BCS Superconductivity and BCS-BEC crossover

Course:
Quantum physics of atoms and ions
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- Differences with the three dimensional case and results that can be obtained in this framework

History of superconductivity

History of superconductivity I

- In the early 1900's there was still a debate about the behaviour of electrons at low temperatures.
- 1911: Kamerlingh Onnes measured the low temperature behaviour of Mercury (Hg)

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Discovery of low-temperature superconductors

- 1933: Meissner and Ochsenfeld discovered the a metal in a superconducting state would expel or screen a magnetic field

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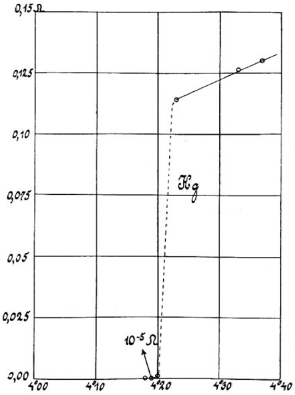
Meissner's effect



Resistance (Ω) versus temperature (K) for mercury from the October, 26th, 1911 experiment.

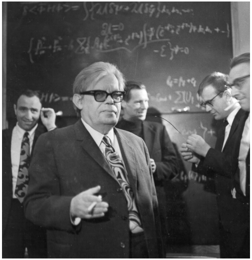
History of superconductivity II

We need a mathematical way to describe superconductivity. During the 1950's, in the midst of the cold war, two approaches developed

- The Russian version (by Bogoliubov, with contribution of the French physicists De Gennes)
  - It can describe inhomogeneous superconductors
- American BCS version (By Bardeen, Cooper and Schrieffer).
  - The analytics can be pursued further

We will focus on the BCS theory of superconductivity

Panel above: Bogoliubov
Panel below: from left to right Bardeen, Cooper and Schrieffer



BCS theory

First attempt of wave function

In 1957 Leon Cooper showed that, in the presence of an attractive potential, two electrons closed to the Fermi surface form a bound state that lowers the overall energy. These two electrons have opposite spin and momentum

$$c^{\dagger}_{\mathbf{k},\uparrow}c^{\dagger}_{-\mathbf{k},\downarrow}|0\rangle \tag{1}$$

So that the wave function of a superconductor should be (with N even)

$$|\psi\rangle_s = \sum_{\mathbf{k}_1,\dots,\mathbf{k}_{N/2}} g_{\mathbf{k}_1}\dots g_{\mathbf{k}_{N/2}} c^{\dagger}_{\mathbf{k}_1,\uparrow}c^{\dagger}_{-\mathbf{k}_1,\downarrow}\dots c^{\dagger}_{\mathbf{k}_{N/2},\uparrow}c^{\dagger}_{-\mathbf{k}_{N/2},\downarrow}|0\rangle \tag{2}$$

Problem: This wave function is too general

Polaron problem

Solution: since the total spin of a two bounded electrons is bosonic, the three American physicists got inspired by the work of Tsung Dao Lee, Francis Eugene Low and David Pines, which considered the 'polaron problem', a variational approach to describe an electron coupled to phonons in a non-perturbative manner.

$$|\psi_{\text{LLP}}\rangle = \prod_{\mathbf{k}} \exp\left(f_{\mathbf{k}} a^{\dagger}_{\mathbf{k}} - f^{*}_{\mathbf{k}} a_{\mathbf{k}}\right) |0\rangle \tag{3}$$

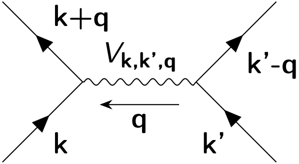
with $[a_{\mathbf{k}}, a_{\mathbf{k'}}] = 0$, $\left[a_{\mathbf{k}}, a^{\dagger}_{\mathbf{k'}}\right] = \delta_{\mathbf{k},\mathbf{k'}}$.
But if $a_{\mathbf{k}} = c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow}$ we need only 1^{st} order expansion of the exponential since $\left(c^{\dagger}_{\mathbf{k},\sigma}\right)^2 = 0$ so (with $|v_{\mathbf{k}}|^2 + |u_{\mathbf{k}}|^2 = 1$)

$$|\psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow}\right) |0\rangle \tag{4}$$

We now specify the BCS Hamiltonian $H = H_0 + H_{int}$, where the interaction comes from the exchange of optical phonons

$$H_0 = \sum_{\mathbf{k},\sigma} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \quad (5)$$

$$H_{int} = \sum_{\substack{\mathbf{k},\mathbf{k'},\mathbf{q} \\ \sigma,\sigma'}} V_{\mathbf{k},\mathbf{k'},\mathbf{q},\sigma,\sigma'} c^\dagger_{\mathbf{k+q},\sigma} c^\dagger_{\mathbf{k'\text{-}q},\sigma'} c_{\mathbf{k'},\sigma'} c_{\mathbf{k},\sigma} \quad (6)$$



The interaction is too general, let

$\mathbf{k+q} = \mathbf{k'}, \sigma = \uparrow$, $\mathbf{k'}$=-$\mathbf{k}$

$\mathbf{k'\text{-}q} = -\mathbf{k'}, \sigma = \downarrow$, $\mathbf{k'}$=$\mathbf{k}$

$\Downarrow$

$H_{int} = \sum_{\mathbf{k},\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} c^\dagger_{\mathbf{k'},\uparrow} c^\dagger_{\text{-}\mathbf{k'},\downarrow} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow}$

Expression for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ I

We recall that

$$|\psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \right) |0\rangle \tag{7}$$

from where we can get

$$\langle \psi_{\text{BCS}} | H_0 | \psi_{\text{BCS}} \rangle = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 \tag{8}$$

$$\langle \psi_{\text{BCS}} | H_{int} | \psi_{\text{BCS}} \rangle = \sum_{\mathbf{k},\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} v^*_{\mathbf{k}} u_{\mathbf{k}} u^*_{\mathbf{k'}} v_{\mathbf{k'}} \tag{9}$$

and now we parametrize

$$u_{\mathbf{k}} = \cos\theta_{\mathbf{k}}, \quad v_{\mathbf{k}} = \sin\theta_{\mathbf{k}} \tag{10}$$

Expression for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ II

$$\langle \psi_{\text{BCS}} | H_0 | \psi_{\text{BCS}} \rangle = \sum_{\mathbf{k}} \xi_{\mathbf{k}} (1 - \cos 2\theta_{\mathbf{k}})$$

$$\langle \psi_{\text{BCS}} | H_{int} | \psi_{\text{BCS}} \rangle = \sum_{\mathbf{k},\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} \cos 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k'}}$$

Performing the minimization with respect to $\theta_{\mathbf{k}}$

$$\frac{\partial}{\partial \theta_{\mathbf{k}}} \langle \psi_{\text{BCS}} | H_0 + H_{int} | \psi_{\text{BCS}} \rangle = 2\xi_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} + \cos \theta_{\mathbf{k}} \sum_{\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} \sin 2\theta_{\mathbf{k'}} = 0 \tag{11}$$

which leads to

$$\xi_{\mathbf{k}} \tan 2\theta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} \sin 2\theta_{\mathbf{k'}} \tag{12}$$

Expression for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ III and gap parameter

We identify the energy gap parameter $\Delta_{\mathbf{k}}$ as

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} u_{\mathbf{k'}} v_{\mathbf{k'}} \tag{13}$$

and now it is easy to derive and expression for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}}\right), \quad v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}}\right) \tag{14}$$

from which we can derive

Gap equation

$$\boxed{\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} \frac{\Delta_{\mathbf{k'}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}}}$$

Interpretation of the gap parameter I

The gap equation is self consistent and it can be solved by assuming the 'Cooper hypothesis'

$$\Delta_{\mathbf{k}} = \begin{cases} \Delta > 0 & \text{for } |\xi_{\mathbf{k}}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \tag{15}$$

$$V_{\mathbf{k},\mathbf{k'}} = \begin{cases} V < 0 & \text{for } |\xi_{\mathbf{k}}|, |\xi_{\mathbf{k'}}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \tag{16}$$

where ω_D is the Debye frequency, and the idea is that

$$\sum_{\mathbf{k'}} \to \int d\xi \, \nu(\epsilon_F), \quad \nu(\epsilon_F) : \text{const. density of states} \tag{17}$$

$$\Downarrow$$

$$\not{\Delta} = \frac{V}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi \, \frac{\nu(\epsilon_F)\not{\Delta}}{\sqrt{\xi^2 + \Delta^2}} = V \, \nu(\epsilon_F) \, \sinh^{-1}\left(\frac{\hbar\omega_D}{\Delta}\right) \tag{18}$$

Interpretation of the gap parameter II

We can get the *weak-coupling limit* from the exact solution

$$\Delta = \frac{\hbar\omega_D}{\sinh\left(\frac{1}{\nu(\epsilon_F)\,V}\right)} \xrightarrow[V\nu(\epsilon_F)\ll 1]{} \Delta \approx 2\omega_D \exp\left\{\left(-\frac{1}{V\nu(\epsilon_F)}\right)\right\}$$

$$\Downarrow$$

BCS NON PERTURBATIVE THEORY

If we relax the condition T=0, at arbitrary temperature we can get

$$1 \approx V\nu(\epsilon_F)\int_{\hbar\omega_D}^{\hbar\omega_D} d\xi \frac{\tanh\frac{\beta}{2}\sqrt{\xi^2+\Delta^2}}{2\sqrt{\xi^2+\Delta^2}}$$

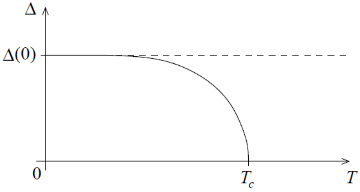


Figure taken from [1]

Gain in energy for superconductors

The ground state energy is

$$E_{GS} = \langle \psi_{\mathrm{BCS}} | H | \psi_{\mathrm{BCS}} \rangle = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right) + \frac{1}{4} \sum_{\mathbf{k},\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} \frac{\Delta_{\mathbf{k}} \Delta_{\mathbf{k'}}}{E_{\mathbf{k}} E_{\mathbf{k'}}} \tag{19}$$

with $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$
From the kinetic part we obtain the energy of a normal metal E_N

$$\sum_{\mathbf{k}} \xi_{\mathbf{k}} = 2\nu(\epsilon_F) \frac{(\hbar\omega_D)^2}{2} + E_N \tag{20}$$

while taking everything into account and assuming $\hbar\omega_D \gg \Delta$

$$\boxed{E_{GS} - E_N = -\frac{1}{2}\nu(\epsilon_F)\Delta^2} \quad \text{with } E_{GS}, E_N < 0 \tag{21}$$

Critical field

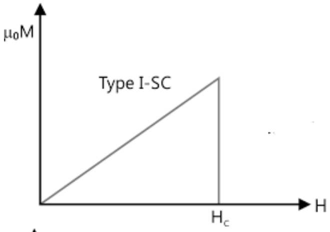
For type-I superconductors, the excess of energy we gain is required for the magnetic-field expulsion. This is the Meissner effect that, together with the electrical resistivity that goes to zero, is one of the two main characteristics of a superconducting material.
So since we have that

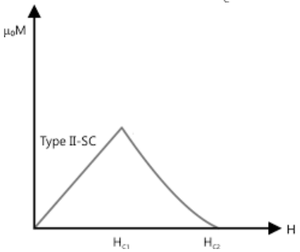
$$E_N - E_{GS} = \frac{H_c^2}{8\pi} \tag{22}$$

where H_c is the critical magnetic field, we get

$$\boxed{\frac{H_c^2}{8\pi} = \frac{1}{2}\nu(\epsilon_F)\Delta^2} \tag{23}$$

Above: Type-I superconductors
Below: Type-II superconductors





BCS-BEC crossover

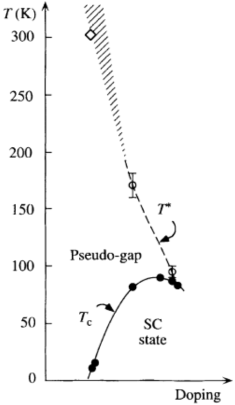
BEC and why we can have BCS-BEC crossover

During the 90's: in cuprates it was experimentally found a gap in the single-particle excitation spectrum at temperature above the critical one for superconductivity, for example for the high-temperature superconductors

$\Downarrow$

Necessity of a theory between BCS and BEC

Schematic phase diagram of $Bi_2Sr_2CaCu_2O_{8+\delta}$ as a function of doping. The filled symbols are the measured T_c for the superconducting phase transition from magnetic susceptibiity. The open symbols are the T* at which the pseudogap closes. Figure taken from [2].

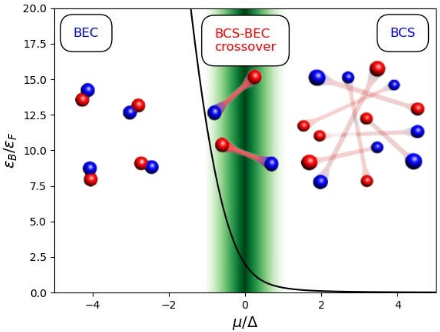


Relevant parameter for the BCS-BEC crossover

We work in two dimensions, where the relevant parameter to study the BCS-BEC crossover is the binding energy of a pair of fermions ϵ_B. It is possible to show that $(x_0 = \mu/\Delta)$ [3]

$$\frac{\epsilon_B}{\epsilon_F} = 2\frac{\sqrt{1+x_0^2} - x_0}{\sqrt{1+x_0^2} + x_0} \quad (24)$$

μ is the chemical potential, Δ is the gap energy



Why two dimensions? Because it is simpler from an algebraic point of view. 3D case require the use of elliptic integrals.
We keep in mind that the relevant values for $\epsilon_B/\epsilon_F \in [0, 1]$

Gap equation I

We start by recalling the bound state equation of a pair of fermions

$$-\frac{1}{g} = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{1}{\frac{\hbar^2 k^2}{m} + \epsilon_B} \tag{25}$$

where $g < 0$ is the strength of the attractive contact potential chosen in order to have pairing between fermions. Ω is the volume of the system.

We recall also the gap equation

$$-\frac{1}{g} = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{1}{2\sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2}} \tag{26}$$

The two equations diverge in the ultraviolet, so we subtract one to the other and we get the regularized gap equation

$$0 = \sum_{\mathbf{k}} \left(\frac{1}{\frac{\hbar^2 k^2}{m} + \epsilon_B} - \frac{1}{2\sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2}} \right) \tag{27}$$

Gap equation II

We work with the two dimensional continuum limit
$\sum_{\mathbf{k}} \to \frac{\Omega}{(2\pi)^2} \int d^2\mathbf{k} = \frac{\Omega}{2\pi} \int dk\ k$ such that

$$0 = \int_0^{k_{max}} \frac{dk}{2\pi}\, k \left[\frac{1}{\frac{\hbar^2 k^2}{m} + \epsilon_B} - \frac{1}{2\sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2}} \right] \tag{28}$$

where we set now an ultraviolet cutoff, k_{max}, in order to send $k_{max} \to \infty$ at the end of the calculation. Performing a change of variable and integrating both terms we reach, with
$\epsilon_{max} = \hbar^2 k_{max}^2 / 2m$

$$\ln|2\epsilon_{max} + \epsilon_B| - \ln|\epsilon_B| = \ln\left|\sqrt{(\epsilon_{max} - \mu)^2 + \Delta^2} + \epsilon_{max} - \mu\right| + \\ - \ln\left|\sqrt{\mu^2 + \Delta^2} - \mu\right|$$

Gap equation III

Sending now ϵ_{max} to infinity and using properties of the logarithmic function we get the full form of the regularized equation

$$\boxed{\epsilon_B = \sqrt{\mu^2 + \Delta^2} - \mu} \tag{29}$$

So we can conclude that even if sending ϵ_{max} to infinity gave us an ultraviolet divergence, the regularization we introduced by subtracting one equation to the other enabled us to mathematically deal with the gap equation.

Number equation I

We want to describe how the number of particles within the system change. We recall the definition of number operator

$$N = 2\sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} = 2\sum_{\mathbf{k}} \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\xi^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}}}\right) \tag{30}$$

so we start by considering the number density

$$n = \frac{N}{\Omega} = \frac{2}{\Omega}\sum_{\mathbf{k}} \frac{1}{2}\left[1 - \frac{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}{\sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2}}\right] \tag{31}$$

$$= \int_0^\infty \frac{dk}{2\pi}\, k \left[1 - \frac{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}{\sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2}}\right]$$

$$n = \frac{m}{2\pi\hbar^2}\left[\sqrt{\mu^2 + \Delta^2} + \mu\right] \tag{32}$$

Number equation II

If we consider a 2D system of N fermionic particles of mass m inside a 2D volume Ω and we assume two possible spin states we have

$$N = 2\sum_{\mathbf{k}} \Theta\left(\epsilon_F - \frac{\hbar^2 k^2}{2m}\right) \tag{33}$$

where Θ is the Heaviside function. WIth the continuum limit

$$n = \frac{N}{\Omega} = \frac{1}{\pi}\int_0^{k_F} dk\ k = \frac{1}{2\pi}k_F^2 \implies n = \frac{m\epsilon_F}{\hbar^2\pi} \tag{34}$$

And finally substituting the last expression in (31)

$$\boxed{2\epsilon_F = \sqrt{\mu^2 + \Delta^2} + \mu} \tag{35}$$

Behaviour of μ and Δ across the crossover

We take the two relations we derived with the number and gap equations

$$\epsilon_B = \sqrt{\mu^2 + \Delta^2} - \mu, \qquad 2\epsilon_F = \sqrt{\mu^2 + \Delta^2} + \mu \tag{36}$$

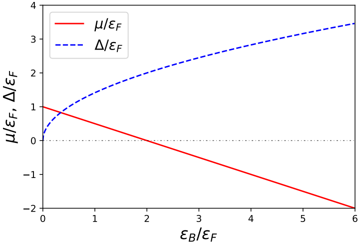
and manipulating

$$\sqrt{\mu^2 + \Delta^2} = \epsilon_B + \mu, \qquad \sqrt{\mu^2 + \Delta^2} = 2\epsilon_F - \mu \tag{37}$$

and with this we can obtain

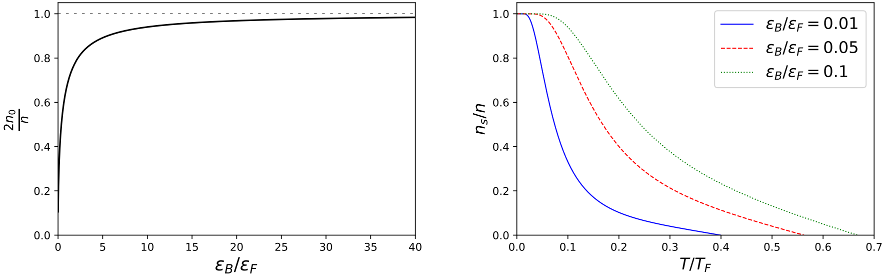
$$\boxed{\mu = \epsilon_F - \frac{\epsilon_B}{2}} \tag{38}$$

$$\boxed{\Delta = \sqrt{2\epsilon_F \epsilon_B}} \tag{39}$$



Condensate fraction n_0 and superfluid density n_s

We can investigate other observables, such as the condensate fraction, which measure the quantity of particles that occupy the same single-particle quantum state (BEC regime), or the superfluid density n_s for different values of the binding energy ϵ_B/ϵ_F



Three dimensional case I

In three dimensions, the 3D scattering length a_s is the relevant parameter for the crossover between BCS ($a_s < 0$) and BEC (a_s >0). It is defined as

$$\frac{m}{4\pi a_s} = \frac{1}{\Omega V} + \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{m}{\mathbf{k}^2} \tag{40}$$

Here we can not use the binding energy between a pair of fermions because in 2D attactive fermions always form biatomic molecules with binding energy ϵ_B due to reduced spacial dimensionality, while in 3D this is not true.
The 3D BCS-BEC crossover is often investigated with the parameter

$$y = \frac{1}{k_F a_s}, \qquad k_F = (3\pi^2 n)^{1/3} \tag{41}$$

Three dimensional case II

The gap energy and chemical potential can be found to be, with $x_0 = \mu/\Delta$

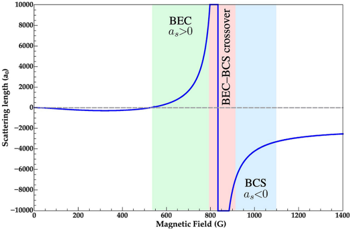
$$\frac{\Delta}{\epsilon_F} = \frac{1}{(x_0 I_5(x_0) + I_6(x_0))^{2/3}}$$
$$\frac{\mu}{\epsilon_F} = \frac{x_0}{(x_0 I_5(x_0) + I_6(x_0))^{2/3}}$$

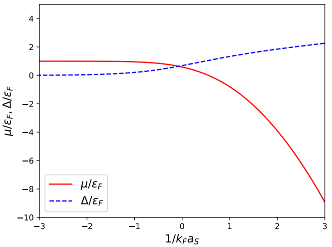
with

$$I_5 = \int_0^\infty dx \frac{x^2}{E_x^3}$$
$$I_6 = \int_0^\infty dx \frac{x^2 \xi_x}{E_x^3}$$

with $\xi_x = \hbar^2 \mathbf{k}^2/(2m\Delta) - \mu/\Delta$ and $E_X = \sqrt{\xi_x^2 + 1}$

Panel above: figure taken from [4]. The magnetic field is relevant due to the Fano-Feshbach technique used to investigate the crossover





Conclusions

- We saw the relevant results for the BCS theory, starting from the polaron work that inspired Bardeen, Cooper and Schrieffer.
- We derived the gap equation, and we showed that it can be exactly solved in the weak coupling limit.
- We then investigate the BCS-BEC crossover, starting from the reasons that pushed scientists to develop this theory.
- We focused on the 2D case, since it is simpler to solve from an analytical point of view, and then we showed how the 3D analysis can be done and which results can be showed.

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Thank you for your attention!

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