Advanced quantum mechanics (20104301)

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Chapter 7: Superconductors

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Chapter 7

Superconductivity

Let us now have a look at another interesting and somewhat surprising phenomenon, namely *superconductivity* (zero electrical resistance). Superconductivity can satisfiable be described within a microscopic theory, which is valid for $T = 0$ and small temperatures. Until now, superconductivity at high temperatures remains to some extend unresolved.

7.1 Introductory thoughts

Superconductivity was first described by Kamerling-Onnes in 1911. He found that mercury, that was cooled under $T_c = 4.15K$, lost its resistance abruptly. For all temperatures below that critical T_c, the same behavior was observed. Today there are more such superconducting substances known, that completely loose their resistance upon cooling under some appropriate critical temperature. One of the most astonishing effects might be the existence of permanent currents, which was also found by Kamerling-Omnes; consider a ring of superconducting material at some $T > T_c$ exposed to an orthogonal magnetic field B. Now cool the ring to $T < T_c$ and switch off the magnetic field. A current will be induced in the ring, that is identical to the current that was there when B was on. Since there is no resistance, the current will stay as it is for ever.

Another effect is the *Meissner-Ochsenfeld-effect*, which states, that in the interior of a superconductor, the magnetic field

$$B = 0. \tag{7.1}$$

Superconductivity remained completely unclear for many years, until Gorter, Casimir and London developed first theories, which were macroscopic in the beginning (we are planning to get back to this later). Herbert Fröhlich observed first, that superconductivity in metals originates from interaction of electrons with phonons (the quasi particles of lattice vibrations). That central insight led to a lot of research in microscopic theories, one of which was the *BCS theory* from Bardeen, Cooper and Schrieffer. It was the first satisfying theory, and – of course – formulated in second quantization. There is no time to go more deeply into that, but let us understand the main ideas.

7.2 BCS theory

7.2.1 Microscopic Hamiltonian

The Hamiltonian of a gas of electrons (i.e. fermions) in a solid body of volume V reads as follows.

Hamiltonian of electrons in solid body:

$$H = H_0 + H_1, \tag{7.2}$$

$$H_0 = \sum_{k,\sigma} \varepsilon_k f^\dagger_{k,\sigma} f_{k,\sigma}, \tag{7.3}$$

$$H_1 = -\frac{1}{2V} \sum_{k,k',\sigma} V_{k,k'} f^\dagger_{k,\sigma} f^\dagger_{-k,-\sigma} f_{-k',-\sigma} f_{k',\sigma}. \tag{7.4}$$

As always $f^\dagger_{k,\sigma}$ denotes the fermionic creation operator with wave number k and spin component σ. Moreover

$$\varepsilon_k = \frac{k^2}{2M} - \mu \tag{7.5}$$

is the kinetic energy, corresponding to the wave number k, where M is the mass of an electron and μ is the chemical potential, which is in a system of exactly N particles (like a Lagrange or more precisely Kuhn Tucker multiplier) fixed by

$$\langle \sum_{k,\sigma} f^\dagger_{k,\sigma} f_{k,\sigma} \rangle = N. \tag{7.6}$$

$V_{k,k'}$ is the effective interaction between the electrons in k-space, which obviously satisfies

$$V_{k,k'} = V_{k',k}. \tag{7.7}$$

7.2.2 Justification of the microscopic Hamiltonian

The central insight is the one from Cooper, supported by Fröhlich's observations, who noticed that the known ground state of non interacting fermions collapses if one allows a small attractive interaction between them. The idea can be roughly summarized as follows.

- On its way through the solid body, the electron deforms the background of positively charged ions. Before, we considered only a classical and fixed background, but in a good microscopic theory we have to allow some movement in it.

- Hence the electron leaves a trace of a slightly higher density of positively charged ions, which again leads to the attraction of another (negatively charged) electron. This effect can be seen like an effective attraction between two electrons. The repulsion among each other is compensated by the mechanism, we talked about in the last chapter on Fermi gases. So the trace of deformation leads to an attraction.
- There is a rather subtle effect, namely that the described attractive electron-electron-interaction is, as a result of the slower movement of ions, retarded compared to the Coulomb interaction between them, which can lead to knowledge about the range of the effective interaction.

Those thoughts should have given some ideas why the Hamiltonian is plausible (even if we do not deliver a full derivation here). The original publication is also not entirely concrete on these matters, but in the meantime, the picture of an effective fermionic interaction mediated via bosonic systems has been understood rather well.

7.2.3 Bogoliubov transformation of the Hamiltonian

We will now try to find the spectrum of the Hamiltonian. We can not find an exact solution, but by using a similar strategy as we did with superfluids, we will finally end up with a quadratic Hamiltonian. The idea is again to do a series of approximations which are highly plausible, given the mindset laid out here, until one arrives at a quadratic Hamiltonian that can be exactly solved. Needless to say, this can also be seen as an invitation that it makes a lot of sense to revisit such derivations, and aim at bounding errors made in approximations in a more rigorous mindset. To proceed, it will be helpful to define the following two new sets of operators $\{A_k\}$ and $\{B_k\}$:

$$f_{k,1/2} = u_k A_k + v_k B_k^\dagger, \tag{7.8}$$

$$f_{-k,-1/2} = u_k B_k - v_k A_k^\dagger, \tag{7.9}$$

with $\{u_k\}, \{v_k\} \in \mathbb{R}$ and

$$u_k = u_{-k}, \tag{7.10}$$

$$v_k = v_{-k}, \tag{7.11}$$

$$u_k^2 + v_k^2 = 1. \tag{7.12}$$

This is, again, a *Bogoliubov transformation*, this time a fermionic one. It is easily found that the inverse transformation reads

$$A_k = u_k f_{k,1/2} - v_k f_{-k,-1/2}^\dagger, \tag{7.13}$$

$$B_k = u_k f_{-k,-1/2} + v_k f_{k,1/2}^\dagger. \tag{7.14}$$

We would like the new coordinates to fulfill the same anti-commutation relations as the old ones, which are

$$\{A_k, A_{k'}^\dagger\} = \delta_{k,k'}, \tag{7.15}$$

$$\{B_k, B_{k'}^\dagger\} = \delta_{k,k'}. \tag{7.16}$$

Inserting these new operators into the above given Hamiltonian and also using anti-commutation relations to order annihilation operators, gives us the new Hamiltonian. (Note that one calls an order of this kind *normal order*)

$$H = E_0 + H_0' + H_1' + H_2', \tag{7.17}$$

where

$$\begin{aligned} E_0 &= 2\sum_k \varepsilon_k v_k^2 - \frac{1}{V}\sum_{k,k'} V_{k,k'} u_k v_k u_{k'} v_{k'}, & (7.18)\\ H_0' &= \sum_p \left(\varepsilon_p (u_p^2 - v_p^2) + \frac{2u_p v_p}{V}\sum_{p'} V_{p,p'} u_{p'} v_{p'}\right) \\ &\times (A_p^\dagger A_p + B_p^\dagger B_p), & (7.19)\\ H_1' &= \sum_p \left(2\varepsilon_p u_p v_p - \frac{u_p^2 - v_p^2}{V}\sum_{p'} V_{p,p'} u_{p'} v_{p'}\right) \\ &\times (A_p^\dagger A_p^\dagger + B_p B_p). & (7.20)\end{aligned}$$

H_2' contains expressions involving higher order polynomials in A_p and B_p, which can be neglected as they represent interactions between quasi particles. The final result will show that the ground state is the vacuum (in terms of quasi particles) and as such, at low energies, there will be little interaction between them.

Now we can again use the freedom we have, to choose $\{u_k\}$ and $\{v_k\}$ such that

$$H_1' = 0, \tag{7.21}$$

which will be the case if

$$2\varepsilon_p u_p v_p = \frac{u_p^2 - v_p^2}{V}\sum_{p'} V_{p,p'} u_{p'} v_{p'}. \tag{7.22}$$

We decide to pick

$$\begin{aligned} u_p &= \frac{1}{\sqrt{2}}\left(1 + \frac{\varepsilon_p}{\sqrt{\Delta_p^2 + \varepsilon_p^2}}\right)^{1/2}, & (7.23)\\ v_p &= \frac{1}{\sqrt{2}}\left(1 - \frac{\varepsilon_p}{\sqrt{\Delta_p^2 + \varepsilon_p^2}}\right)^{1/2}, & (7.24)\end{aligned}$$

where Δ_p is determined by the anti-commutation relations as

$$\Delta_p = \frac{1}{2V}\sum_{k'} \frac{V_{p,p'}\Delta_{p'}}{\sqrt{\Delta^2(p') + \varepsilon_{k'}^2}}, \tag{7.25}$$

Kicking out H_1' in this fashion was no approximation but just our freedom to choose the pre-factors in the Bogoliubov transformation (which was of course a reason for doing the transformation in the first place). The new Hamiltonian then becomes

$$H = E_0 + H_0', \tag{7.26}$$

with

$$\begin{aligned} E_0 &= \sum_p \frac{1}{\sqrt{\Delta_p^2 + \varepsilon_p^2}} \\ &\times \left(\varepsilon_p \left(\sqrt{\Delta_p^2 + \varepsilon_p^2} - \varepsilon_p \right) - \Delta_p^2/2 \right), \end{aligned} \tag{7.27}$$

and

$$H_0' = \sum_p \sqrt{\Delta_p^2 + \varepsilon_p} (A_p^\dagger A_p + B_p^\dagger B_p). \tag{7.28}$$

This procedure, similar to the one we did for superfluids, leaves us with a, not only quadratic Hamiltonian, but it even takes the form of uncoupled harmonic oscillators and is thus solved. We have followed a very similar logic here as before when discussing superfluidity.

7.2.4 Discussion of the interaction

Since this can be seen like a "first date" with the ideas of superconductivity, we only consider the case $T = 0$ and say $\mu = k_0^2/(2M)$. All energies are thus expressed in terms of the chemical potential, upon choosing ε_k. We will make the following assumption about the interaction potential:

$$V_{p,p'} = \begin{cases} C, & \text{if } |\varepsilon_p|, |\varepsilon_{p'}| \leq \omega_c, \\ 0, & \text{otherwise.} \end{cases} \tag{7.29}$$

with $C \in \mathbb{R}$ being some constant.

Here $\omega_c \ll k_0^2/(2M)$. So the interaction occurs only between electrons with some momentum in a small sphere around the momentum k_0. It is consistent with all said above to assume

$$\Delta_p = \begin{cases} \Delta, & \text{if } |\varepsilon_p| \leq \omega_c, \\ 0, & \text{otherwise.} \end{cases} \tag{7.30}$$

In the limit of a large volume V, the constant Δ can be found by solving the integral equation

$$\Delta = \Delta \frac{C}{2(2\pi)^3} \int dp \frac{1}{\sqrt{\Delta^2 + \varepsilon_p^2}}, \tag{7.31}$$

where one integrates over all k for which

$$|\varepsilon_k| \leq \omega_c \tag{7.32}$$

The integral becomes one dimensional as

$$\Delta = \Delta \frac{C}{2\pi^2} \int_{\sqrt{k_0^2 - 2M\omega_c}}^{\sqrt{k_0^2 + 2M\omega_c}} dp p^2 \left(\Delta^2 + \frac{1}{4M^2} (p^2 - k_0^2)^2 \right)^{-1/2}. \tag{7.33}$$

Introducing the new variables $p = k_0 + x$ and using that $k_0^2 \gg 2M\omega_c$, we get

$$\Delta \approx \Delta \frac{Ck_0^2}{4\pi^2} \int_{-M\omega_c/k_0}^{M\omega_c/k_0} dx \left(\Delta^2 + \frac{k_0^2}{M^2} x^2 \right)^{-1/2}. \tag{7.34}$$

And finally

$$\Delta \approx \Delta \frac{Ck_0}{4\pi^2} \log \frac{\sqrt{\Delta^2 + \omega_c^2} + \omega_c}{\sqrt{\Delta^2 + \omega_c^2} - \omega_c}. \tag{7.35}$$

This is a curious expression, since Δ is contained in both sides of the equation.

7.2.5 The spectrum of the Hamiltonian

We found the spectrum of the Hamiltonian to be

$$E_0 + \sum_k \sqrt{\varepsilon_k^2 + \Delta_k^2} (N_A(k) + N_B(k)), \tag{7.36}$$

where $N_A(k)$ and $N_B(k)$ are the number of quasi particles A and B with wave number k respectively. There are now two possible solutions to Eq. (7.35), one is trivially $\Delta = 0$. It corresponds to a state with neither any A nor B quasi particles and the energy is just

$$E_{gs} = 0. \tag{7.37}$$

Also $k_0 = p_F$ and u_p (Eq.7.23) and v_p (Eq.7.24) can be chosen to be

$$u_p = 1,\ v_p = 0 \quad \text{for } \varepsilon_p > 0 \tag{7.38}$$

and

$$u_p = 0,\ v_p = 1 \quad \text{for } \varepsilon_p < 0, \tag{7.39}$$

where $\varepsilon_p >< 0$ implies $|p| >< p_F$. If $|p| > p_F$, it follows

$$A_p = f_{p,1/2}, \tag{7.40}$$
$$B_p = f_{-p,-1/2}. \tag{7.41}$$

Those operators thus annihilate fermions outside the Fermi sphere. Otherwise, if $|p| < p_F$:

$$A_p = -f^\dagger_{-p,-1/2}, \tag{7.42}$$
$$B_p = f^\dagger_{p,1/2}. \tag{7.43}$$

As such, they fill up fermionic holes in the Fermi sphere. The ground state with energy $E_{gs} = 0$, is the one, where all states up to $|p| \leq p_F$ are filled up and all states with $|p| > p_F$ are empty. Exited states have some fermions that jumped up to $|p| > p_F$. For sufficiently large systems, the spectrum is thus continuous. If C is positive and large enough, that is, if there is enough attractive interaction between fermions of opposite momentum and different spins near the Fermi level, there exists another solution for Eq. (7.35).

Energy gap of the superconducting solution : We find the solution

$$\Delta = 2\omega_c \frac{e^{-D/C}}{1 - e^{-2D/C}}, \quad (7.44)$$

$$D = \frac{2\pi^2}{Mk_0}, \quad (7.45)$$

which gives rise to an energy gap of 2Δ between the ground and first excited state.

This solution is called *superconducting solution* and the ground state energy is $E_{gs} < 0$. Hence it is the real ground state of the system. Fixing the particle number, one finds an energy gap of 2Δ between the ground state energy and the first excited energy. In fact,

$$A_p^\dagger A_p - B_p^\dagger B_p = f_{p,1/2}^\dagger f_{p,1/2} - f_{-p,-1/2}^\dagger f_{-p,-1/2}. \quad (7.46)$$

In the ground state one finds

$$\langle f_{p,\sigma}^\dagger f_{p,\sigma} \rangle = \langle f_{-p,-\sigma}^\dagger f_{-p,-\sigma} \rangle. \quad (7.47)$$

Which corresponds to electrons appearing in pairs; pairs with opposite k and spin, the so called *Cooper pairs*:

$$(k, 1/2; -k, -1/2). \quad (7.48)$$

It is energetically favourable for the electrons to come in such pairs, in fact, the ground state is well described by the BCS ground state vector.

BCS ground state vector:

$$|\psi_{\text{BCS}}\rangle = \prod_k \left(u_k + v_k f_{k,1/2}^\dagger f_{-k,-1/2}^\dagger \right) |\emptyset\rangle. \quad (7.49)$$

"Divorcing" such a pair generates two unpaired electrons and $N_A + N_B = 2$, such that the first excited energy is 2Δ above the ground state, and precisely that energy gap is responsible for superconductivity, as too much energy is needed to generate such an excitation. Thus no dissipation occurs.