé's approximants method (Carbotte).

Real Axis


2.5
2
1.5
1
Z(iω,k)
[Ha]
0.0002
0.0001
0
ϕ(iω,k)
-0.02
-0.01
0
0.01
0.02
ξk [Ha]
Im
Re
4
3
2
1
0
Z(ω,k)
Ha
0.0005
0
-0.0005
ϕ(ω,k)
0.002
0.004
0.006
ξk [Ha]

Excitation spectrum

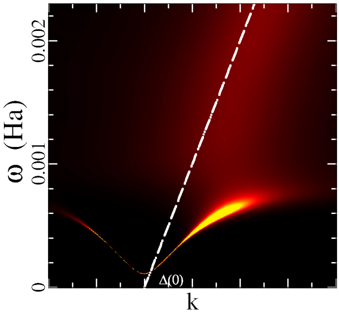
the poles of

$$G^{11}(\mathbf{k},\omega) = -\frac{\omega Z(\omega) + \xi_{\mathbf{k}}}{\left[Z(\omega)\omega\right]^2 + \xi_{\mathbf{k}}^2 + \phi^2(\omega)}. \tag{18}$$

give the elemental excitations of the Superconductor.
The minimum excitation energy is $\omega = \Delta = \phi(\omega)/Z(\omega)$ This is therefore the binding energy for electrons in a Cooper pair.

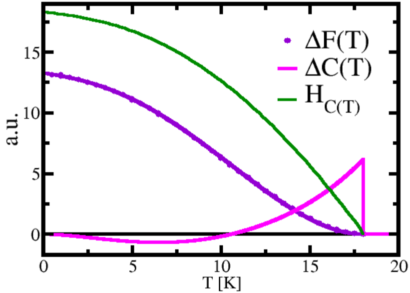
Spectral function

the imaginary part of G^{11} is the electron spectral function. It Shows how the non interacting (Kohn-Sham) band structure is modified by the presence of phonons. And by the superconducting condensation (Scalapino and Schrieffer).



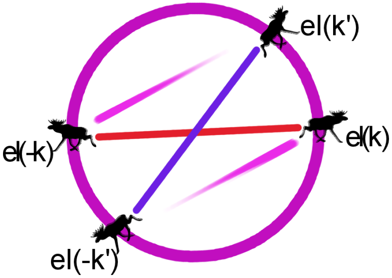
and many other properties can be derived

- Free energy difference from the normal state (ΔF)
- Critical magnetic fields (H_C)
- jumps in the specific heat at the superconducting transition
- ... (Carbotte)



That's all

The Eliashberg's theory of phononic superconductivity is a powerful technique that allows to describe in a reliable way the superconducting state.
A basic implementation is included in, from which many physical properties can be simulated (directly or with a little bit of post-processing)



References

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