Quantum Theory of Solids
Lecture notes - Spring 2020

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Digitialized lecture notes for the course "TFY4210 - Quantum Theory of Many-Particle Systems" held by Prof. Asle Sudbø spring 2020. These notes follow the pdf containing the hand written lecture notes, which are based upon the lecture notes for the course "FY8302 - Quantum Theory of Solids"

Website: https://www.ntnu.edu/studies/courses/TFY4210

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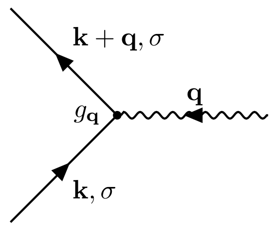


Figure 1: Diagram of electron-phonon vertex

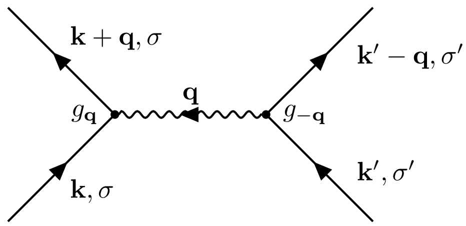


Figure 2: Diagram of the effective electron-phonon interaction

3 Quasi-particles in interacting electron-systems. Fermi-liquids.

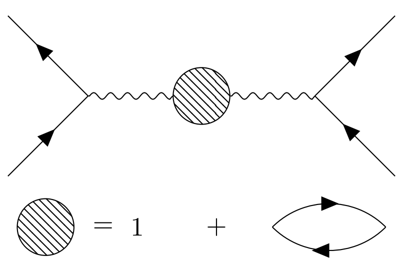
3.1 Fermi-liquids

3.2 Screening of the Coulomb-interaction

3.3 Phonon mediated electron-electron interaction

Due to the electron-phonon coupling depicted in fig. 1, we will get an effective phonon-mediated interaction between electrons, depicted in fig. 2

This is an exchange of a virtual phonon. The above diagram is the effective interaction to second order in g_q if we regard the wavy line as a bare phonon Green's function. We could also imagine that we replaced this by



which would include an effective interaction computed correctyly up to order $\mathcal{O}(g^4)$. In fact, we might replace $D_0 + D_0 \Pi D_0 + \ldots$ by D! Thus computing the effective interaction up to infinite order in g. Another, often used approach would be to replace by **TODO:** *SETT INN DIAGRAM*

Here, we have resummed a subset of diagrams to infinite order in g in order to get an effective interaction between electrons. Under the assumption that g is weak, we will keep terms only to $\mathcal{O}(g^2)$.

$$V_{\text{eff}}(q,\omega) = |g_q^2| \frac{2\omega_q}{\omega^2 - \omega_q^2} \tag{3.1}$$

Thus, the interaction part of the Hamiltonian becomes

$$\mathcal{H} = \sum_{\substack{k,k',q\\ \sigma,\sigma'}} V_{\text{tot}}(q,\omega) c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma} \tag{3.2}$$

$$V_{\text{tot}}(q,\omega) = \frac{e^2}{4\pi\varepsilon q^2} + V_{\text{eff}}(q,\omega), \tag{3.3}$$

where the first term is the Coulomb-interaction. Furthermore, ω is the energy transfer between scattering electrons when they exchange a phonon

$$\omega = \varepsilon_{k+q} - \varepsilon_k \tag{3.4}$$

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Note the singularities in V_{tot} when $|\omega| \to \omega_q$. In particular, note the negative singularity when $|\omega| \to \omega_q^-$. This singularity persists when Coulomb-repulsion is included. For most frequencies, the Coulomb-interaction completely dominates. However, in a narrow ω-region close to ω_q, the extremely weak electron-phonon coupling will always beat the Coulomb-interaction! This frequency is slightly smaller than ω_q. For small ω, V_{tot} is repulsive. For large ω, V_{tot} is repulsive. For $|\omega| \lesssim \omega_q$, V_{tot} is attractive.

Let us try to give a physical picture for this: When an electron moves past an ion, they interact. The electron pulls slightly on the heavy, positively charged ion. Electrons are light, and move much faster than the heavy ions. The electron this moves quickly out of the scattering zone, while the ion relaxes slowly back to its equilibrium position. The ion in its out-of-equilibrium position represents excessive positive charge in that position, which can pull another electrn towards it. This is effectively a charge-dipole interaction. If the second electron "waits" a little for the first electron to get away (thus reducing Coulomb-repulsion) but does not wait for too long (such that the ion has relaxed back to its equilibrium position), then the second electron can be attracted the scattering region. Effectively, the second electron is attracted to the scattering region because the first electron was there. This is an effective electron-electron attraction. It only works if the electron waits a little, but not for too long. A minimum time corresponds to a maximum frequency, while a maximum time corresponds to a minimum frequency. This implies that V_{tot} is attractive if $\omega_{\min} < \omega < \omega_{\text{masx}}$, as depicted in **TODO:** *Sett in figurer og referanse til figuren (s.7)* We may view the effective electron-electron attrraction as a result of an electron locally deforming an elastic medium. Think of a rubber membrane that you put a little metal sphere on. The membrane is stretched, dipping down where you put the first sphere. If you put another little sphere on the membrane, it will fall into the dip, i.e. it will be attracted to the first particle. This is also how gravity works: A mass deforms space-time (an elastic medium) and thus attracts another mass.

Disclaimer: The above two analogs are classical. There will be an important quantum effect coming into play here, which we will come back to. here, it will suffice to not that, classically, one can keep adding particles to the dip, such that all particles will be gathered in the same one, forming a large heavy object. This is not how it works quantum mechanically with fermions. Note also that in V_{tot}, and the two different simplified models for $\bar{V}$, they are only attractive up to a maximum ω, i.e. only after a minimum amount of time. The second particle has to wait a minimum amount of time for the interaction to be attractive. This is called retardation.

> The electrons avoid the Coulomb-interactions by avoiding each other, not in space, but in time.

3.4 Magnon mediated electron-electron interaction

We have seen how a boson (a phonon) with a linear coupling to electrons could give an effective attractive interaction aming electrons. What is we couple the electrons linearly to other bosons? One obvious thing to investigate, is to consider the coupling of electrons to magnons. For simplicity, we consider itinerant electrons coupled to spin-fluctuations in a ferromagnetic insulatior. (FMI) The question is if the spin-fluctuations of the FMI can give rise to an attractive interaction aming electrons. We therefore consider a system of itinerant electrons with Hamiltonian

$$\mathcal{H}_{\text{el}} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma}. \tag{3.5}$$

In this system, we envisage a regular lattice of localized spins with ferromagnetic coupling, with Hamiltonian

$$\mathcal{H}_{\text{spin}} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{3.6}$$

The localized spins are denoted by capital letter $\mathbf{S}$. The coupling between the localized spins (FMI) and the itinerant electron spins $\mathbf{s}_i$ (lower case) is given by

$$\mathcal{H}_{\text{el-spin}} = -J_{sd} \sum_{i} \mathbf{S}_i \cdot \mathbf{s}_i. \tag{3.7}$$

As a minimal model, we have assumed that the electrons are hopping around on the same regular lattice that the localized spins are located. Using the

Holstein-Primakoff transformation, ignoring the classical ground-state energy, and expressing operators in momentum space, we have

$$\mathcal{H}_{\text{spin}} = \sum_q \omega_q a_q^\dagger a_q \tag{3.8}$$

$$\omega_q = 2JS(z - \gamma(\mathbf{q})) \tag{3.9}$$

$$\gamma(\mathbf{q}) = \sum_\delta \mathrm{e}^{i\mathbf{q}\cdot\delta}, \tag{3.10}$$

where δ connects site i to all its nearest neighbors. One important fact ato make note of at once, is that $\omega_q \sim q^2$ for small q. For the phonon-case, with acoustical phonons, $\omega_q \sim q$. Thus ω_q for small q is much smaller for ferromagnetic magnons than acoustical phonons. We will return to this point. Consider next the electron-spin coupling:

$$\begin{aligned}\mathcal{H}_{\text{el-spin}} &= -J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i &(3.11)\\ &= -J_{sd} \sum_i (S_{iz}s_{iz} + S_{ix}s_{ix} + S_{iy}s_{iy}) &(3.12)\\ &= -J_{sd} \sum_i \left(S_{iz}s_{iz} + \frac{1}{2}\left(S_{i+}s_{i-} + S_{i-}s_{i+}\right)\right), &(3.13)\end{aligned}$$

where $S_{i\pm} = S_{ix} \pm iS_{iy}$, $S_{iz} = S - a_i^\dagger a_i$, $S_{i+} = \sqrt{2S}a_i$, $S_{i-} = \sqrt{2S}a_i^\dagger$. $\mathbf{s}_i = \frac{1}{2}c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta}$ with implicit summation over repeated indices α, β.

$$\implies s_{iz} = \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) = \frac{1}{2}\sum_\sigma \sigma c_{i\sigma}^\dagger c_{i\sigma}$$

$$\sigma^x = \left(\begin{smallmatrix}0 & 1\\ 1 & 0\end{smallmatrix}\right) \qquad \sigma^y = \left(\begin{smallmatrix}0 & -i\\ i & 0\end{smallmatrix}\right) \qquad \sigma^z = \left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$$

$$\sigma^\pm = \sigma^z \pm i\sigma^y \qquad \sigma^+ = \begin{pmatrix}0 & 2\\ 0 & 0\end{pmatrix} \qquad \sigma^- = \begin{pmatrix}0 & 0\\ 2 & 0\end{pmatrix}$$

Thus, we have

$$\begin{aligned}\mathcal{H}_{\text{el-spin}} = &-J_{sd}S \sum i, \sigma\sigma c_{i\sigma}^\dagger c_{i\sigma} + J_{sd}\sum_{i,\sigma} \sigma a_i^\dagger a_i c_{i\sigma}^\dagger c_{i\sigma}\\ &- \frac{J_{sd}\sqrt{2S}}{2}\sum_i \left(a_i c_{i\downarrow}^\dagger c_{i\uparrow} + a_i^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}\right)\end{aligned} \tag{3.14}$$

For the remainder of the calculation, we focus on the linear coupling of magnons to electrons, and ignore the second term. Thus, we focus on el-el interaction mediated by the vertices in fig. 3.

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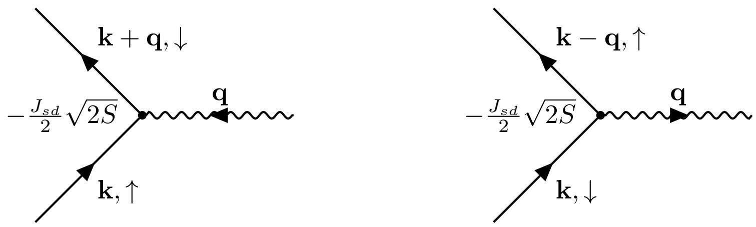

(a) Spin-1 magnon is dumped into electron, flipping ↓→↑

(b) Spin-1 magnon is excited, taking with it a spin-1, flipping ↑→↓

Figure 3: The two interaction vertices of interest

4 The Cooper-problem

5 The Bardeen-Cooper-Scheiffer theory of superconductivity

This is essentially the many-particle version of the Cooper-problem. Superconductivity: **TODO:** *Sett inn figur*

Note that a non analytic function like this usually suggests that there is some phase-transition in the system, so we are essentially looking at a phase transition of the electron gas. T_C : A sharply defined temperature

$$\rho(T) = \begin{cases} 0 & \text{if } T < T_C \\ \text{nonzero} & \text{if } T > T_C \end{cases} \tag{5.1}$$

T_C is denoted the critical temperature. Superconductivity was discovered experimentally in 1911 by Heike Kammerlingh Onnes in Leiden, measuring low-T $\rho(T)$ in ultra pure Mercury (Hg). This was 15 years before the discovery of quantum mechanics. It turns out that the phenomena is purely a quantum effect. So in 1911, there was no hope of giving a correct explanation for what is happening. It took 46 years to figure out what is going on. The most important reasons for this, is that apart from having to invent quantum mechanics first, completely novel and radical ideas had to be formulated in order to solve the problem[1]. Historically, one important clue to figuring out what is happening, was the experimental observations that T_C varied with ion mass. (Isotope substitution on elemental superconductors). This indicated that lattice-vibrations somehow were involved in the early discovered superconductors. (Recall that electron-phonon-coupling $\sim \frac{1}{\sqrt{M}}$). This "isotope-effect" was announced in 1950 on elemental Mercury, and the measured shift in T_C was 0.01K, something that

[1] From in the lecture: illustration of the Meissner effect. The Higgs providing a mass to the em-field in the metal blob drawn is the expectation value of the Cooper pair operator. Superconductivity is that the photon acquires a mass through the Higgs field, which is a cooper pair. Lots of analogs to the standard model.

required very careful and precise measurements. We may guess what will happen with T_C by appealing to what we found in the Cooper-problem, where we surmised a Cooper-pair dissociation temperature $T^* \sim \Delta$ and

$$\Delta = 2\hbar\omega_0 \mathrm{e}^{-\frac{1}{\lambda}} \tag{5.2}$$

ω_0: A typical phonon-frequency, if we assume that the effective attractions originates with e-ph coupling. $\omega_0 \sim \frac{1}{\sqrt{M}} \to T^* \sim \frac{1}{\sqrt{M}}$. This means that $\sqrt{M}T_C$ =constant! This relation is validated very well in experiments on elemental superconductors such as Hg, Sn, and Tl. Previously, we have derived an effective e-e interaction, including Coulomb-interactions and e-ph–e interactions, $\tilde{V}_{\text{eff}}$.

$$\begin{aligned} \mathcal{H} = &\sum_{k,\sigma} (\varepsilon_k - \mu)\, c^\dagger_{k\sigma} c_{k\sigma} \\ &+ \sum_{\substack{k,k',q \\ \sigma,\sigma'}} \tilde{V}_{\text{eff}} c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma} \end{aligned} \tag{5.3}$$

Notice the global U(1)-symmetry of this Hamiltonian. This is on the standard form for a second-quantized electron-gas, now including the (potentially singular) effects of e-ph- coupling

$$\tilde{V}_{\text{eff}} = \frac{2|g_q|^2 \omega_q}{\omega^2 - \omega_q^2} + V_{\text{Coulomb}}(q) \tag{5.4}$$

TODO: *Sett inn figure*

ω : Energy-transfer in scattering. $\omega = \varepsilon_{k+q} - \varepsilon_k, \quad \varepsilon_{k'} = \varepsilon_{k'-q} + \omega$. The effect of the repulsive interaction can be calculated pertubatively. In any case, this repulsion is not a singular perturbation. We therefore set it aside for the moment, and consider

$$\tilde{V}_{\text{eff}} = \frac{2|g_q|^2 \omega_q}{\omega^2 - \omega_q^2}. \tag{5.5}$$

This interaction as attractive (< 0) if

$$(\varepsilon_{k+q} - \varepsilon_k)^2 < \omega_q^2$$

or

$$(\varepsilon_{k'-q} - \varepsilon_{k'})^2 < \omega_q^2$$

We now focus on those scattering processes that give attraction between electrons. The processes giving repulsion do nothing more than what the Coulomb interaction does. We will include these effects later on. We now simplify this in a series of steps. The scattering caused by the weak e-ph-e coupling can only take place in a thin shell around the Fermi-surface. Thus $\varepsilon_k, \varepsilon_{k'}, \varepsilon_{k+q}, \varepsilon_{k'-q}$ must all lie within a thin shell around the Fermi surface. Let us take a look at the relevant kinematics seen in fig. 4. We see that in general, the state with

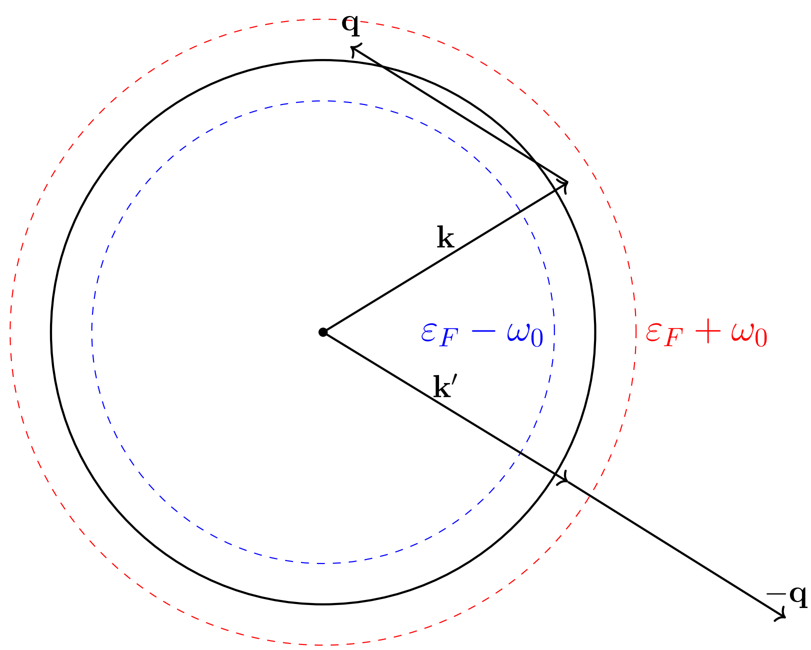

Figure 4: Thin shell around the Fermi surface.

momenta $k' - q$ will lie outside the shell, even if $\varepsilon_k, \varepsilon_{k'}, \varepsilon_{k+q}$ lie within the shell. There is an important special case where $\varepsilon_{k'-q}$ will always lie within shell if $\varepsilon_k, \varepsilon_{k'}, \varepsilon_{k+q}, \varepsilon_{k'-q}$ is within shell, namely the case when $k' = -k$. This choice will this maximize the scattering phase-space for attractive interactions. We will retain only such terms: $k' = -k$.

A second simplification: $\sigma' = -\sigma$. The spatial extent of attractive interaction is small. We may essentially think of it (in real space) as an attractive Hubbard-interaction. Thus, we end up with the following simplified Hamiltonian

$$\mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,q,\sigma} \tilde{V}_{\text{eff}} c^\dagger_{k+q,\sigma} c^\dagger_{-(k+q),-\sigma} c_{-k,-\sigma} c_{k\sigma}. \tag{5.6}$$

Now redefine variables $k \to k', \quad k+q \to k, \quad \tilde{V}_{\text{eff}} \to V_{k,k'}/2$ (spin independent interaction). Thus we can write eq. (5.6) as

$$\mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,k'} V_{k,k'} c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} c_{-k',\downarrow} c_{k,\uparrow}, \tag{5.7}$$

with $V_{k,k'}$ being attractive if k, k' lie in a small vicinity of the Fermi-surface, and zero otherwise. eq. (5.7) is the so called BCS-model of superconductivity. Althought it has been motivated by an attractive e-ph-e interaction, the above model is in fact more general than that, and can be applied to any system with an effective (somehow) attractive electron-electron interaction. This model in spirit is very much like the model we looked at for the Cooper-problem. The difference is that $V_{k,k'}$ in the BCS-model works between all electrons in a thin shell around the Fermi-surface, while the Cooper-problem only considered interactions between two such electrons. The Hamiltonian can not be treated exactly. Moreover, from the Cooper-problem, there is every reason to believe that in order to get correct eigenvalues, we cannot use perturbations theory. We must therefore treat $\mathcal{H}$ both approximately and non-perturbatively. This is what we will do next. We will transform this many-body problem to a self-consistent one-particle problem. This is done very much like what we do when we perform a mean-field approximation on spin-systems:

$$\begin{aligned} c_{-k\downarrow}c_{k\uparrow} &= \underbrace{\langle c_{-k\downarrow}c_{k\uparrow}\rangle}_{\equiv b_k} + \underbrace{c_{-k\downarrow}c_{k\uparrow} - \langle c_{-k\downarrow}c_{k\uparrow}\rangle}_{\delta b_k} \\ &= b_k + \delta b_k. \end{aligned} \tag{5.8}$$

Here, b_k is a statistical average [2] Now insert the definitions in eq. (5.8) and the Hermitian conjugate into eq. (5.7) and ignore terms $\mathcal{O}((\delta b)^2)$ Consider the interaction term:

$$\begin{aligned} \sum_{k,k'} V_{k,k'} c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} c_{-k',\downarrow} c_{k,\uparrow} &= \sum_{k,k'} V_{k,k'} \left(b^\dagger_k + \delta b^\dagger_k\right)\left(b_{k'} + \delta b_{k'}\right) \\ &= \sum_{k,k'} V_{k,k'} \left(b^\dagger_k b_{k'} + b^\dagger_k \delta b_{k'} + \delta b^\dagger_k b_{k'}\right) + \mathcal{O}((\delta b)^2) \\ &\simeq \sum_{k,k'} V_{k,k'} \left(b^\dagger_k b_{k'} + b^\dagger_k c_{-k'\downarrow} c_{k'\uparrow} + b_{k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - 2 b^\dagger_k b_{k'}\right). \end{aligned}$$

Giving the b's a finite expectation value breaks the U(1)-symmetry of the system. There is no way to gradually break this symmetry, it either happens or not.

[2] with respect to the "correct" Hamiltonian.