Quantum Theory of Solids

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Foreword

Digitialized lecture notes for the course “TFY4210 - Quantum Theory of Many-Particle Systems” held by Prof. Asle Sudbø spring 2020. These notes follow that of the hand written lecture notes, which are based upon the lecture notes for the course “FY8302 - Quantum Theory of Solids”, originally written in 1996.
Course website: https://www.ntnu.edu/studies/courses/TFY4210

Initial contributors

The transcription of lecture notes was started in the spring of 2020. Several people has contributed to the initial transcription.

- **Øyvind Muldal Taraldsen** wrote the indtroductory chapters on many-particle system, up until the section on atomic orbital basis. (Lecture notes week 1-2 and start of 3.)
- **Ola Lajord** transcribed the section on many-boson systems, and much of the section on the transformation from Hubbard model to antiferromagnet. (Lecture notes week 4).
- **Snorre Bergan** did the initial transcription of magnon mediated superconductivity and the Cooper problem. (Most of lecture notes week 9)
- **Niels Henrik Aase** took care of the Ginzburg-Landau theory of superconductivity, including figures. (Lecture notes week 11)
- **Karl Kristian Ladegård Lockert** transcribed most of the remaining lecture notes, and many figures in sections transcribed by other contributors. (Lecture notes week 3,5-8, start of 9, and 10)

Completion

The completion of transcription is done during the summer of 2021 by Karl Kristian.

CONTENTS

CHAPTER 1

INTRODUCTION

Many-particle systems are systems where interactions between the particle-constituents of the system are important. When quantum effects are important, we talk about quantum many-body systems. The sort of systems we will consider in this course are made up of aggregate states of various atoms, and may typically be separated, a priori, into interacting states of electrons and ions:

1. Electrons interacting among themselves.
2. Ions interacting among themselves.
3. Interactions between electrons and ions.

What we seek to explain, is what determines the various physical states such a system may take up. Why are some materials metals, insulators, superfluids, superconductors, ferromagnets, antiferromagnets? The plethora of states appears quite bewildering. A major objective of this course is to see how to give a unifying description of all these systems, a "theory of everything" (almost).

In principle, the answer to the above question is obtained by solving the Schrödinger-equation for the many-body quantum-mechanical state $|\psi\rangle$:

$$\mathcal{H}\,|\psi\rangle = i\hbar\frac{\partial\,|\psi\rangle}{\partial t} \tag{1.0.1}$$

$\mathcal{H}$: Operator that generates dynamics. Here, $\mathcal{H}$ is the Hamiltonian of the system, this $\mathcal{H}$ consists of three parts:

1. $\underline{\mathcal{H}_{e-e}}$: Describes the electrons with interactions among themselves.
2. $\underline{\mathcal{H}_{i-i}}$: Describes the ions with interactions among themselves.
3. $\underline{\mathcal{H}_{e-i}}$: Describes the interactions between ions and electrons.

The Hamiltonian we consider will furthermore describe a priori non-relativistic systems, which means we can separate $\mathcal{H}$ into kinetic energy, T, and potential energy, V,

$$\mathcal{H} = T + V \tag{1.0.2}$$

$$\underline{\mathcal{H}_{e-e} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i,j} V_{e-e}^{Coulomb}(\mathbf{r}_i - \mathbf{r}_j)} \tag{1.0.3}$$

m : Electron mass
$\mathbf{p}_i$: Electron momentum
$\mathbf{r}_i$: Electron coordinate
$V_{e-e}^{\text{Coulomb}}(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$
e : Electron charge (e defined as positive)
ε_0 : Vacuum-permittivity

$$\underline{\mathcal{H}_{i-i} = \sum_i \frac{\mathbf{P_i}^2}{2M} + \sum_{i,j} V_{i-i}^{Coulomb}(\mathbf{R_i} - \mathbf{R_j})} \tag{1.0.4}$$

M : Ion mass
$\mathbf{P}_i$: Ion momentum
$\mathbf{R}_i$: Ion coordinate
$V_{i-i}^{\text{Coulomb}}(\mathbf{R}) = \frac{Z^2e^2}{4\pi\varepsilon_0}\frac{1}{R}$
Ze : Ionic charge

$$\underline{\mathcal{H}_{e-i} = \sum_{i,j} V_{e-i}^{Coulomb}(\mathbf{R}_i - \mathbf{r}_j)} \tag{1.0.5}$$

$V_{e-i}^{\text{Coulomb}}(\mathbf{R}) = \frac{-Ze^2}{4\pi\varepsilon_0}\frac{1}{R}$

NB! Note that the kinetic energy of the entire system is the sum of kinetic energies of each individual particle. The potential energy of the system is the sum of potential energy of pairs of particles, this later statement is an approximation. In principle, we can include three-, four-, five-, ... body interactions, but these will be ignored to a good approximation. Thus, the total Hamiltonian for a many-body system is a sum of one-particle terms and two-particle terms. This is an enormous simplification. NB!! There exists physical systems in condensed matter physics where this may not be a good approximation.

Observables are represented by operators $\hat{O}$. A measurable quantity is then

$$\langle \hat{O} \rangle = \langle \psi | \, \hat{O} \, | \psi \rangle \,, \tag{1.0.6}$$

which is the expectation value of $\hat{O}$ in the many-body quantum state. $|\psi\rangle$ is computed at zero temperature $T = 0$; i.e. $|\psi\rangle$ is a ground state. Often, we would like to compute expectation-values of $\hat{O}$ at $T > 0$. This can be done by introducing a statistical parameter

$$\beta = \frac{1}{k_B T}; \tag{1.0.7}$$

k_B : Boltzman's constant.

Partition function:

$$\mathcal{Z} = \mathrm{Tr}\left(\mathrm{e}^{-\beta \mathcal{H}}\right) \tag{1.0.8}$$

$$\langle \hat{O} \rangle_T = \frac{1}{Z} \mathrm{Tr}\left(\hat{O} \mathrm{e}^{-\beta \mathcal{H}}\right) \tag{1.0.9}$$

Thermal average involves also excited states.

The systems are assumed to be overall charge-neutral. The above Hamiltonian is formulated as a classical Hamiltonian in terms of coordinates and momenta of electrons and ions. We are seeking a quantum formulation of such a system, which means we need to find a useful formalism of operators and states in order to proceed.

For the systems that will be considered in this course, quantum particles come in two varieties:
  i) Fermions.
  ii) Bosons.
We first proceed by setting up a formulation for fermions (electrons are fermions).

CHAPTER 2

MANY-PARTICLE STATES FOR FERMIONS

2.1 N-particle vacuum state

Many-particle states will be built up by constructing a basis using products of single-particle states. Let λ be some set of quantum numbers that uniquely specifies a single-particle quantum state.

Example: λ could be the set of quantum numbers of the hydrogen-atom.
$\lambda = (n, l, m, \sigma)$

$$\begin{aligned} n &: \text{Main quantum number.} \\ l &: \text{Orbital angular momentum quantum number.} \\ m &: \text{Quantization of angular momentum along z-axis.} \\ \sigma &: \text{Spin quantum number.} \end{aligned}$$

Motion in 3 dimensions $\implies$ 3 quantum numbers : (n, l, m)
Spin: 1 quantum number.

$$\begin{array}{ll} \text{Corresponding state:} & |n_\lambda\rangle \\ \text{Adjoint state:} & \langle n_\lambda| = (|n_\lambda\rangle)^\dagger \end{array}$$

Vacuum-state (unoccupied state): $|0_\lambda\rangle$
Introduce creation and annihilation operators.

$$\begin{array}{ll} \text{Creation:} & c_\lambda^\dagger \\ \text{Annihilation:} & c_\lambda \end{array}$$

$$\begin{aligned} |1_\lambda\rangle &= c_\lambda^\dagger |0_\lambda\rangle \\ |0_\lambda\rangle &= c_\lambda |1_\lambda\rangle \\ 0 &= c_\lambda |0_\lambda\rangle \end{aligned}$$

In general, we will use a set og quantum numbers that are convenient. Exactly what this means in practice will become clear later, when we start looking at specific systems.

Many-body state:

$$|N\rangle = |n_{\lambda_1}, n_{\lambda_2}, n_{\lambda_3}, ..., n_{\lambda_N}\rangle$$

N-particle vacuum-state:

$$\begin{aligned} &|0\rangle = |0_{\lambda_1}, 0_{\lambda_2}, ..., 0_{\lambda_N}\rangle \\ &|N\rangle : \text{Fock-basis} \end{aligned} \tag{2.1.1}$$

We regard fermions as quantized excitations of a matter field, in the same way as we regard photons as quantized excitations of an electromagnetic field.

Field operators for a fermion: $\psi^\dagger(x,t):$ Creates a fermion in some quantum state at point $(\boldsymbol{r}, s) = x$ at time t.

$$\psi^\dagger(x,t) = \sum_\lambda c_\lambda^\dagger(t)\varphi_\lambda^*(x) \tag{2.1.2}$$

$\varphi_\lambda(\boldsymbol{r}, s)$: Wave-function for quantum state with quantum numbers $\underline{\lambda}$.

Quantization:

$$\{\psi^\dagger(x,t), \psi(x,t)\} = \delta(\boldsymbol{r} - \mathbf{r}')\delta(s, s') \tag{2.1.3}$$

Note that t is the same in $\psi^\dagger$ and ψ!

$$\{A, B\} = AB + BA \tag{2.1.4}$$

The set of wavefunctions $\varphi_\lambda(\boldsymbol{r})$ are assumed to constitute a complete set i.e. any function $f(\boldsymbol{r})$ can be expressed in terms of $\{\varphi_\lambda(\boldsymbol{r})\}$

$$f(\boldsymbol{r}, s) = \sum_\lambda a_\lambda \varphi_\lambda(\boldsymbol{r}, s) \tag{2.1.5}$$

$\{\varphi_\lambda(\boldsymbol{r}, s)\}$ is furthermore assumed to be orthonormalized

$$\sum_{\boldsymbol{r},s} \varphi^*_\lambda(\boldsymbol{r},s)\varphi_{\lambda'}(\boldsymbol{r},s) = \delta_{\lambda,\lambda'}, \tag{2.1.6}$$

where

$$\delta_{\lambda,\lambda'} = \begin{cases} 1; & \lambda = \lambda' \\ 0; & \lambda \neq \lambda' \end{cases}$$

$$\begin{aligned}
\sum_{\boldsymbol{r}} \varphi^*_{\lambda'}(\boldsymbol{r},s) f(\boldsymbol{r},s) &= \sum_\lambda \sum_{\boldsymbol{r}} \varphi^*_{\lambda'}(\boldsymbol{r},s)\varphi_\lambda(\boldsymbol{r},s) \\
&= \sum_\lambda \delta_{\lambda,\lambda'} \\
&= \lambda'
\end{aligned}$$

$$\begin{aligned}
f(\boldsymbol{r},s) &= \sum_\lambda \sum_{\mathbf{r}',s} \varphi^*_\lambda(\mathbf{r}',s') f(\boldsymbol{r},s')\varphi_\lambda(\boldsymbol{r},s) \\
&= \sum_{\mathbf{r}',s'} \left[\sum_\lambda \varphi^*_\lambda(\mathbf{r}',s')\varphi_\lambda(\boldsymbol{r},s) \right] f(\mathbf{r}',s') \\
&= \sum_{\mathbf{r}',s'} \delta(\boldsymbol{r}-\mathbf{r}')\delta_{s,s'} f(\mathbf{r}',s')
\end{aligned}$$

2.2 Completeness relation

$$\sum_\lambda \varphi^*_\lambda(\boldsymbol{r},s)\varphi_\lambda(\boldsymbol{r},s) = \delta(\boldsymbol{r}-\mathbf{r}')\delta_{s,s'} \tag{2.2.1}$$

Futhermore:

$$\begin{aligned}
\{\psi^\dagger(x',t),\psi(x,t)\} &= \delta_{x',x} \\
&= \sum_{\lambda_1}\sum_{\lambda_2} \{c^\dagger_{\lambda_1}, c_{\lambda_2}\}(\boldsymbol{r},s)\varphi^*_{\lambda_1}(\boldsymbol{r},s)\varphi_{\lambda_2}
\end{aligned} \tag{2.2.2}$$

If $\{c^\dagger_{\lambda_1}, c_{\lambda_2}\} = \delta_{\lambda_1,\lambda_2}$ then equation (2.2.2) is satisified.

$$\{c^\dagger_{\lambda_1}, c_{\lambda_2}\} = \delta_{\lambda_1,\lambda_2} \tag{2.2.3}$$

In addition:

$$\{\psi^\dagger(x',t),\psi^\dagger(x,t)\} = 0 \implies \{c^\dagger_{\lambda'}, cd_\lambda\} = 0 \tag{2.2.4}$$

$$\{\psi(x',t),\psi(x,t)\} = 0 \implies \{c_{\lambda'}, c_\lambda\} = 0 \tag{2.2.5}$$

$$c^\dagger_\lambda c^\dagger_\lambda |0\rangle = 0 \tag{2.2.6}$$

Cannot create more than one fermion in one single-particle state. (Pauli-principle) $\Longrightarrow$

$$
\begin{aligned}
c_\lambda c_\lambda \left|n_\lambda\right\rangle &= 0 \\
\{c^\dagger_{\lambda_1}, c_{\lambda_2}\} &= \delta_{\lambda_1,\lambda_2} \\
\lambda_1 \neq \lambda &: \\
\left|n_{\lambda_1} n_{\lambda_2}\right\rangle &= -\left|n_{\lambda_2} n_{\lambda_1}\right\rangle
\end{aligned}
$$

A fermionic two-particle sstate is antisymmetric under interchange of the constituent single-particle states.

The next step is now to express operators representing observables in terms of creation and destruction operators. This is called second quantization.

2.3 Operators

Definitions:

1. One-particle operator is an operator representing an observable of the following classical form

$$U = \sum_{i=1}^{N} U_i(\boldsymbol{r}_i, \mathbf{P}_i). \tag{2.3.1}$$

   U_i depends only on the coordinate and momentum of one particle $(\boldsymbol{r}_i, \mathbf{P}_i)$.

2. Two-particle operator is an operator representing an observable of the following classical form

$$V = \sum_{i,j} V_{ij}(\boldsymbol{r}_i, \mathbf{P}_i, \boldsymbol{R}_j, \mathbf{P}_j). \tag{2.3.2}$$

   V_{ij} depends on the coordinates and momenta of two particles, $(\boldsymbol{r}_i, \mathbf{P}_i)$ and $(\boldsymbol{R}_j, \mathbf{P}_j)$. For the situations we will consider V_{ij} will depend only on $\mathbf{r}_i$ and $\boldsymbol{R}_j$, not $\mathbf{P}_i, \mathbf{P}_j$.

Matrix elements of single-particle operators.

$$\hat{U}\left|N\right\rangle = \sum_i \hat{U}_i \left|N\right\rangle$$

$\hat{U}_i$ Only works on *one* element in $|N\rangle$:

$$\hat{U}_i = \underbrace{\hat{U}_i \left| n_{\lambda_1}, \cdots, \; n_{\lambda_i} \; , \cdots, n_{\lambda_N} \right\rangle}_{\text{Works on this element only}}$$

Examples of one-particle operators:

1. Kinetic energy T

$$\hat{T} = \sum_{i=1}^{N} \frac{\hat{p_i}^2}{2m} |N\rangle \,, \tag{2.3.3}$$

spin-independent (does not involve spin-coordinate).

2. Crystal potential that electrons move through in a solid

$$\hat{V} = \sum_i \hat{V}_i |N\rangle \tag{2.3.4}$$

$$\hat{V}_i = \sum_j \hat{V}_{ij}(\boldsymbol{r}_i - \boldsymbol{R}_j), \tag{2.3.5}$$

spin-independent, (no spin-coordinate).
$\boldsymbol{r}_i$: Electron-coordinate
$\boldsymbol{R}_j$: Ion-coordinate

The matrix element of a 1-p operator sandwiched between two many-particle states:

$$\begin{aligned}
\langle N'| \hat{U} |N\rangle &= \sum_i \langle N'| \hat{U}_i |N\rangle \\
&= \sum_i \left\langle n'_1, \cdots, \; n'_i \; , \cdots, n'_N \right| \underbrace{\hat{U}_i \left| n_1, \cdots, \; n_i \; , \cdots, n_N \right\rangle}_{\text{i-th element}} \\
&= \sum_i \left\langle \tilde{N}' \middle| \tilde{N} \right\rangle \langle n'_i| U_i |n_i\rangle \qquad (2.3.6) \\
\left|\tilde{N}\right\rangle &= \prod_{k \neq i} |n_k\rangle \\
\left|\tilde{N}'\right\rangle &= \prod_{k \neq i} |n'_k\rangle
\end{aligned}$$

Normalization:

$$\frac{\langle N'|\,\hat{U}\,|N\rangle}{\langle N'|N\rangle} = \sum_i \frac{\langle \tilde{N}'|\tilde{N}\rangle}{\langle \tilde{N}'|\tilde{N}\rangle} \cdot \frac{\langle n_i'|\,\hat{U}_i\,|n_i\rangle}{\langle n_i'|n_i\rangle}$$
$$= \sum_i \frac{\langle n_i'|\,\hat{U}_i\,|n_i\rangle}{\langle n_i'|n_i\rangle} \tag{2.3.7}$$

> One-particle operators are defined by matrix-elements in a one-particle Hilbert-space $\{|n_i\rangle\}$, $i = 1, \cdots, N$.

Matrix elements of <u>two-particle operators</u>

$$\hat{V}\,|N\rangle = \sum_{i,j} \hat{V}_{ij}\,\Big|n_1, \cdots,\ n_i\ , \cdots,\ n_j\ , \cdots, n_N\Big\rangle \tag{2.3.8}$$

Works only on these two elements

<u>Example: Coulomb-interactions</u>
Matrix element:

$$\langle N'|\hat{V}|N\rangle = \sum_{i,j} \big\langle n_1', \cdots, n_i', \cdots, n_j', \cdots, n_N'\big|\,\hat{V}_{ij}\,|n_1, \cdots, n_i, \cdots, n_j, \cdots, n_N\rangle \tag{2.3.9}$$

$$= \sum_{i,j} \prod_{k\neq(i,k)} \langle n_k'|n_k\rangle\,\big\langle n_i', n_j'\big|\,\hat{V}_{ij}\,|n_i, n_j\rangle \tag{2.3.10}$$

<u>Normalization:</u>

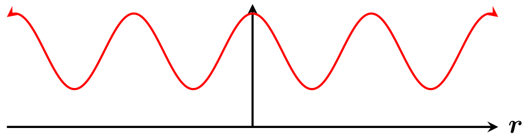
$$\frac{\langle N'|\,\hat{V}\,|N\rangle}{\langle N'|N\rangle} = \sum_{ij} \frac{\big\langle n_i', n_j'\big|\,\hat{V}_{ij}\,|n_i, n_j\rangle}{\big\langle n_i', n_j'\big|n_i, n_j\big\rangle} \tag{2.3.11}$$

> Matrix elements of two-particle operators are computed in a Hilbert-space of two-particle states.

For the 2-particle operators we consider

$$\hat{V}_{ij} = \hat{V}_{ji}, \qquad i \neq j \tag{2.3.12}$$
$$\text{If } i = j \implies \hat{V}_{ij} = 0,$$

because otherwise a 2-particle operator would operate on a 1-particle state, which it does not.



2.4 Interacting electron gas

Interacting electron gas in a periodic crystal potential $U(\boldsymbol{r})$

$$\mathcal{H} = \sum_i \left[\frac{\mathbf{P}_i^2}{2m} + U(\boldsymbol{r}_i)\right] + \sum_{ij} V_{e-e}^C(\boldsymbol{r}_i - \boldsymbol{R}_j) \tag{2.4.1}$$

This is, in general, a very hard problem to solve. In particular, it is the Coulomb-term which makes it really hard.

One-particle term:

$$\mathcal{H}_1 = \sum_i \mathcal{H}_1(\boldsymbol{r}_i, \mathbf{P}_i) \tag{2.4.2}$$

$$\mathcal{H}_1(\boldsymbol{r}_i, \mathbf{P}_i) = \frac{\mathbf{P}_i^2}{2m} + U(\boldsymbol{r}_i) \tag{2.4.3}$$

Two-particle term:

$$\mathcal{H}_2 = \sum_{ij} V_{e-e}^C(\boldsymbol{r}_i - \boldsymbol{R}_j \tag{2.4.4}$$

We will first work out the second-quantized form of the two terms in $\mathcal{H}_1(\boldsymbol{r}_i, \mathbf{P}_i)$.

We define $\varphi_\lambda(\boldsymbol{r}, s)$ as follows: Solutions to the single-particle Schrödinger-equation

$$\mathcal{H}_1 \varphi_\lambda = \varepsilon_\lambda \varphi_\lambda \tag{2.4.5}$$

$$\mathcal{H}_1 = -\frac{\hbar^2}{2m}\nabla^{\mathbf{2}} + U(\boldsymbol{r}); \qquad \nabla^{\mathbf{2}} : \text{Laplace-operator} \tag{2.4.6}$$

The task is now to find a second-quantized form of $\mathcal{H}_1$ which will yield the same matrix elements as 2.4.6.

Consider:

$$\langle\lambda_1|\,\mathcal{H}_1\,|\lambda_2\rangle\,; \qquad \langle\lambda_1|\lambda_2\rangle = \delta_{\lambda_1,\lambda_2} \tag{2.4.7}$$

Completeness relation:

$$\langle \boldsymbol{r}, s|\lambda_1\rangle = \varphi_{\lambda_1} \qquad \text{(some wavefunction)}$$

Normalized states: $\langle\lambda|\lambda\rangle = 1$

$$\sum_{\lambda} \varphi^*_{\lambda}(\boldsymbol{r}, s)\varphi_{\lambda}(\mathbf{r}', s') = \delta(\boldsymbol{r} - \mathbf{r}')\delta_{s,s'} \tag{2.4.8}$$

$$\sum_{\boldsymbol{r},s} \varphi^*_{\lambda'}(\boldsymbol{r}, s)\varphi_{\lambda}(\boldsymbol{r}, s) = \delta_{\lambda,\lambda'} \tag{2.4.9}$$

$$\langle\lambda|\lambda'\rangle = \delta_{\lambda,\lambda'} \implies \sum_{\boldsymbol{r},s} |\boldsymbol{r}, s\rangle\,\langle\boldsymbol{r}, s| = 1; \quad \sum_{x} |x\rangle\,\langle x| = 1 \tag{2.4.10}$$

Now we use this version of the completeness relations to evaluate the matrix element $\langle\lambda_1|\,\mathcal{H}_1\,|\lambda_2\rangle$

$$\begin{aligned} \langle\lambda_1|\,\mathcal{H}_1\,|\lambda_2\rangle &= \sum_{\boldsymbol{r},s}\sum_{\mathbf{r}',s'} \langle\lambda_1|\boldsymbol{r}, s\rangle\,\langle\boldsymbol{r}, s|\,\mathcal{H}_1\,|\mathbf{r}', s'\rangle\,\langle\mathbf{r}'|\lambda_2\rangle \\ &= \sum_{\boldsymbol{r},s}\sum_{\mathbf{r}',s'} \varphi^*_{\lambda_1}(\boldsymbol{r}, s)\,\langle\boldsymbol{r}, s|\,\mathcal{H}_1\,|\mathbf{r}', s'\rangle\,\varphi_{\lambda_2}(\mathbf{r}', s') \end{aligned} \tag{2.4.11}$$

$$\mathcal{H}_1 = \frac{\mathbf{p}^2}{2m} + U(\boldsymbol{r}) \qquad \text{Classical} \tag{2.4.12}$$

$$\mathbf{p} = \frac{\hbar}{i}\boldsymbol{\nabla}; \qquad \boldsymbol{\nabla} : \text{Gradient operator} \tag{2.4.13}$$

$$\mathcal{H}_1 = -\frac{\hbar^2\nabla^{\mathbf{2}}}{2m} + U(\hat{r}) \qquad \text{Quantum mechanical} \tag{2.4.14}$$

$$U(\hat{r})\,|r\rangle = U(\boldsymbol{r})\,|r\rangle \tag{2.4.15}$$

$\boldsymbol{r}$: Position : eigenvalue of the position operator

$$\hat{r}\,|\boldsymbol{r}, s\rangle = \boldsymbol{r}\,|\boldsymbol{r}, s\rangle \tag{2.4.16}$$

$$U(\hat{r})\,|\boldsymbol{r}, s\rangle = U(\boldsymbol{r})\,|\boldsymbol{r}, s\rangle \tag{2.4.17}$$

$$\langle\boldsymbol{r}, s|\,\mathcal{H}_1\,|\mathbf{r}', s'\rangle = \left[-\frac{\hbar^2}{2m}\nabla^{\mathbf{2}} + U(\boldsymbol{r})\right]\delta_{\boldsymbol{r},\mathbf{r}'}\delta_{s,s'} \tag{2.4.18}$$

$$\begin{aligned} \langle\lambda_1|\,\mathcal{H}_1\,|\lambda_2\rangle &= \sum_{\boldsymbol{r},s} \varphi^*_{\lambda_1}(\boldsymbol{r}, s)\left[-\frac{\hbar^2}{2m}\nabla^{\mathbf{2}} + U(\boldsymbol{r})\right]\varphi_{\lambda_2}(\boldsymbol{r}, s) \\ &\equiv \varepsilon_{\lambda_1,\lambda_2} \end{aligned} \tag{2.4.19}$$

$\varphi_\lambda(\boldsymbol{r}, s)$: Some complete set of functions, by assumption.

Let us now give an alternative form of $\mathcal{H}_1$, which will yield the same matrix elements.
Anzats:

$$\mathcal{H}_1 = \sum_{\lambda_1,\lambda_2} h_{\lambda_1,\lambda_2} c^\dagger_{\lambda_1} c_{\lambda_2} \tag{2.4.20}$$

where h_{λ_1,λ_2} is some complex number. Then:

$$\begin{aligned}
\langle\lambda_1| \mathcal{H}_1 |\lambda_2\rangle &= \langle 0| c_{\lambda_1} \left(\sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2} c^\dagger_{\lambda'_1} c_{\lambda'_2} \right) c^\dagger_{\lambda_2} |0\rangle \\
&= \sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2} \langle 0| c_{\lambda_1} c^\dagger_{\lambda'_1} c_{\lambda'_2} c^\dagger_{\lambda_2} |0\rangle \\
&= \sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2} \langle 0| (\delta_{\lambda_1,\lambda'_1} - c^\dagger_{\lambda'_1} c_{\lambda_1})(\delta_{\lambda_2,\lambda'_2} - c^\dagger_{\lambda_2} c_{\lambda'_2}) |0\rangle \\
&= \sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2} \delta_{\lambda_1,\lambda'_1} \delta_{\lambda_2,\lambda'_2} \langle 0|0\rangle \qquad (c_\lambda |0\rangle = 0) \\
&= h_{\lambda_1,\lambda_2}
\end{aligned} \tag{2.4.21}$$

Choose $h_{\lambda_1,\lambda_2} = \varepsilon_{\lambda_1,\lambda_2} \implies$ Same matrix-elements for

$$\mathcal{H}_1 = -\frac{\hbar^2}{2m} \nabla^{\mathbf{2}} + U(\hat{r}) \tag{2.4.22}$$

and

$$\boxed{\mathcal{H}_1 = \sum_{\lambda_1,\lambda_2} \varepsilon_{\lambda_1,\lambda_2} c^\dagger_{\lambda_1} c_{\lambda_2}} \tag{2.4.23}$$

Thus, 2.4.23 is a useful 2nd quantized form of $\mathcal{H}_1$.

This expression may be simplified. Consider now a judicial choice of the complete set $\{\varphi_\lambda(x)\}$:
Let φ_λ be defined by

$$\left(-\frac{\hbar^2}{2m} \nabla^{\mathbf{2}} + U(\boldsymbol{r}) \right) \varphi_\lambda(x) = \varepsilon_\lambda \varphi_\lambda(x) \tag{2.4.24}$$

i.e. φ_λ are eigenfunctions of $\mathcal{H}_1$

Then:

$$\begin{aligned}
\varepsilon_{\lambda_1,\lambda_2} &= \sum_x \varphi^*_{\lambda_1}(x)\left(-\frac{\hbar^2}{2m}\nabla^{\mathbf{2}} + U(\boldsymbol{r})\right)\varphi_{\lambda_2}(x) \\
&= \sum_x \varphi^*_{\lambda_1}(x)\varepsilon_{\lambda_2}\varphi_{\lambda_2}(x) \\
&= \varepsilon_{\lambda_2}\sum_x \varphi^*_{\lambda_1}(x)\varphi_{\lambda_2}(x) \\
&= \varepsilon_{\lambda_2}\delta_{\lambda_1,\lambda_2}
\end{aligned} \tag{2.4.25}$$

giving that,

$$\mathcal{H}_1 = \sum_{\lambda_1} \varepsilon_{\lambda_1} c^\dagger_{\lambda_1} c_{\lambda_1} \tag{2.4.26}$$

This form of $\mathcal{H}_1$ has an intuitively appealing form: $c^\dagger_{\lambda_1} c_{\lambda_1}$ is a number operator. It counts the number of particles in state $|\lambda_1\rangle$.
ε_λ is the single-particle energy in this state. Thus, $\mathcal{H}_1$ is an operator that counts the energy in the system coming from all the possible states of the system.

General one-particle operators:

$$T(x,\mathbf{p}) = T(x, \frac{\hbar}{i}\boldsymbol{\nabla}) \tag{2.4.27}$$

Could in principle depend on spin-coordinate s !

$$\langle\lambda_1|\, T\, |\lambda_2\rangle = \sum_x \varphi^*_{\lambda_1}(x) T(x, \frac{\hbar}{i}\boldsymbol{\nabla})\varphi_{\lambda_2}(x) \tag{2.4.28}$$

$$\boxed{\begin{aligned}
T &= \sum_{\lambda_1,\lambda_2} \langle\lambda_1|\, T(x,\mathbf{p})\, |\lambda_2\rangle\, c^\dagger_{\lambda_1} c_{\lambda_2} \\
&= \sum_{\lambda_1,\lambda_2} t_{\lambda_1,\lambda_2} c^\dagger_{\lambda_1} c_{\lambda_2}
\end{aligned} \qquad (2.4.29)}$$

This expression for $\mathcal{H}_1$ and T in second quantized form applies for any choice of sets of quantum numbers λ.

We next proceed by setting up a general form of second quantized form of 2-particle operators.

$$\mathcal{H} = \sum_i \mathcal{H}_1(\mathbf{p}_i, \boldsymbol{r}_i) + \sum_{i,j} \mathcal{H}_2(\boldsymbol{r}_i, \boldsymbol{r}_j) \tag{2.4.30}$$

Second-quantized form (general):

$$\begin{aligned}\mathcal{H} &= \sum_{\lambda_1,\lambda_2} \langle\lambda_1|\, \mathcal{H}_1 \,|\lambda_2\rangle\, c^\dagger_{\lambda_1} c_{\lambda_2} \\ &+ \sum_{\lambda_1} \cdots \sum_{\lambda_4} \langle\lambda_1, \lambda_2|\, \mathcal{H}_2 \,|\lambda_3, \lambda_4\rangle\, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}\end{aligned} \tag{2.4.31}$$

2.5 Plane-wave basis

i) Plane-wave basis: $\varphi_\lambda(\boldsymbol{r}, s) = \frac{1}{\sqrt{V}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}} \chi_\sigma(s)$

Completeness:

$$\sum_{\boldsymbol{k}} \sum_{\sigma} \varphi^*_{\boldsymbol{k},\sigma}(\boldsymbol{r'}, s')\varphi_{\boldsymbol{k},\sigma}(\boldsymbol{r}, s) = \delta_{\boldsymbol{r},\boldsymbol{r'}}\delta_{s,s'} \tag{2.5.1}$$

Orthogonality:

$$\sum_{\boldsymbol{r}} \sum_{s} \varphi^*_{\boldsymbol{k'},\sigma'}(\boldsymbol{r}, s)\varphi_{\boldsymbol{k},\sigma}(\boldsymbol{r}, s) = \delta_{\boldsymbol{k},\mathbf{k'}}\delta_{\sigma,\sigma'} \tag{2.5.2}$$

Field-operators are given by

$$\psi^\dagger(\boldsymbol{r}, s, t) = \sum_{\boldsymbol{k},\sigma} c^\dagger_{\boldsymbol{k},\sigma}(t) \left(\frac{1}{\sqrt{V}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}} \chi_\sigma(s)\right) \tag{2.5.3}$$

$$\{c_{k,\sigma}(t), c^\dagger_{k',\sigma'}\} = \delta_{k,k'}\delta_{\sigma,\sigma'} \tag{2.5.4}$$

$$\{c_{k,\sigma}(t), c_{k',\sigma'}\} = 0 \tag{2.5.5}$$

$$\{c^\dagger_{k,\sigma}(t), c^\dagger_{k',\sigma'}\} = 0 \tag{2.5.6}$$

Orthonormality, spatial part

$$\frac{1}{V} \sum_{\boldsymbol{r}} \mathrm{e}^{i\boldsymbol{r}\cdot(\boldsymbol{k}-\mathbf{k}')} = \delta_{\boldsymbol{k},\boldsymbol{k'}} \tag{2.5.7}$$

Orthonormality, spin part

$$\sum_s \chi^*_{\sigma_1}(s)\chi_{\sigma_2}(s) = \delta_{\sigma_1,\sigma_2} \tag{2.5.8}$$

Completeness, spatial part

$$\frac{1}{V}\sum_{\boldsymbol{k}} \mathrm{e}^{i\mathbf{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta_{\boldsymbol{r},\boldsymbol{r}'} \tag{2.5.9}$$

Completeness, spin part

$$\sum_\sigma \chi^*_\sigma(s')\chi_\sigma(s) = \delta_{s',s} \tag{2.5.10}$$

The plane-waves are eigenfunctions of $\mathcal{H}_{10} \equiv -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 \implies$

$$\mathcal{H}_{10} = \sum_{\boldsymbol{k}_1,\sigma_1}\sum_{\boldsymbol{k}_2,\sigma_2} \langle \boldsymbol{k}_1,\sigma_1|\,\mathcal{H}_{10}\,|\boldsymbol{k}_2,\sigma_2\rangle\, c^\dagger_{\boldsymbol{k}_1,\sigma_1} c_{\boldsymbol{k}_2,\sigma_2} \tag{2.5.11}$$

$$\langle \boldsymbol{k}_1,\sigma_1|\,\mathcal{H}_{10}\,|\boldsymbol{k}_2,\sigma_2\rangle = \frac{1}{V}\sum_{\boldsymbol{r}} \mathrm{e}^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}} \sum_s \chi^*_{\sigma_1}(s)\chi_{\sigma_2}(s)\frac{\hbar^2k_2^2}{2m} \tag{2.5.12}$$

$$\mathcal{H}_{10} = \sum_{\mathbf{k_1},\sigma_1} \frac{\hbar^2k_1^2}{2m} c^\dagger_{\boldsymbol{k}_1,\sigma_1} c_{\boldsymbol{k}_1,\sigma_1}$$

$$\mathcal{H}_{10} = \sum_{\boldsymbol{k},\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k,\sigma}\ ; \qquad \varepsilon_k = \frac{\hbar^2k^2}{2m}$$

The next contribution to $\mathcal{H}_1$ is the crystal potential $U(\boldsymbol{r}_i) = \mathcal{H}_{11}(r_i)$
$\sum_i U(\boldsymbol{r}_i) \to \sum_{\lambda_1,\lambda_2} \langle\lambda_1|\,\mathcal{H}_{11}\,|\lambda_2\rangle\, c^\dagger_{\boldsymbol{k}_1,\lambda_1} c_{\lambda_2}$

$$\begin{aligned}\langle\lambda_1|\,\mathcal{H}_{11}\,|\lambda_2\rangle &= \sum_{\boldsymbol{r}}\sum_s \frac{1}{\sqrt{V}}\mathrm{e}^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}\chi^*_{\sigma_1}(s)U(\boldsymbol{r})\frac{1}{\sqrt{V}}\mathrm{e}^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}\chi_{\sigma_2}(s) \\ &= \frac{1}{V}\sum_{\boldsymbol{r}} \mathrm{e}^{i(\boldsymbol{k}_2-\mathbf{k}_1)\cdot\boldsymbol{r}}U(\boldsymbol{r})\sum_s \chi^*_{\sigma_1}(s)\chi_{\sigma_2}(s)\end{aligned} \tag{2.5.13}$$

Introduce Fourier-transform of the crystal-potential

$$\tilde{U}(\mathbf{q}) \equiv \frac{1}{V}\sum_{\boldsymbol{r}} \mathrm{e}^{-i\mathbf{q}\cdot\boldsymbol{r}}U(\boldsymbol{r}) \tag{2.5.14}$$

$$U(\boldsymbol{r}) = \sum_{\mathbf{q}} \tilde{U}(\mathbf{q})\mathrm{e}^{i\mathbf{q}\boldsymbol{r}} \tag{2.5.15}$$

$$\langle\lambda_1|\,\mathcal{H}_{11}\,|\lambda_2\rangle = \delta_{\sigma_1,\sigma_2}\tilde{U}(\boldsymbol{k}_1-\mathbf{k}_2) \tag{2.5.16}$$

$$\sum_{\lambda_1}\sum_{\lambda_2} \langle\lambda_1|\,\mathcal{H}_{11}\,|\lambda_2\rangle\, c^\dagger_{\lambda_1} c_{\lambda_2} = \sum_{\boldsymbol{k}_1}\sum_{\boldsymbol{k}_2}\sum_{\sigma} \tilde{U}(\boldsymbol{k}_1-\boldsymbol{k}_2) c^\dagger_{\mathbf{k}_1,\sigma} c_{\mathbf{k}_2,\sigma}$$
$$= \sum_{\boldsymbol{k},\mathbf{q},\sigma} \tilde{U}(\mathbf{q}) c^\dagger_{\boldsymbol{k}+\mathbf{q},\sigma} c_{\boldsymbol{k},\sigma}$$

Where we have defined $\mathbf{q} \equiv \boldsymbol{k}_1 - \boldsymbol{k}_2$; $\boldsymbol{k}_2 \equiv \boldsymbol{k}$.

Scattering of plane-waves $|\boldsymbol{k},\sigma\rangle \to |\boldsymbol{k}+\mathbf{q},\sigma\rangle$ by crystal lattice. Momentum $\mathbf{q}$ is transferred to fermions (electrons) from the lattice. Spin is conserved in the scattering.

$$\mathcal{H}_1 = \sum_i \left[\frac{p_i^2}{2m} + U(\boldsymbol{r}_i)\right] \implies \tag{2.5.17}$$

$$\mathcal{H}_1 = \sum_{\boldsymbol{k},\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{\boldsymbol{k},\mathbf{q},\sigma} \tilde{U}(\mathbf{q}) c^\dagger_{k+q,\sigma} c_{k,\sigma} \quad ; \ \varepsilon_k = \frac{\hbar^2 k^2}{2m} \tag{2.5.18}$$

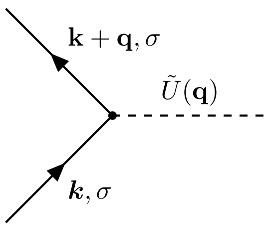


Illustration of the scattering event

Next, we second-quantize the Coulomb interaction in the plane-wave basis.

Electron-electron interaction:

$$\mathcal{H}_2 = \sum_{\lambda_1}\cdots\sum_{\lambda_4} \langle\lambda_1,\lambda_2|\,V^C_{e-e}\,|\lambda_3,\lambda_4\rangle\, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4} \tag{2.5.19}$$

$$\begin{aligned} &\langle\lambda_1,\lambda_2|\,V^C_{e-e}(\boldsymbol{r}_i-\boldsymbol{r}_j)\,|\lambda_3,\lambda_4\rangle \\ &= \sum_{s_1}\cdots\sum_{s_4} \chi^*_{\sigma_1}(s_1)\chi^*_{\sigma_2}(s_2)\chi_{\sigma_3}(s_3)\chi_{\sigma_4}(s_4) \\ &\cdot \frac{1}{V^2}\sum_{\boldsymbol{r}_1\cdots\boldsymbol{r}_4} \mathrm{e}^{-i\boldsymbol{k}_1\boldsymbol{r}_1 - i\mathbf{k}_2\cdot\boldsymbol{r}_2 + i\mathbf{k}_3\cdot\boldsymbol{r}_3 + i\mathbf{k}_4\cdot\boldsymbol{r}_4} \\ &\cdot V^C_{e-e}(\boldsymbol{r}_3-\boldsymbol{r}_4)\delta_{s_2,s_3}\delta_{s_1,s_4}\delta_{\boldsymbol{r}_2,\boldsymbol{r}_3}\delta_{\boldsymbol{r}_1,\boldsymbol{r}_4} \end{aligned} \tag{2.5.20}$$

Spin-part: Four sums over s's reduce to two:

$$\sum_{s_1}\sum_{s_2}\chi^*_{\sigma_1}(s_1)\chi^*_{\sigma_2}(s_1)\chi_{\sigma_3}(s_2)\chi_{\sigma_4}(s_2) = \delta_{\sigma_1,\sigma_2}\delta_{\sigma_3,\sigma_4}$$

Spatial part: Again, four sums over $\boldsymbol{r}$ reduce to 2:

$$\sum_{\boldsymbol{r}_1}\sum_{\boldsymbol{r}_2} V^C_{e-e}(\boldsymbol{r}_2-\boldsymbol{r}_1)\frac{1}{V^2}\mathrm{e}^{i(\boldsymbol{k}_4-\mathbf{k}_1)\cdot\boldsymbol{r}_1}\mathrm{e}^{i(\mathbf{k}_3-\mathbf{k}_2)\cdot\boldsymbol{r}_2}$$

Rewrite plane-wave factors in such a way that we can factor out a Fourier-transform of $V^C_{e-e}(\boldsymbol{r}_2-\boldsymbol{r}_1)$. We therefore need a plane-wave factor of the type $\mathrm{e}^{i\mathbf{q}\cdot(\boldsymbol{r}_2-\boldsymbol{r}_1)}$. Since the spatial argument of V^C_{e-e} is $\boldsymbol{r}_2-\mathbf{r}_1$ here.

$$\mathrm{e}^{i(\boldsymbol{k}_4-\mathbf{k}_1)\cdot\boldsymbol{r}_1}\mathrm{e}^{i(\mathbf{k}_3-\mathbf{k}_2)\cdot\boldsymbol{r}_2} = \mathrm{e}^{i(\mathbf{k}_4-\mathbf{k}_1+\mathbf{k}_3-\mathbf{k}_2)\cdot\boldsymbol{r}_1}\mathrm{e}^{i(\mathbf{k}_3-\mathbf{k}_2)\cdot(\boldsymbol{r}_2-\boldsymbol{r}_1)}$$

Define $\boldsymbol{r}_2-\boldsymbol{r}_1\equiv\boldsymbol{r}$ and sum over $(\mathbf{r},\boldsymbol{r}_1)$ instead of $(\mathbf{r}_1,\boldsymbol{r}_2)$

$$\begin{aligned}\sum_{\boldsymbol{r}} V^C_{e-e}\mathrm{e}^{i(\boldsymbol{k}_3-\mathbf{k}_2)\cdot\boldsymbol{r}}\frac{1}{V^2}\sum_{\boldsymbol{r}_1}\mathrm{e}^{i(\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_1-\mathbf{k}_2)\cdot\boldsymbol{r}_1} &= \sum_{\boldsymbol{r}} V^C_{e-e}\mathrm{e}^{i(\mathbf{k}_3-\mathbf{k}_2)\cdot\boldsymbol{r}}\frac{1}{V}\delta_{\boldsymbol{k}_3+\mathbf{k}_4,\mathbf{k}_1+\mathbf{k}_2}\\ &= \tilde{V}^C_{e-e}(\boldsymbol{k}_2-\boldsymbol{k}_3)\delta_{\boldsymbol{k}_3+\boldsymbol{k}_4,\boldsymbol{k}_1+\boldsymbol{k}_2}\end{aligned}$$

Fourier-transform of Coulomb-potential:

$$\tilde{V}^C_{e-e}(\mathbf{q}) \equiv \frac{1}{V}\sum_{\boldsymbol{r}}\mathrm{e}^{-i\mathbf{q}\cdot\boldsymbol{r}}V^C_{e-e}(\boldsymbol{r})$$

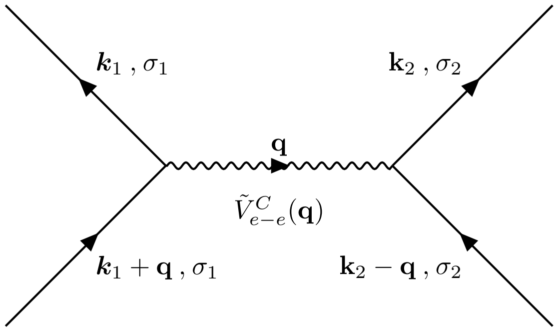
Thus, we have so far

$$\mathcal{H}_2 = \sum_{\boldsymbol{k}_1\ldots\mathbf{k}_4}\sum_{\sigma_1,\sigma_2}\tilde{V}^C_{e-e}(\mathbf{k}_2-\mathbf{k}_3)\delta_{\boldsymbol{k}_3+\mathbf{k}_4,\mathbf{k}_1+\mathbf{k}_2}c^\dagger_{\boldsymbol{k}_1,\sigma_1}c^\dagger_{\mathbf{k}_2,\sigma_2}c_{\mathbf{k}_3,\sigma_2}c_{\boldsymbol{k}_4,\sigma_1},$$

defining $\mathbf{q}\equiv\boldsymbol{k}_2-\boldsymbol{k}_3 \implies \boldsymbol{k}_3=\boldsymbol{k}_2-\mathbf{q}, \quad \boldsymbol{k}_4=\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3=\boldsymbol{k}_1-\mathbf{q}$. Thus, sum over $\boldsymbol{k}_1,\boldsymbol{k}_2,\mathbf{q}$:

$$\mathcal{H}_2 = \sum_{\boldsymbol{k}_1,\mathbf{k}_2,\mathbf{q}}\sum_{\sigma_1,\sigma_2}\tilde{V}^C_{e-e}(\mathbf{q})c^\dagger_{\mathbf{k}_1,\sigma_1}c^\dagger_{\mathbf{k}_2,\sigma_2}c_{\mathbf{k}_3-\mathbf{q},\sigma_2}c_{\mathbf{k}_1+\mathbf{q},\sigma_1}$$

This is a scattering process between two electrons. Diagrammatically, we may view the scattering event as:



Note that the spin of each electron is conserved in the scattering, since Coulomb-interaction is a purely electrostatic, spin-independent potential. This in total, we have

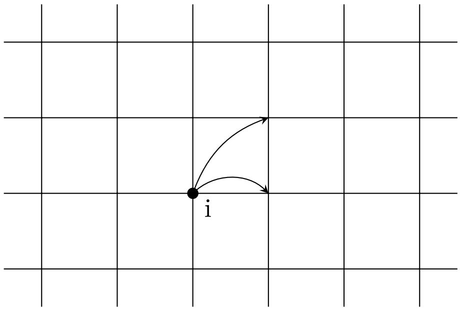
$$\begin{aligned} \mathcal{H} = & \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\mathbf{q}\sigma} \tilde{U}(\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k},\sigma} \\ & + \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\mathbf{q}} \sum_{\sigma_1,\sigma_2} \tilde{V}^C_{e-e}(\mathbf{q}) c^\dagger_{\boldsymbol{k}_1,\sigma_1} c^\dagger_{\boldsymbol{k}_2,\sigma_2} c_{\boldsymbol{k}_3-\mathbf{q},\sigma_2} c_{\boldsymbol{k}_1+\mathbf{q},\sigma_1} \end{aligned}$$

For a static crystal, $\tilde{U}(\mathbf{q})$ is some given fixed external potential that electrons move in. In that case, it is the Coulomb term which makes the problem really hard, since it represents a genuine many-particle problem. On the other hand, if the lattice it self has dynamics, then this introduces additional scattering of electrons, now off quantized lattice vibrations (phonons). In that case, the second term involving $\tilde{U}(\mathbf{q})$ will include phonons, and this turns the $\tilde{U}(\mathbf{q})$- term also into a genuine many-body problem. We will later in the course return to the important problem of studying coupling between electrons and phonons.

2.6 Atomic orbital basis

ii) Atomic orbital basis (lattice fermions)

We now consider a system where fermions most of the time stay localized on sites on a lattice. Occasionally, they may tunnel from one lattice site to another. This tunneling arises because the long-distance (away from lattice sites) tails of the atomic orbitals (Wannier-functions) may overlap.



Two tunneling processes ("hopping") on a 2D rectangular lattice, from lattice site i to its nearest and next-nearest neighbors. The long distance tails of the Wannier-functions fall off exponentially (recall the wave-functions of the Hydrogen-atom). Therefore, hopping is most likely to occur from a lattice site i to its nearest neighbor. The next most probable hopping event is a direct hopping from i to its next-nearest neighbor, or two hopping via an intermediate nearest neighbor. Which process is most likely is a matter of some detail: The two factors that mostly determine this is the distance between atoms on the lattice, and the type of atoms which are situated on the lattice points. If $\Delta\mathbf{r}$ is the separation between the electron and the ionic position, then the Wannier-functions fall off approximately as $\mathrm{e}^{-\Delta\mathbf{r}/\lambda}$

$$\lambda = c\frac{a_0}{Z}$$

c: Constant of order unity
a_0: Bohr-radius
Z: Number of protons in the nucleus

For heavy atoms, Wannier orbitals are more tightly localized around atoms than in lighter elements.
Crystal potential (rigid crystal)

$U = \sum_i U(\mathbf{r}_i)$
$U(\mathbf{r}_i) = \sum_j U(\mathbf{r}_i, \mathbf{R}j)$
$\mathbf{r}_i$: Electronic coordinate ; $\mathbf{R}j$: Ionic coordinate.

$U_a(\mathbf{r}_i, \mathbf{R}j)$: Potential energy that electron at $\mathbf{r}_i$ feels from ion located at $\mathbf{R}j$. The dominant contribution to this is when $i = j$, i.e. when the electron and ion is on the same site i. We single out this contribution as follows

$$U = \sum_i U_a(\mathbf{r}_i, \mathbf{r}_i) + \sum_i \sum_{j\neq i} U_a(\mathbf{r}_i, \mathbf{R}j).$$

The point of this splitting is that the basis functions $\{\varphi_\lambda\}$ that we will choose, will be the eigenfunctions of the total Hamilton-operator for isolated atoms. This is a very natural choice for a system where electrons spend most of the time on isolated atoms and only relatively rarely hop from one site to the other.

Schrödinger-equation for isolated atoms:

$$\left[\frac{\mathbf{p}_i^2}{2m} + U_a(\mathbf{r}_i, \mathbf{R}_i)\right] \varphi_{\alpha,\sigma}(\mathbf{r}_i, s_i) = \varepsilon_{\alpha,\sigma,i}\varphi_{\alpha,\sigma}(\mathbf{r}_i, s_i)$$

α: Index for atomic orbital
σ: Spin quantum number
$\mathbf{r}_i$: Spatial coordinate of electron on lattice site i
σ_i: Spin-coordinate of electron on lattice site ir
$\varepsilon_{\alpha,\sigma,i}$: Energy of electron in orbital α on lattice site$i$. In principle this energy could vary from lattice site to lattice site, but for most systems we will let $\varepsilon_{\alpha,\sigma,i} = \varepsilon_{\alpha,\sigma}$ i.e. independent of the position on the lattice. In principle, $\varepsilon_{\alpha,\sigma}$ could depend on spin. If we now bring in the rest of the crystal potential (from the surrounding atoms) in the one-particle Hamiltonian, the basis set $\{\varphi_\lambda\}$ that we have chosen, are no longer eigenfunctions of the Hamiltonian. This leads to scattering from one state $|\lambda\rangle$ to another state $|\lambda'\rangle$, and this in term gives rise to tunneling, or hopping, of electrons on the lattice. Thus, the hopping of electrons around on the lattice, which represents kinetic energy, originates with the crystal potential from surrounding atoms working on an electron. The details are as follows:

$$\varphi_{\alpha,\sigma,j}(\mathbf{r}_i, s_i) = \Phi^W_{\alpha,j}(\mathbf{r}_i) \cdot \chi_\sigma(s_i)$$
$$\lambda = (\alpha, \sigma, j)$$

(Note: α must be thought of as consisting of two numbers: (l,m) of a hydrogen-like atom.)

Field operator:

$$\psi_j^\dagger(\mathbf{r}_i, s_i, t) = \sum_{\alpha,\sigma} c^\dagger_{\alpha,\sigma,i}\Phi^*_{\alpha,j}(\mathbf{r}_i) \cdot \chi^*_\sigma(s_i)$$

$$\{c_{\alpha,\sigma,i}, c^\dagger_{\alpha',\sigma',i'}\} = \delta_{\alpha,\alpha'}\delta_{\sigma,\sigma'}\delta_{i,i'}$$

Other commutators are zero.

Orthogonality:

$$\sum_{\mathbf{r}} \sum_{s} \varphi^*_{\alpha,\sigma,j}(\mathbf{r}, s)\varphi_{\alpha',\sigma',j'}(\mathbf{r}, s) \cong \delta_{\alpha,\alpha'}\delta_{\sigma,\sigma'}\delta_{j,j'}$$

Completeness:

$$\sum_{\alpha,\sigma,j} \varphi^*_{\alpha,\sigma,j}(\mathbf{r}, s)\varphi_{\alpha,\sigma,j}(\mathbf{r}', s') \cong \delta_{\mathbf{r},\mathbf{r}'}\delta_{s,s'}$$

Forslag for del-overskrift.

2.6.1 Single particle Hamiltonian

$$\mathcal{H}_1 = \sum_i \left(\frac{\mathbf{p}_i^2}{2m} + U_a(\mathbf{r}_i, \mathbf{R}_i) \right) + \sum_i \sum_{j\neq i} U_a(\mathbf{r}_i, \mathbf{R}_j)$$

Since the basis-functions are assumed to be eigenfunctions of the first term, we have:

$$\sum_i \frac{\mathbf{p}_i^2}{2m} + U_a(\mathbf{r}_i, \mathbf{R}_i) \implies \sum_{\alpha,\sigma,i} \varepsilon_{\alpha,\sigma,i} c^\dagger_{\alpha,\sigma,i} c_{\alpha,\sigma,i} \tag{2.6.1}$$

Consider now the term

$$\begin{aligned}
&\sum_i \sum_{j\neq i} U_a(\mathbf{r}_i, \mathbf{R}_j) \\
\implies H_{12} &= \sum_{\lambda_1,\lambda_2} \langle\lambda_1| \sum_{j\neq i} U_a(\mathbf{r}_i, \mathbf{R}_j) |\lambda_2\rangle \, c^\dagger_{\lambda_1} c_{\lambda_2} \\
&= \sum_{\alpha_1,\sigma_1,i_1} \sum_{\alpha_2,\sigma_2,i_2} \langle\alpha_1, \sigma_1, i_1| \sum_{j\neq i_2} U_a \, |\alpha_2, \sigma_2, i_2\rangle \, c^\dagger_{\alpha_1,\sigma_1,i_1} c_{\alpha_2,\sigma_2,i_2}
\end{aligned}$$

The matrix element:

$$\begin{aligned}
&\langle\alpha_1, \sigma_1, i_1| \sum_{j\neq i_2} U_a \, |\alpha_2, \sigma_2, i_2\rangle \\
&= \sum_s \sum_{\mathbf{r}} \varphi^*_{\alpha_1,\sigma_1,i_1}(\mathbf{r}, s) \underbrace{\left[\sum_{j\neq i_2} U_a(\mathbf{r}, \mathbf{R}_j) \right]}_{\text{Sum from surrounding atoms}} \varphi_{\alpha_2,\sigma_2,i_2}(\mathbf{r}, s)
\end{aligned}$$

Here, we have used

$$\langle\mathbf{r}, s|U_a(\mathbf{r}, \mathbf{R}_j)|\mathbf{r}', s'\rangle = U_a(\mathbf{r}, \mathbf{R}_j)\delta_{\mathbf{r},\mathbf{r}'}\delta_{ss'}. \tag{2.6.2}$$

This may be simplified further, using the fact that $U_a(\mathbf{r}, \mathbf{R}_j)$ is purely electrostatic and spin-independent. We use the fact that set $\{\varphi_{\alpha,\sigma,i}(\mathbf{r}, s)\}$ factorize into a spatial part and a spin-part. Denoting the spin-independent quantity

$$\sum_j U_a(\mathbf{r}, \mathbf{R}_j) \equiv A(\mathbf{r}), \tag{2.6.3}$$

The matrix element is

$$\sum_{\mathbf{r}} \sum_{s} \Phi^{W*}_{\alpha_1,i_1}(\mathbf{r}) A(\mathbf{r}) \Phi^{W}_{\alpha_2,i_2}(\mathbf{r}) \cdot \chi^*_{\sigma_1}(s) \chi_{\sigma_2}(s). \tag{2.6.4}$$

Summing over s and using orthogonality of the χ's, we obtain

$$\langle \alpha_1, \sigma_1, i_1 | A(\mathbf{r}_i) | \alpha_2, \sigma_2, i_2 \rangle = \delta_{\sigma_1 \sigma_2} \sum_{\mathbf{r}} \Phi^{W*}_{\alpha_1,i_1}(\mathbf{r}) A(\mathbf{r}) \Phi^{W}_{\alpha_2,i_2}(\mathbf{r}) \tag{2.6.5}$$

Spin is conserved during the hopping process. The remaining spatial integration may be computed, since the crystal potential is assumed to be known, and so are the required Wannier-functions. We define the following matrix-elements:

Index i i $A(\mathbf{r}_i)$.

$$t^{\alpha_2,i_2}_{\alpha_1,i_1} \equiv \sum_{\mathbf{r}} \Phi^{W*}_{\alpha_1,i_1}(\mathbf{r}) A(\mathbf{r}) \Phi^{W}_{\alpha_2,i_2}(\mathbf{r}). \tag{2.6.6}$$

We may now write down the second-quantized version of the single-particle contribution to the Hamiltonian for lattice fermions.

$$\boxed{\mathcal{H}_1 = \sum_{\alpha\sigma i} \varepsilon_{\alpha\sigma i} c^\dagger_{\alpha\sigma i} c_{\alpha\sigma i} + \sum_{\substack{\alpha_1 i_1 \\ \alpha_2 i_2 \\ \sigma}} t^{\alpha_2,i_2}_{\alpha_1,i_1} c^\dagger_{\alpha_1\sigma_1 i_1} c_{\alpha_2\sigma_2 i_2}} \tag{2.6.7}$$

The first term is simply the energy of electrons on isolated atoms on the lattice. The second term describes spin-conserving hopping of electrons from a state (α_2, i_2) to a state (α_1, i_1). That is, electron hop from lattice site i_2 to i_1, and in the process, they may end up in a different atomic orbital α_1, than the one they started in (α_2).

$$(\alpha_1, i_1) \xleftarrow{\text{Spin is conserved}} (\alpha_2, i_2)$$

Before we consider the two-particle contribution to $\mathcal{H}_1$, let us simplify the one-particle term. First, we specialize to the important case where $\varepsilon_{\alpha\sigma i} = \varepsilon_{\alpha\sigma}$

i.e. translationally invariant system. Furthermore, we assume $\varepsilon_{\alpha\sigma}$ to be spin-independent, $\varepsilon_{\alpha\sigma} = \varepsilon_\alpha$. Further simplification is obtained by noting that only the most loosely bound electrons around an atom will be able to “escape” the atom and hop to a neighboring site. We will focus only on these electrons, which means we will focus on a small subset of orbitals α, and ignore the orbitals containing tightly bound electrons.

The simplest case is obtained by considering the case where only electrons in one particular orbital (the most loosely bound electrons) can hop from one site to the other. Then we may drop the orbital index altogether, and we have

$$\mathcal{H}_1 = \sum_{\sigma,i} \varepsilon c^\dagger_{\sigma,i} c_{\sigma i} + \sum_{\substack{i,j \\ \sigma}} t_{ij} c^\dagger_{\sigma,i} c_{\sigma,j}. \tag{2.6.8}$$

We may now set $\varepsilon = 0$ (a referecnce energy). Furthermore,

$$-t_{ij} \equiv \sum_{\mathbf{r}} \Phi_i^{W*}(\mathbf{r}) A(\mathbf{r}) \Phi_j^W(\mathbf{r}). \tag{2.6.9}$$

t_{ij} can be computed from first-principles, since A and Φ^W are known. However, we will rather consider t_{ij} as a phenomenological parameter that can be fittet to numerical or experimental results. Thus, wee finally have

$$\mathcal{H}_1 = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{\sigma i} c_{\sigma_j}. \tag{2.6.10}$$

Typically, one limits the hopping to nearest and next-nearest neighbor hopping. Note that t_{ij} in principle could be complex.

2.6.2 Two-particle Hamiltonian

Forslag for del-overskrift.

Next:

$$\sum_{ij} V_{e-e}(\mathbf{r}_i - \mathbf{r}_j) \to \sum_{\lambda_1,\ldots,\lambda_4} \langle \lambda_1 \lambda_2 | V_{e-e} | \lambda_3 \lambda_4 \rangle \, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}. \tag{2.6.11}$$

Here, $\lambda = (i, \sigma)$. No orbital index, since we are only considering one (some) orbital. We therefore need to consider the matrix element

$$\langle i_1\sigma_1\, i_2\sigma_2 | V_{e-e} | i_3\sigma_3\, i_4\sigma_4 \rangle$$
$$= \sum_{x_1,\ldots,x_4} \varphi^*_{i_1\sigma_1}(x_1) \varphi^*_{i_2\sigma_2}(x_2) V_{e-e}(x_3, x_4) \varphi_{i_3\sigma_3}(x_3) \varphi_{i_4\sigma_4}(x_4) \delta_{x_2 x_3} \delta_{x_4 x_1},$$

where $x = (\mathbf{r}, s)$. V_{e-e} is spin-independent, so

$$V_{e-e}(x_3, x_4) = V_{e-e}(\mathbf{r}_3, \mathbf{r}_4) = V_{e-e}(|\mathbf{r}_3 - \mathbf{r}_4|). \tag{2.6.12}$$

Thus, we have, after using the Kronecker-deltas and performing sums over x_3, x_4

$$\begin{aligned}\langle i_1\sigma_1\, i_2\sigma_2|V_{e-e}|i_3\sigma_3\, i_4\sigma_4\rangle \\ &= \sum_{\mathbf{r}_1}\sum_{\mathbf{r}_2} \Phi^{W*}_{i_1}(\mathbf{r}_1)\Phi^{W*}_{i_2}(\mathbf{r}_2)V_{e-e}(|\mathbf{r}_1 - \mathbf{r}_2|)\Phi^{W}_{i_3}(\mathbf{r}_2)\Phi^{W}_{i_4}(\mathbf{r}_1) \\ &\quad \cdot \sum_{s_1,s_2} \chi^*_{\sigma_1}(s_1)\chi^*_{\sigma_2}(s_2)\chi_{\sigma_4}(s_1)\chi_{\sigma_3}(s_2)\end{aligned}$$

Performing the spin-summation:

$$\sum_{s_1,s_2} \cdots \to \delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}. \tag{2.6.13}$$

Define

$$V_{i_1,i_2,i_3,i_4} \equiv \sum_{\mathbf{r}_1}\sum_{\mathbf{r}_2} \Phi^{W*}_{i_1}(\mathbf{r}_1)\Phi^{W*}_{i_2}(\mathbf{r}_2)V_{e-e}(|\mathbf{r}_1 - \mathbf{r}_2|)\Phi^{W}_{i_3}(\mathbf{r}_2)\Phi^{W}_{i_4}(\mathbf{r}_1). \tag{2.6.14}$$

This quantity expresses the Coulomb-interaction as a scattering matrix element of two electrons initially located around lattice sites (i_3, i_4) into two electrons located around lattice sites (i_1, i_2).

Depending on exactly what (i_3, i_4) and (i_1, i_2) are, this scattering element has various physical interpretations. For instance, in the same way that the single particle crystal potential could give rise to single-particle hopping, V_{e-e} may give rise to pair-hopping. Of course, V_{e-e} will also give rise to electrostatic density-density interactions.

Thus, we have the second-quantized version of the lattice Hamiltonian

$$\boxed{\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{\substack{i_1,\ldots,i_4 \\ \sigma_1,\sigma_2}} V_{i_1,\ldots,i_4} c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} c_{i_3\sigma_2} c_{i_4\sigma_1}. \qquad (2.6.15)}$$

2.6.3 Special cases in scattering matrix

Forslag for deloverskrift. De står ikke i notatene, men for ryddighets skyld kanskje fornuftig?

All i equal

Consider next special cases for $(i_1, \dots, i_4)$. We expect the largest contribution to $V_{i_1,\dots,i_4}$ when $i_1 = \dots = i_4 (= i)$. In this case, $\Phi_i^W(\mathbf{r})$ are all peaked around the same point

$$V_{iiii} = \sum_{\mathbf{r}_1} \sum_{\mathbf{r}_2} |\Phi_i^W(\mathbf{r_1})|^2 V_{e-e}(|\mathbf{r}_1 - \mathbf{r}_2|) |\Phi_i^W(\mathbf{r}_2)|^2 \equiv U_i. \tag{2.6.16}$$

Since $|\Phi_i^W|^2$ represents a density, U represents a density-density electrostatic interaction. However, there is a subtle feature pertaining to this interaction, as a result of the fact that we only consider one orbital per site: The Hamiltonian reads, considering $i_1 = i_2 = i_3 = i_4$

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\substack{i \\ \sigma_1,\sigma_2}} U_i c_{i\sigma_1}^\dagger c_{i\sigma_2}^\dagger c_{i\sigma_2} c_{i\sigma_1}. \tag{2.6.17}$$

σ_3 brukes ikke oven-for?

Since the operators $(c_{i\sigma}^\dagger, c_{i\sigma})$ create and destroy fermions, we can at most accomodate one fermion per state $|i,\sigma\rangle$. Therefore, in the operator $c_{i\sigma_1}^\dagger c_{i\sigma_2}^\dagger c_{i\sigma_2} c_{i\sigma_3}$, we must have

$$\left.\begin{aligned} \sigma_1 &= -\sigma_2 \\ \sigma_2 &= -\sigma_3 \end{aligned}\right\} \implies \sigma_3 = \sigma_1 = -\sigma_2. \tag{2.6.18}$$

Thus, upon anti-commuting $c_{i\sigma_3}$ through $c_{i\sigma_2}$ and $c_{i\sigma_2}^\dagger$, we may write this operator as

$$c_{i,\sigma_1}^\dagger c_{i,-\sigma_1}^\dagger c_{i,-\sigma_1} c_{i,\sigma_1} = c_{i,\sigma_1}^\dagger c_{i,\sigma_1} c_{i,-\sigma_1}^\dagger c_{i,-\sigma_1} = n_{i,\sigma_1} n_{i,-\sigma_1}, \tag{2.6.19}$$

where $n_{i,\sigma_1} = c_{i,\sigma_1}^\dagger c_{i,\sigma_1}$ is a number operator. Thus, the Hamiltonian becomes

$$\boxed{\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} U_i n_{i,\sigma} n_{i,-\sigma}.} \tag{2.6.20}$$

This is the so-called Hubbard-model, which we may view as an "Ising-model" of correlated fermion systems. In most cases, we consider $U_i = U$ independent of i. In that case, it may be solved exactly in one dimension. In two and higher dimensions, no exact solution exists. In fact, very little is known about the properties of this model in more than one dimension, except at a very special point. If we have one fermion pr. site, and $U \gg t_{ij}$, the properties are known, and we will investigate them. When there is more or less than one fermion pr. site on the lattice, the nature of the ground state and the excitations of the model, are not known. This model is very important in contemporary condensed matter systems. The two-dimensional version is particularily important. It serves as a paradigm model for the physics of high-temperature superconducting copper-oxides, and it also serves, with minor modifications as a model for strongly correlated topological quantum systems, i.e. systems with ground states that have a certain robustness against scattering which is protected by non-trivial topological structure in the space of eigenfunctions. The minor modification of the Hubbard model which is required to have it describe correlated topological quantum systems, is to allow the hopping amtrix element t_{ij} to become spin-dependent $t_{ij} \rightarrow t_{ij}^{\sigma\sigma'}$ and complex.

$$\boxed{\mathcal{H} = -\sum_{i,j,\sigma,\sigma'} t_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} + U \sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma}. \qquad (2.6.21)}$$

This model is often referred to as the Kane-Mele-Hubbard model, here written in a very general form since the complex and spin-dependent $t_{ij}^{\sigma\sigma'}$ is not specified. Note that so far, there is no reference to precisely what lattice this model is defined on.

In the Hubbard-model, we ignore electron-electron two-particle interactions except for when two electrons occupy the same site i (and if they do, they must have opposite spins). This is clearly a drastic simplification. Nevertheless, the model serves as a useful model if instead of computing U from first principles, we regard it as a phenomenological parameter where screening of the Coulomb potential has been taking into account. The spin-structure of the density-density interaction $Un_{i\sigma}n_{i-\sigma}$ is interesting. It gives rise to antiferromagnetism, as we will see.

The case $i_1 = i_2, i_3 = i_4$

Overskrift?

Consider next the case

$$\left.\begin{matrix} i_1 = i_2 \\ i_3 = i_4 \end{matrix}\right\} i_1 \neq i_3 \qquad\qquad \left.\begin{matrix} i_1 \rightarrow i \\ i_3 \rightarrow j \end{matrix}\right\} i \neq j.$$

We now get a contribution to the two-particle Hamiltonian given by

$$\sum_{\substack{i,j \\ \sigma_1,\sigma_2}} V_{iijj} c_{i\sigma_1}^{\dagger} c_{i\sigma_2}^{\dagger} c_{j\sigma_2} c_{j\sigma_1}. \qquad (2.6.22)$$

Again, we see that $\sigma_1 = -\sigma_2$. This term describes a hopping of a two-particle spin-singlet from site j to site i.

$$\begin{tikzcd}(\uparrow \times \downarrow)_j \arrow[rr, bend left] & & (\uparrow \times \downarrow)_i\end{tikzcd}$$

I.e. it is not a density-density interaction.

The case $i_1 = i_4, i_2 = i_3$

Consider next the case

$$\left.\begin{aligned} i_1 &= i_4 \\ i_2 &= i_3 \end{aligned}\right\} i_1 \neq i_2 \qquad\qquad \left.\begin{aligned} i_1 &\to i \\ i_2 &\to j \end{aligned}\right\} i \neq j.$$

Contribution to two-particle Hamiltonian is given by

$$\sum_{\substack{i,j \\ \sigma_1,\sigma_2}} V_{ijji} c^\dagger_{i\sigma_1} c^\dagger_{j\sigma_2} c_{j\sigma_2} c_{i\sigma_1}. \tag{2.6.23}$$

Anti-commute $c_{i\sigma_1}$ through $c_{j\sigma_2}$ and $c^\dagger_{j\sigma_2}$ to obtain

$$\sum_{\substack{i,j \\ \sigma_1,\sigma_2}} V_{ijji} n_{i\sigma_1} n_{j\sigma_2} = \sum_{i,j} V_{ijji} n_i n_j \quad ; \quad n_i = \sum_\sigma n_{i\sigma}. \tag{2.6.24}$$

This is a purely electrostatic density-density interaction with no spin-structure. (The naive expectation).

The case $i_1 = i_4, i_2 = i_3$

Consider finally the case

$$\left.\begin{aligned} i_1 &= i_3 \\ i_2 &= i_4 \end{aligned}\right\} i_1 \neq i_2 \qquad\qquad \left.\begin{aligned} i_1 &\to i \\ i_2 &\to j \end{aligned}\right\} i \neq j.$$

Contribution to the two-particle Hamiltonian given by

$$\sum_{\substack{i,j \\ \sigma_1,\sigma_2}} V_{ijij} c^\dagger_{i\sigma_1} c^\dagger_{j\sigma_2} c_{i\sigma_2} c_{j\sigma_1}. \tag{2.6.25}$$

Anti-commute $c_{i\sigma_2}$ through $c^\dagger_{j\sigma_2}$

$$-\sum_{\substack{i,j \\ \sigma_1,\sigma_2}} V_{ijij} c^\dagger_{i\sigma_1} c_{i\sigma_2} c^\dagger_{j\sigma_2} c_{j\sigma_1}. \tag{2.6.26}$$

There are no restrictions on the values that σ_1 and σ_2 can take, and so σ_1 and σ_2 may or may not be equal. When $\sigma_1 = \sigma_2$, the term $c^\dagger_{i\sigma_1} c_{i\sigma_2}$ simply counts the number of particles in spin-state σ_1 on lattice site i. If $\sigma_1 \neq \sigma_2$, then $c^\dagger_{i\sigma_1} c_{i\sigma_2}$ represents a spin-flip on site i. Let us therefore investigate this a bit further.

Consider the operator

$$\sum_{\sigma_1,\sigma_2} c^\dagger_{i\sigma_1} c_{i\sigma_2} c^\dagger_{j\sigma_2} c_{j\sigma_1}$$

$$\begin{aligned} &= c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\uparrow} && \text{(spin up - spin up)} \\ &+ c^\dagger_{i\uparrow} c_{i\downarrow} c^\dagger_{j\downarrow} c_{j\uparrow} && \text{(flip up - flip down)} \\ &+ c^\dagger_{i\downarrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\downarrow} && \text{(flip down - flip up)} \\ &+ c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{j\downarrow} c_{j\downarrow} && \text{(spin down - spin down).} \end{aligned}$$

NB! These terms clearly have a spin-structure. These operators, which are two-particle operators, work on a Hilbert-space of two-particle states $|i\sigma, j\sigma'\rangle$. $c^\dagger_{i\sigma_1} c_{i\sigma_2}$ works on the first factor, while $c^\dagger_{j\sigma_2} c_{j\sigma_1}$ works on the second factor. We next introduce a basis for "up" and "down" spin states on lattice sites i and j

“[...] which can be factored as $|i\sigma\rangle \otimes |j\sigma'\rangle$.” (For å gjøre betydningen av kommende “factor” mer tydelig.)

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.6.27}$$

$$\begin{aligned} c^\dagger_\uparrow c_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} & c^\dagger_\uparrow c_\uparrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= 0 \\ c^\dagger_\downarrow c_\downarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= 0 & c^\dagger_\downarrow c_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ c^\dagger_\uparrow c_\downarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= 0 & c^\dagger_\uparrow c_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ c^\dagger_\downarrow c_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} & c^\dagger_\downarrow c_\uparrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= 0 \end{aligned}$$

NB! Look for representation by 2×2 matrices. The task now is to find 2×2 matrices that perform these actions on $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

$$\begin{aligned} c^\dagger_\uparrow c_\uparrow &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & c^\dagger_\downarrow c_\downarrow &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ c^\dagger_\uparrow c_\downarrow &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & c^\dagger_\downarrow c_\uparrow &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \end{aligned}$$

Any 2×2-matrix may be expressed in terms of the Paul-matrices, since Pauli-matrices form a complete basis in the space of 2×2-matrices. On the other hand, we know that Pauli-matrices form a representation of spin-$\frac{1}{2}$ spin-operators (quantum spins). Since the contribution to the two-particle Hamiltonian under consideration is a product of two factors $c^\dagger_{i\sigma} c_{i\sigma'}$, it appears that this contribution essentially represent spin-spin interactions. The details are as follows: The Pauli matrices are given by

and identity matrix

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.6.28}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.6.29}$$

$$c^\dagger_\uparrow c_\uparrow = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(I + \sigma_z) \tag{2.6.30}$$

$$c^\dagger_\downarrow c_\downarrow = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(I - \sigma_z) \tag{2.6.31}$$

$$c^\dagger_\uparrow c_\downarrow = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x + i\sigma_y) = \frac{1}{2}\sigma^+ \tag{2.6.32}$$

$$c^\dagger_\downarrow c_\uparrow = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x - i\sigma_y) = \frac{1}{2}\sigma^-. \tag{2.6.33}$$

Thus, we obtain

$$\begin{aligned}
&-\sum_{\substack{i,j \\ \sigma_1,\sigma_2}} V_{ijij} c^\dagger_{i\sigma_1} c_{i\sigma_2} c^\dagger_{j\sigma_2} c_{j\sigma_1} \\
&= -\sum_{i,j} V_{ijij} \left[\frac{1}{2}(I + \sigma_{iz}) \frac{1}{2}(I + \sigma_{jz}) + \frac{1}{2}(I - \sigma_{iz}) \frac{1}{2}(I - \sigma_{jz}) \right. \\
&\qquad\qquad\qquad \left. + \frac{1}{2}\sigma_i^+ \frac{1}{2}\sigma_j^- + \frac{1}{2}\sigma_i^- \frac{1}{2}\sigma_j^+ \right] \\
&= -\sum_{i,j} \frac{V_{ijij}}{4} \left(2 + \sigma_{iz} + \sigma_{jz} + \sigma_{iz}\sigma_{jz} \right. \\
&\qquad\qquad \left. -\sigma_{iz} - \sigma_{jz} + \sigma_{iz}\sigma_{jz} + \sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+ \right) \\
&= -\sum_{i,j} \frac{V_{ijij}}{2} \left(1 + \sigma_{iz}\sigma_{jz} + \frac{1}{2}\left(\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+ \right) \right).
\end{aligned}$$

Legge inn en bemerkning på hva multiplikasjon er her? F.eks $\sigma_{iz} = \sigma_{iz} \otimes I_2$ og $2 = 2I_2 \otimes I_2$.

The first term is just a constant, which we may absorb into the single-particle site-energy term which we have used as a reference energy 0. Note how linear terms cancel!. We then finally get the contribution

$$-\sum_{i,j}\frac{V_{ijij}}{2}\left(\sigma_{iz}\sigma_{jz}+\sigma_{ix}\sigma_{jx}+\sigma_{iy}\sigma_{jy}\right)=-\sum_{i,j}\frac{V_{ijij}}{2}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j. \tag{2.6.34}$$

Introduce the spin operators: $\boldsymbol{S}=\frac{\hbar}{2}\boldsymbol{\sigma}$, and set $\hbar=1$. Then, we get

$$-\sum_{i,j}2V_{ijij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j\equiv-\sum_{i,j}J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j. \tag{2.6.35}$$

This part of the Hamiltonian is just the Heisenberg model, and we observe that the origin of the exchange interaction between spins here is rooted in Coulomb interaction V_{e-e}. Thus far, we therefore have

$$\begin{aligned}\mathcal{H}=&-\sum_{\substack{i,j\\\sigma}}t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i,\sigma}n_{i,\sigma}n_{i,-\sigma}\\&+\sum_{\substack{i,j\\\sigma}}P_{ij}c_{i,\sigma}^{\dagger}c_{i,-\sigma}^{\dagger}c_{jk,-\sigma}c_{j,\sigma}+\sum_{i,j}V_{ij}n_in_j-\sum_{i,j}J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j\quad;(i\neq j)\end{aligned}$$

with

$$\begin{array}{ll}U\equiv V_{iiii} & P_{ij}\equiv V_{iijj}\\ V_{ij}\equiv V_{ijji} & J_{ij}\equiv 2V_{ijij},\end{array}$$

Faktor to i $J_{ij} = 2V_{ijij}$ mangler i notater.

where $V_{i_1i_2i_3i_4}$ has been defined previously (see eq. (2.6.14)).

So far, we have thus considered the cases where either all $(i_1i_2i_3i_4)$ are equal, or where they are pair-wise equal. The first case means that all the four Wannier orbitals are located on the same site whereas the second case means that two Wannier orbitals are centered around one site and the other two are centered on one other site. Of course, it is possible to have cases where two Φ^W's are located on one site and the two other are located on two different other sites, or where all four Φ^W's are all located on different sites. However, such contributions to $V_{i_1i_2i_3i_4}$ will be very small due to the exponential decay of Φ^W away from their centers. We therefore ignore these contributions in what follows.

One important point to note is that J_{ij} may, depending on details, be either positive or negative. Thus, this model may give rise to both ferromagnetism or anti-ferromagnetism. For the cases where we may ignore single- and two-particle hopping (see next section) the model describes a magnetic insulator.

Ok overskrift?

2.6.4 Generalization of hopping term

A generalization of this model is obtained by letting t_{ij} become spin-dependent

$$t_{ij} \rightarrow t_{ij}^{\sigma\sigma'}. \tag{2.6.36}$$

Then, we have for the hopping term

$$\mathcal{H}_1 = -\sum_{\substack{i,j \\ \sigma,\sigma'}} t_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} \tag{2.6.37}$$

i.e. the fermions are allowed to flip spin during the hopping process, and $\uparrow$-spins could in principle hop at a different rate than $\downarrow$-spins even while conserving spins. This model is referred to as the Kane-Mele model. Even this simple model has highly non-trivial properties at least on certain special lattices in two and three dimensions, and given specific choices of $t_{ij}^{\sigma\sigma'}$.

Physical origin og spin-dependence in $t_{ij}^{\sigma\sigma'}$

The fact that $t_{ij}^{\sigma\sigma'}$ may contain elements for which $\sigma \neq \sigma'$, suggest that there is some coupling between the motion of the fermion, and its spin. From atomic physics, we know of such a coupling: Spin-orbit coupling (SOC). In a hydrogen-like atom, this coupling is of the general form

$$E_{\text{SOC}} = \lambda Z^2 \alpha^2 \frac{1}{r^3} \boldsymbol{S} \cdot \boldsymbol{L}, \tag{2.6.38}$$

where
λ is some constant determining the strength of SOC,
r is the distance of electron away from nucleus in atom,
$\boldsymbol{S}$ is the electron spin,
Z is the atomic number = # protons in nucleus.

$$\begin{aligned} \alpha &= \frac{1}{137} = \text{fine-structure constant} \\ &= \frac{e}{4\pi\epsilon_0 \hbar c}, \end{aligned}$$

which implies that SOC is a relativistic effect! ($c^{-1} > 0$). $\boldsymbol{L} = \mathbf{r} \times \boldsymbol{p}$ = angular momentum, and $\boldsymbol{p}$ is linear momentum.

The Coulomb potential $V_C = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$ gives

$$\boldsymbol{\nabla} V_C \sim \frac{1}{r^3}\mathbf{r} \simeq \gamma \boldsymbol{\sigma} \cdot (\boldsymbol{\nabla} V_C \times \boldsymbol{p}) \tag{2.6.39}$$

on general form, to leading order in $\frac{1}{c}$. The strength of SOC is determined by γ. Suppose now that we replace the Coulomb potential by the ionic crystal potential $U(\mathbf{r}_i)$. Then we get an additional piece to the Hamiltonian, given by

$$\mathcal{H}_{\text{SOC}} = \gamma\boldsymbol{\sigma}(\boldsymbol{\nabla}U \times \boldsymbol{p}) \quad ; \boldsymbol{p} = -i\hbar\boldsymbol{\nabla}, \tag{2.6.40}$$

where again, γ is some parameter giving the strength of the SOC.

$\mathcal{H}_{\text{SOC}}$ is a leading relativistic correction to the non-relativistic Hamiltonian, which wo now can second-quantize following the route we used in finding t_{ij}. Following our general recipe, we now write down the second quantized version of this, for lattice fermions

$$\langle\lambda_1|\gamma\boldsymbol{\sigma}(\boldsymbol{\nabla}U \times \boldsymbol{p})|\lambda_2\rangle = t^{\text{SOC}}_{\lambda_1\lambda_2}. \tag{2.6.41}$$

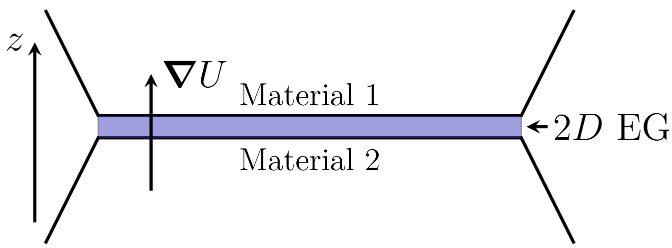
The $\boldsymbol{\sigma}$-operator works on the spin-part of the wave-function, and the matrix element factors as

$$\begin{aligned} t^{\text{SOC}}_{\lambda_1\lambda_2} &= \gamma\,\langle\sigma_1|\boldsymbol{\sigma}|\sigma_1\rangle \cdot \underbrace{\sum_{\mathbf{r}} \Phi^{W*}_{i_1}(\mathbf{r}) \left[\boldsymbol{\nabla}_{\mathbf{r}} U \times \frac{\hbar}{i}\boldsymbol{\nabla}_{\mathbf{r}}\right] \Phi^{W}_{i_2}(\mathbf{r})}_{\equiv \mathbf{R}_{i_1 i_2}} \\ &= t^{\sigma_1\sigma_2}_{i_1 i_2} = \gamma\left[\sigma^z_{\sigma_1\sigma_2}R^z_{i_1i_2} + \sigma^x_{\sigma_1\sigma_2}R^x_{i_1i_2} + \sigma^y_{\sigma_1\sigma_2}R^y_{i_1i_2}\right]. \end{aligned}$$

On matrix form, using the standard representation of the spin-operators,

$$t^{\text{SOC}}_{i_1i_2} = \gamma\begin{pmatrix} R^z_{i_1i_2} & R^x_{i_1i_2} + iR^y_{i_1i_2} \\ R^x_{i_1i_2} - iR^y_{i_1i_2} & -R^z_{i_1i_2} \end{pmatrix}. \tag{2.6.42}$$

This should be added to the usual spin-independent hopping term. To proceed further and compute $\mathbf{R}_{i_1i_2}$, we must specify $\boldsymbol{\nabla}U$. A simple model which is often used is one appropriate for a two-dimensional electron gas living at the interface of two different materials in a sandwich heterostructure.



In this case, there will typically be a $\boldsymbol{\nabla}U = \frac{\partial U}{\partial z}\hat{e}_z$ perpendicular to the plane of motion, which is in the (x, y)-plane. Let us approximate

$$\frac{\partial U}{\partial z} = E = \text{constant} \implies \boldsymbol{\nabla}U = E\hat{z}. \tag{2.6.43}$$

The motion is in the (x, y)-plane, i.e.

$$\boldsymbol{p} = p_x \hat{e}_x + p_y \hat{e}_y. \tag{2.6.44}$$

This model for spin-orbit coupling is often called Rashba spin-orbit coupling. In this case, $\mathbf{R}_{i_1 i_2}$ is a vector in the (x, y)-plane, such that $R^z_{i_1 i_2} = 0$.

Problems

Problem 2.1. In class, we have seen how to formulate a second-quantized version of the Hamiltonian of a non-relativistic many-particle system in a general basis,

$$\mathcal{H} = \sum_{\lambda_1,\lambda_2} \varepsilon_{\lambda 1,\lambda_2}\ c^\dagger_{\lambda_1} c_{\lambda_2} + \sum_{\lambda_1,\lambda_2\lambda_3,\lambda_4} v_{\lambda_1,\lambda_2\lambda_3,\lambda_4}\ c^\dagger_{\lambda_1}\ c^\dagger_{\lambda_2} c_{\lambda_3}\ c_{\lambda_4}$$

where $\varepsilon_{\lambda_1,\lambda_2}$ and $v_{\lambda_1,\lambda_2\lambda_3,\lambda_4}$ are matrix elements of the one-particle and two-particle contributions to the Hamiltonian, computed using a complete set of basis functions $\{\phi_\lambda(x)\}$.

a) Write down an expression for the Hamitonian in a general basis for the case where the system is materially open and coupled to particle reservoir. (In the above version, it is materially closed).

b) Give an explicit form of this Hamiltonian using a Bloch-basis for $\{\phi_\lambda(x)\}$

$$\phi_\lambda(x) = \phi_{\mathbf{k},\sigma}(\mathbf{r}, s) = \frac{1}{\sqrt{V}}\ e^{i\mathbf{k}\cdot\mathbf{r}}\ u_{\mathbf{k}}(\mathbf{r})\ \chi_\sigma(s)$$

in the notation used in class. (Hint: The Bloch functions may be taken to be eigenfunctions of the one-particle problem).

Problem 2.2. Show by an explicit calculation that the following relations hold for the spin-part of the wavefunction $\chi_\sigma(s)$ of $S = 1/2$ particles:

$$\sum_\sigma \chi^*_\sigma(s)\chi_\sigma(s') = \delta_{s,s'}$$
$$\sum_s \chi^*_\sigma(s)\chi_{\sigma'}(s) = \delta_{\sigma,\sigma'}$$

Problem 2.3. Consider the following two-body potential that could enter into the two-particle contribution to a many-body Hamiltonian

$$V(\mathbf{r}) = V(r) = \frac{A}{r}\ \exp(-r/\lambda_{TF})$$

Compute the Fourier-transform of this potential. Give an interpretation of the quantity λ_{TF}. Here A is a dimensionful constant that we need not specify further.

Problem 2.4. Consider a tight binding Hamiltonian with nearest-neighbor hopping on a general two dimensional Bravais lattice with N lattice points, in contact with a particle reservoir. The chemical potential of the system is denoted μ. The nearest-neighbor hopping element is given by t. The Hamiltonian is given by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}$$

Here, $(c^\dagger_{i,\sigma}, c_{i,\sigma})$ create and destroy particles in spin-state σ on site i. Introduce Fourier-transformed operators

$$c^\dagger_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i c^\dagger_{i,\sigma} \; \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_i}$$
$$c_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i c_{i,\sigma} \; \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_i}$$

where $\mathbf{r}_i$ is the position at lattice site i.

a) Show that Hamiltonian may be written on form

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} \; c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

and give an expression for $E_{\mathbf{k}}$ for a general two-dimensional Bravais lattice.

Missing fig: Square lattice

b) Specialize to the case of a two-dimensional square lattice, see Figure **??**, and give the expression for $E_{\mathbf{k}}$ in this case.

c) Imagine that we now consider a model on a *honeycomb* lattice, see Figure **??**. Explain what the *principal* difference between this lattice and the square lattice is.

Missing fig: Honeycomb lattice

d) Write down a tight-binding model for this system, conidering only nearets neighbor interactions, and find $E_{\mathbf{k}}$. (Hint: You need to introduce two distinct types of fermions, one type for the red atoms and one type for the blue atoms).

Problem 2.5. Consider a tight-binding model in a uniform external magnetic field h directed along the z-direction. The Hamiltonian is given by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} - h \sum_{i,\sigma} \sigma c^\dagger_{i\sigma} c_{i\sigma}$$

in the same notation as in Problem 1. The last term is the second-quantized version of the Zeeman-term $-\mathbf{h} \cdot \mathbf{S} = -h \sum_i S_{iz} = -h \sum_i \left[c^\dagger_{i,\uparrow} c_{j,\uparrow} - c^\dagger_{i,\downarrow} c_{j,\downarrow} \right] = -h \sum_{i,\sigma} \sigma c^\dagger_{i\sigma} c_{i\sigma}$.

a) Introduce the same Fourier-transform as in Problem 1, and show that the Hamiltonian may be written on the form

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k},\sigma} \; c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

and give an expression for $E_{\mathbf{k},\sigma}$ for a general two-dimensional Bravais lattice.

b) Consider instead another variant of the tight-binding model, now in the absence of a magnetic field, but with a spin-dependent hopping matrix element. (In lectures Week 4, we discuss what the origin of such spin-dependent hopping could be). The Hamiltonian is given by, with a general spin-dependent hopping matrix element $t_{ij}^{\sigma\sigma'}$

$$\mathcal{H} = - \sum_{\langle i,j \rangle, \sigma, \sigma'} t_{ij}^{\sigma\sigma'} c^\dagger_{i,\sigma'} c_{j,\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}$$

Consider a special case $t_{ij}^{\sigma\sigma'} = t_{ij}^{\sigma\sigma} \delta_{\sigma,\sigma'}$, with $t_{ij}^{\uparrow\uparrow} \neq t_{ij}^{\downarrow\downarrow}$. Introduce the same Fourier-transform as in Problem 1, and show that the Hamiltonian may be written on the form

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k},\sigma} \; c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

and give an expression for $E_{\mathbf{k},\sigma}$ for a general two-dimensional Bravais lattice.

c) Compare with the results in Problem 2 **a)**, and show that this sort of spin-dependent hopping may be interpreted as particles moving in a $\mathbf{k}$-dependent external magnetic field along the z-axis.

Problem 2.6. A non-interacting electron gas has a Hamiltonian which in a grand canonical ensemble may be written on the form

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) \; c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

where $\varepsilon_{\mathbf{k}}$ is the single-particle excitation energy and μ is a chemical potential. Let us now subject this system to magnetic field directed along, say, the $\hat{z}$-axis. This adds a term $-\mathbf{B} \cdot \mathbf{S}$ to the Hamiltonian. Here, $\mathbf{S}$ is the total spin of the system, $\mathbf{S} = \sum_i \mathbf{S}_i$ for spins $\mathbf{S}_i$ on lattice site i. We have seen in HW # 2 that $\mathcal{H}$ may be written on the form

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu_\sigma) \; c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

where $\mu_\sigma = \mu + \sigma B$.

a) Denote the spin-dependent density of states of this system by $D_\sigma(\omega)$, where

$$D_\sigma(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \delta(\omega - (\varepsilon_{\mathbf{k}} - \mu_\sigma))$$

Let $\varepsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$. Compute $D_\sigma(\omega)$ in 2 and 3 dimensions. (Hint: Convert the summation over $\mathbf{k}$ to a d-dimensional integral

$$\sum_{\mathbf{k}} \to (L/a)^d \int d^d k / (2\pi)^d$$

Here N is the number of lattice sites, a is the lattice constant of the lattice, and L is the sidelength of the volume V of the system, $V = L^d$.)

b) Compute the zero-temperature magnetization of this system, $M = N_\uparrow - N_\downarrow$, where N_σ is the total number of particles with spin σ in the system. (Hint: Here you must invoke the Pauli principle and occupy states up to some maximum energy, say ε_F, which will determine the total number of particles $N = N_\uparrow + N_\downarrow$ in the system. Express therefore your answer also in terms of ε_F.)

Problem 2.7. Consider a $S = 1/2$ fermionic tight-binding model on a two-dimensional square lattice with N lattice sites, describing a spin-orbit coupled system in an external magnetic field, given by the Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} -t & s_{ij}^{\uparrow\downarrow} \\ s_{ij}^{\downarrow\uparrow} & -t \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{pmatrix} - \sum_{i\sigma} \mu_\sigma n_{i\sigma}$$

Here, $\langle i, j \rangle$ denotes that i and j are nearest neighbor lattice sites on the square lattice. μ_σ is the chemical potential for particles with spin σ, $c_{i,\sigma}^+, c_{i,\sigma}$ are fermionic creation and destruction operators, and $n_i = \sum_\sigma n_{i\sigma}$ are number operators, $n_{i\sigma} = c_{i,\sigma}^+ c_{i,\sigma}$. t represents a nearest-neighbor hopping without spin-flip in the hopping process, while $s_{ij}^{\uparrow\downarrow} = (s_{ji}^{\downarrow\uparrow})^*$ represents a nearest-neighbor spin-flipping hopping elements (spin-orbit coupling) which depend on the direction of the vector that connects lattice site i with lattice site i, $s_{ij}^{\downarrow\uparrow} = s_{i,i+\delta}^{\downarrow\uparrow} = s_\delta$ where δ is a unit vector in x- or y-direction. For Rashba spin-orbit coupling (see lecture notes Week 4), we set $s_{\pm\hat{x}} = \mp i\eta$ and $s_{\pm\hat{y}} = \pm\eta$.

a) Introduce Fourier-transformed fermion operators

$$c_{\mathbf{k},\sigma}^+ = \frac{1}{\sqrt{N}} \sum_i c_{i,\sigma}^+ e^{-i\mathbf{k}\cdot\mathbf{r}_i}$$
$$c_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i c_{i,\sigma} e^{i\mathbf{k}\cdot\mathbf{r}_i}$$

where $\mathbf{r}_i$ is the position on the lattice corresponding to lattice site i. Show that the Hamitonian given above may be written on the form

$$\mathcal{H} = \sum_{\mathbf{k}} \begin{pmatrix} c_{k\uparrow}^\dagger & c_{k\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} \varepsilon_{\mathbf{k}} - \mu - h & \gamma_{\mathbf{k}} \\ \gamma_{\mathbf{k}}^* & \varepsilon_{\mathbf{k}} - \mu + h \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix}$$

and give expressions for $\varepsilon_{\mathbf{k}}, \gamma_{\mathbf{k}}, \gamma_{\mathbf{k}}^*$ as well as μ and h, in terms of the parameters of the Hamiltonian.

b) This Hamiltonian may further be diagonalized in terms of new fermion operators $\alpha_{\mathbf{k}}^\pm$ and $\alpha_{\mathbf{k}}^{\dagger\pm}$. Show, by introducing the unitary transformation

$$S = \frac{1}{\sqrt{r_{\mathbf{k}}^2 + |\gamma_{\mathbf{k}}|^2}} \begin{pmatrix} r_{\mathbf{k}} & \gamma_{\mathbf{k}} \\ \gamma_{\mathbf{k}}^* & -r_{\mathbf{k}} \end{pmatrix}$$

that the Hamiltonian may be written on the form

$$\begin{aligned}
\mathcal{H} &= \sum_{\mathbf{k}} \begin{pmatrix} c_{k\uparrow}^\dagger & c_{k\downarrow}^\dagger \end{pmatrix} SS^{-1} \begin{pmatrix} \varepsilon_{\mathbf{k}} - \mu - h & \gamma_{\mathbf{k}} \\ \gamma_{\mathbf{k}}^* & \varepsilon_{\mathbf{k}} - \mu + h \end{pmatrix} SS^{-1} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} \\
&= \sum_{\mathbf{k}} \left[E_{\mathbf{k}}^{+} \; \alpha_{\mathbf{k}}^{\dagger +} \alpha_{\mathbf{k}}^{+} + E_{\mathbf{k}}^{-} \; \alpha_{\mathbf{k}}^{\dagger -} \alpha_{\mathbf{k}}^{-} \right]
\end{aligned}$$

and give expressions for $E_{\mathbf{k}}^{\pm}$. Here, $r_{\mathbf{k}} = -h + \sqrt{h^2 + |\gamma_{\mathbf{k}}|^2}$.

c) The spectrum of these particles in general have global minima at four distinct finite $\mathbf{k}$, provided that the Zeeman-field is not too large. Give a physical interpretation of the fact that the lowest energy state is located at these finite wave-vectors (momenta). (Hint: Think about what a state with a finite momentum represents).

CHAPTER 3

MAGNETIC INSULATORS AND MAGNONS

3.1 From the Hubbard-model to the quantum antiferromagnetic Heisenberg model.

We now return to the Hubbard model and consider this in a special, but important, limit.

The general starting point is:

$$\begin{aligned}\mathcal{H} = &\sum_{\lambda_1,\lambda_2} \langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle\, c^\dagger_{\lambda_1} c_{\lambda_2} \\ &+ \sum_{\substack{\lambda_1,\lambda_2,\\ \lambda_3,\lambda_4}} \langle\lambda_1\lambda_2|\mathcal{H}_2|\lambda_3\lambda_4\rangle\, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}\end{aligned} \tag{3.1.1}$$

Lattice fermions:

i) One type of fermions

ii) Lattice translational invariance (discrete)

iii) One orbital pr. site and at most two fermions pr. site

Under such circumstances the Hamiltonian takes the form:

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{\substack{i_1,i_2,i_3,i_4\\ \sigma_1,\sigma_2}} \langle i_1 i_2|V|i_3 i_4\rangle \cdot c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} c_{i_3\sigma_3} c_{i_4\sigma_4} \tag{3.1.2}$$

Further simplifications

iv) Nearest-neighbor hopping only ($t_{ij} = t$)

v) Hubbard interaction only ($i_1 = i_2 = i_3 = i_4, V_{iiii} = U$)

vi) $\boxed{U/t \gg 1}$ NB!!

This gives:

$$\mathcal{H} = -t \sum_{\substack{\langle i,j \rangle \\ \sigma}} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma} \tag{3.1.3}$$

$$n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} \tag{3.1.4}$$

The Hubbard model, as written above, is valid for arbitrary ratio U/t, but we will consider it in the case $U/t \gg 1$, where the fermions are said to be strongly correlated.

vii) We now study the model at half-filling. That is, the number of fermions on the lattice is N, where N is the # of lattice points. On average, there is one fermion pr. lattice site. The lattice is therefore half-filled, since the maximum # fermions on the lattice is $2N$.

Since $U/t \gg 1$, we regard the unperturbed Hamiltonian $\mathcal{H}_0$ to be

$$\mathcal{H}_0 = U \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} \tag{3.1.5}$$

This problem is easy to solve exactly, since it is completely local (it can be solved for each site independently).

We will regard the hopping term as a perturbation.

Unperturbed ground state:

$$\mathcal{H}_0 \left|\psi_0\right\rangle = E_0 \left|\psi_0\right\rangle \tag{3.1.6}$$

$E_0 = 0$

$\left|\psi_0\right\rangle$: One fermion on each lattice site. Massively degenerate, since the distribution of $\uparrow$ and $\downarrow$ does not matter.

$N_f = N_{f\uparrow} + N_{f\downarrow} = N$

$N_{f\uparrow} = N_{f\downarrow} = N/2$

N_f: # fermions

$N_{f\uparrow}$: # fermions with spin $\uparrow$

$N_{f\downarrow}$: # fermions with spin $\downarrow$

$|\psi_0\rangle$: linear combination of states like $|\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow \ldots\rangle$ with equally many $\uparrow$ and $\downarrow$.

There are 2^N such states. From degenerate perturbation theory: Find specifi linear combination of these 2^N states that changes little when perturbation is introduced. Imagine that we have found this. Call this state $|\psi_0\rangle$ from now on.

$$\mathcal{H}_{\text{hop}} = -\sum_{\substack{\langle i,j\rangle \\ \sigma}} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} : \qquad \text{Perturbation.} \tag{3.1.7}$$

1. order correction to E_0:

$$\begin{aligned} \Delta E^{(1)} &= \langle\psi_0|\mathcal{H}_{\text{hop}}|\psi_0\rangle & (3.1.8) \\ &= -\sum_{\substack{\langle i,j\rangle \\ \sigma}} t_{ij} \langle\psi_0|c^\dagger_{i\sigma} c_{j\sigma}|\psi_0\rangle & (3.1.9) \end{aligned}$$

$c^\dagger_{i\sigma} c_{j\sigma} |\psi_0\rangle$: A state where i is double occupied and j is unoccupied. This new state is orthogonal to $|\psi_0\rangle \implies \Delta E^{(1)} = 0$.

2. order correction to E_0:

$$\Delta E^{(2)} = \frac{\langle\psi_0|\mathcal{H}_{\text{hop}}|n\rangle \langle n|\mathcal{H}_{\text{hop}}|\psi_0\rangle}{E_0 - E_n} \tag{3.1.10}$$

$|n\rangle$: Some intermediate excited eigenstate of $\mathcal{H}_0$:

$$\mathcal{H}_0 |n\rangle = E_n |n\rangle . \tag{3.1.11}$$

Which $|n\rangle$ will contribute to $\Delta E^{(2)}$? They must be such that

$$\langle\psi_0|\mathcal{H}_{\text{hop}}|n\rangle \neq 0 \tag{3.1.12}$$

$$-\sum_{\substack{\langle i,j\rangle \\ \sigma}} t_{ij} \langle\psi_0|c^\dagger_{i\sigma} c_{j\sigma}|n\rangle \neq 0 \tag{3.1.13}$$

$$c^\dagger_{i\sigma} c_{j\sigma} |n\rangle \sim |\psi_0\rangle \tag{3.1.14}$$

This means that $|n\rangle$ has to be a state with site j doubly occupied and site i unoccupied, thus $E_n = U + E_0 = U$.

Hence:

$$\Delta E^{(2)} = -\frac{1}{U}\sum_n \langle\psi_0|\mathcal{H}_{\text{hop}}|n\rangle\ \langle n|\mathcal{H}_{\text{hop}}|\psi_0\rangle \tag{3.1.15}$$

$$= -\frac{1}{U}\ \langle\psi_0|\mathcal{H}^2_{\text{hop}}|\psi_0\rangle \tag{3.1.16}$$

Thus, $\Delta E^{(2)}$ is equivalent to a first-order correction to E_0 from an effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = -\frac{1}{U}\mathcal{H}^2_{\text{hop}} \tag{3.1.17}$$

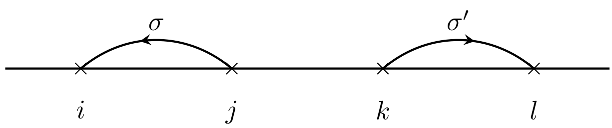
Since $\mathcal{H}_{\text{eff}}$ is the product of two one-particle Hamiltonians, it is in fact a two-particle Hamiltonian. Let us consider this in some more detail.

$$\mathcal{H}_{\text{eff}} = -\frac{1}{U}\sum_{\langle i,j\rangle,\sigma}\sum_{\langle l,k\rangle,\sigma'} t_{ij}t_{lk}\ c^\dagger_{i\sigma}c_{j\sigma}\ c^\dagger_{l\sigma'}c_{k\sigma'} \tag{3.1.18}$$

A non-zero correction to the ground-state requires certain restrictions on (i,j) and (l,k). Namely, <u>after</u> $c^\dagger_{i\sigma}c_{j\sigma}\ c^\dagger_{l\sigma'}c_{k\sigma'}$ has acted on $|\psi_0\rangle$, the resulting state must $\sim |\psi_0\rangle$,

$$c^\dagger_{i\sigma}c_{j\sigma}\ c^\dagger_{l\sigma'}c_{k\sigma'}\,|\psi_0\rangle \sim |\psi_0\rangle\,. \tag{3.1.19}$$

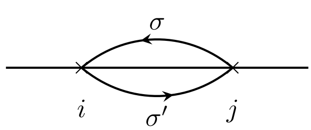
<u>In general:</u>



$$\langle\psi_0|\mathcal{H}^2_{\text{hop}}|\psi_0\rangle \neq 0 \quad \text{requires} \tag{3.1.20}$$

$$i = k, \quad l = j \implies t_{ij}t_{lk} \to t_{ij}t_{ji} = t_{ij}t^*_{ij} = |t_{ij}|^2 \geq 0 \tag{3.1.21}$$

That is, two fermions (one with spin σ, the other with spin σ') is swapped between sites i and j



This process is an exchange-process.

Now, we have

$$\mathcal{H}_{\text{eff}} = -\frac{1}{U}\sum_{\substack{i,j\\ \sigma,\sigma'}} |t_{ij}|^2 c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} \tag{3.1.22}$$

$$= -\frac{1}{U}\sum_{\substack{i,j\\ \sigma,\sigma'}} |t_{ij}|^2 c^\dagger_{i\sigma} c_{i\sigma'} (\delta_{\sigma\sigma'} - c^\dagger_{j\sigma'} c_{j\sigma}) \tag{3.1.23}$$

The first term just contributes to the single-site energy. Absorb the first in the site-energy.

The remaining term is then

$$\mathcal{H}_{\text{eff}} = \frac{1}{U}\sum_{\substack{\langle i,j\rangle\\ \sigma,\sigma'}} |t_{ij}|^2 c^\dagger_{i\sigma} c_{i\sigma'} c^\dagger_{j\sigma'} c_{j\sigma} \tag{3.1.24}$$

Such an operator, we have already studied, and we know that, apart from an additive constant which we absorb in a reference zero-point of energy, it may be written as a spin-spin interaction

$$\mathcal{H}_{\text{eff}} = \frac{4}{\hbar^2 U}\frac{1}{2}\sum_{i,j} |t_{ij}|^2 \mathbf{S}_i \cdot \mathbf{S}_j \tag{3.1.25}$$

where $\mathbf{S}_i = (S_{ix}, S_{iy}, S_{iz})$ are spin-operators $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$.

$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$: Pauli-matrices (SU(2)-matrices: 2x2 unitary matrices with determinant = 1)

$$[S_{ix}, S_{jy}] = i\frac{\hbar}{2} S_{iz}\delta_{ij} \text{ etc: Quantum spins.} \tag{3.1.26}$$

$$\text{Define} \quad J_{ij} \equiv -\frac{2|t_{ij}|^2}{\hbar^2 U} < 0 \tag{3.1.27}$$

$$\underline{\mathcal{H}_{\text{eff}} = -\sum_{\langle i,j\rangle} J_{ij}\mathbf{S_i}\cdot\mathbf{S_j}} \tag{3.1.28}$$

Since $J_{ij} < 0$ in this case, it favors spins that are anti-parallell on neighboring lattice sites. This hints at the existence of antiferromagnetism in such strongly correlated fermion-systems, at least close to half-filling.

$\mathcal{H}_{\text{eff}}$ should be regarded as the effective low-energy Hamiltonian of the Hubbard-model in the strong-coupling limit $U/t \gg 1$, at half-filling. There are no terms in $\mathcal{H}_{\text{eff}}$ that describes single-particle hopping processes on the lattice. There are no itinerant fermions in this low-energy model. It therefore describes a quantum antiferromagnetic insulator. The crucial feature that contributes to this fact, is that the system is assumed to be at 1/2-filling.

Let us also give a heuristic argument for why the Hubbard model, at 1/2-filling in the strongly coupled regime, gives rise to antiferromagnetism.

Localizing electrons on individual sites means that their wavefunctions are packed together tightly around the sites. Thus, they must contain many Fourier-components. This costs much kinetic energy. To lower this energy, it is advantageous to spread the wavefunctions out in space. This is facilitated by hopping to neighboring sites. To facilitate hopping, this means that spins on neighboring sites must have opposite spins (recall that we are at 1/2-filling). Therefore, antiferromagnetic order will facilitate this hopping to a maximum extent.

- Coulomb interactions give rise to ferromagnetism (Hund's rule)

- Kinetic energy gives rise to antiferromagnetism

It is a matter of detail which effect will dominate, and this explains the existence of ferromagnetism in some compounds, and antiferromagnetism in other compounds

$$\mathcal{H} = -\sum_{i,j} J_{ij}^{\text{tot}} \mathbf{S_i} \cdot \mathbf{S_j} \tag{3.1.29}$$

$$J_{ij}^{\text{tot}} = -\frac{2|t_{ij}|^2}{U} + A\sum_{\mathbf{k}} \frac{|I_{ij}|^2}{k^2} \tag{3.1.30}$$

$$I_{jk}(\mathbf{k}) = \sum_{\mathbf{r}} \phi_i^*(\mathbf{r})\phi_j(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{3.1.31}$$

$$A = \frac{e^2}{\Omega_d \varepsilon_0} \tag{3.1.32}$$

3.2 Second quantization for bosons

Setting up a second-quantized version of a Hamiltonian for bosons follows much of the same path as for fermions. Again, we define creation and destruction operators for states with q.n.'s λ

$$a_\lambda^\dagger |0\rangle = |\lambda\rangle \quad ; \; a_\lambda |n_\lambda\rangle \sim |n_\lambda - 1\rangle \tag{3.2.1}$$

$$(a_\lambda^\dagger)^{n_\lambda} \sim |n_\lambda\rangle \; ; \; a_\lambda |0\rangle = 0 \tag{3.2.2}$$

Main difference from fermions: it is allowed to occupy a single-particle state with an arbitrary number of particles.
Commutation relations:

$$[a_\lambda, a_{\lambda'}^\dagger] = \delta_{\lambda\lambda'} \tag{3.2.3}$$

$$[a_\lambda, a_{\lambda'}] = 0 \tag{3.2.4}$$

$$[a_\lambda^\dagger, a_{\lambda'}^\dagger] = 0 \tag{3.2.5}$$

$$([A, B] \equiv AB - BA) \tag{3.2.6}$$

Field operator:

$$\left.\begin{array}{ll} A^\dagger(x,t) & = \sum_\lambda a_\lambda^\dagger \varphi_\lambda^*(x) \\ A(x,t) & = \sum_\lambda a_\lambda \varphi_\lambda(x) \end{array}\right\} \quad [A(x,t), A^\dagger(x',t)] = \delta_{x,x'} \tag{3.2.7}$$

$\{\varphi_\lambda(x)\}$: Complete set of functions which may be chosen conveniently, precisely as in the fermionic case.

The general form of the Hamiltonian is identical in form to the fermionic case:

$$\boxed{\mathcal{H} = \sum_{\lambda_1,\lambda_2} \varepsilon_{\lambda_1,\lambda_2} a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger + \sum_{\lambda_1,\ldots,\lambda_4} V_{\lambda_1\ldots\lambda_4} a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger a_{\lambda_3} a_{\lambda_4}} \tag{3.2.8}$$

NB!! The above form holds for bosons that are material particles, for instance Helium-4 atoms or cold-atom systems such as Rb^{87}. Bosons could also be non-material and interacting. An example would be quantized lattice vibrations, i.e. phonons. For such systems, one could have interaction terms with an unequal number of creation and destruction operators. Such interaction terms do not conserve number of particles (Examples of this would be quantized anharmonic lattice vibrations, or quantum spin-fluctuations beyond linear spin-wave theory. We will consider such cases in the following).

An important application of this will be in studying quantized lattice vibrations and how they couple to electrons. Another important application is in the study of the low-temp. properties of quantum spin-systems.

3.3 Low temperature properties of magnetic insulators

We will consider fluctuation effects in quantum spin models of localized spins, i.e. magnetic insulators. In order to do this, we will consider spin-fluctuations that are small around some ordere state. Under such circumstances, we may find convenient representations of spin-operators in terms of boson-operators.

We will consider two main cases:

i) Ferromagnetic insulators described by a Hamiltonian

$$\mathcal{H} = -\sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad J_{ij} > 0 \tag{3.3.1}$$

with a ground state where spins are ordered in parallell to each other. For the most part, we consider nearest-neighbor interactions.

ii) Antiferromagnetic insulators on a biparticle lattice, described by

$$\mathcal{H} = -\sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad J_{ij} < 0 \tag{3.3.2}$$

with a classical ground state where spins are ordered oppositely on neighboring lattice points. A simple biparticle lattice would be a 2D square lattice or a 3D cubic lattice. Again, for the most part, we consider nearest-neighbor spin-spin interactions. Including longer range interactions is no essential complication.

The spin-operators for $S = 1/2$ spins satisfy the following commutation relations:

$$[S_{ix}, S_{jy}] = i\hbar S_{iz} \delta_{ij} \tag{3.3.3}$$

+ cyclic permutations, which may be written more compactly as

$$[S_{i\alpha}, S_{j\beta}] = i\hbar \varepsilon_{\alpha\beta\gamma} \delta_{j\gamma} \delta_{ij} \tag{3.3.4}$$

$(\alpha, \beta, \gamma) \in (x, y, z)$ and $\varepsilon_{\alpha\beta\gamma}$ is the totally anti-symmetric tensor (Levi-Civita tensor). We will set $\hbar = 1$ in the following.

3.3.1 Ferromagnetic case

We assume that all spins are nearly completely ordered along the z-axis, and will introduce a boson-operator representation of the spins under this assumption. This representation must give correct commutation relations for spins.

$$S_{iz} = S - a_i^\dagger a_i, \quad S = 1/2 \tag{3.3.5}$$

Introduce $S_{i\pm} = S_{ix} \pm iS_{iy}$. These are spin-flip operators

$$S_+ \left|\downarrow\right\rangle = \left|\uparrow\right\rangle \tag{3.3.6}$$

$$S_- \left|\uparrow\right\rangle = \left|\downarrow\right\rangle \tag{3.3.7}$$

$$S_{i+} = \sqrt{2S}\left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2} a_i \tag{3.3.8}$$

$$S_{i-} = \sqrt{2S}\left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2} a_i^\dagger = (S_{i+})^\dagger \tag{3.3.9}$$

The assumption of nearly-ordered spins is equivalent to the statement that we can approximate the boson-representation of spins by ignoring all terms beyond quadratic order in boson-operators.

$$S_{iz} = S - a_i^\dagger a_i \tag{3.3.10}$$

$$\left.\begin{array}{l} S_{i+} \approx \sqrt{2S} a_i \\ S_{i-} \approx \sqrt{2S} a_i^\dagger \end{array}\right\} \text{corrections to this involve cubic terms in } a, a^\dagger \tag{3.3.11}$$

$(a, a^\dagger)$: Satisfy boson comm. relations. Consider the nearest-neighbor case.

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{3.3.12}$$

$$= -J \sum_{\langle i,j \rangle} [S_{iz}S_{jz} + S_{ix}S_{jx} + S_{iy}S_{jy}] \tag{3.3.13}$$

$$= -J \sum_{\langle i,j \rangle} [S_{iz}S_{jz} + S_{i+}S_{j-}] \tag{3.3.14}$$

$$\approx -J \sum_{\langle i,j \rangle} [(S - a_i^\dagger a_i)(S - a_j^\dagger a_j) + 2S a_i a_j^\dagger] \tag{3.3.15}$$

$$\approx -J \sum_{\langle i,j \rangle} [S^2 - S(a_i^\dagger a_i + a_j^\dagger a_j) + 2S a_j^\dagger a_i] \tag{3.3.16}$$

With no spin-fluctuations present, we ignore terms involving boson-operators. In that case

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S^2 \tag{3.3.17}$$

which is simply the ground-state energy. Let us denote it by E_0, and use it as our reference energy ($E_0 \to 0$). Thus, we consider only the fluctuation part of the Hamiltonian from now.

$$\mathcal{H} = 2SJ \sum_{\langle i,j \rangle} (a_i^\dagger a_i - a_i^\dagger a_j); \;\; J > 0 \tag{3.3.18}$$

Missing figure: Nearest-neighbor hopping

$$a_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} a_k^\dagger \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_i} \tag{3.3.19}$$

$$a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} a_k \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_i} \tag{3.3.20}$$

We must next insert these representations into $\mathcal{H}$. $(a, a^\dagger)$ destroy and create quantized spin-fluctuations: magnons.

$$\sum_{\langle i,j \rangle} a_i^\dagger a_j = \sum_{\mathbf{r_i}} \sum_{\delta} \frac{1}{N} \sum_{\mathbf{k}_1} \sum_{\mathbf{k}_2} a_{k_1}^\dagger \mathrm{e}^{i\mathbf{k}_1\mathbf{r}_i} a_{k_2} \mathrm{e}^{-i\mathbf{k}_2\mathbf{r}_j} \tag{3.3.21}$$

$$= \frac{1}{N} \sum_{\mathbf{k}_1} \sum_{\mathbf{k}_2} a_{k_1}^\dagger a_{k_2} \underbrace{\sum_{\mathbf{r}_i} \mathrm{e}^{i(\mathbf{k}_1 - \mathbf{k}_2)\cdot\mathbf{r}_i}}_{=N\delta_{\mathbf{k}_1,\mathbf{k}_2}} \underbrace{\sum_{\delta} \mathrm{e}^{-i\mathbf{k}_2\cdot\delta}}_{\equiv\gamma(\mathbf{k}_2)} \tag{3.3.22}$$

$$= \sum_{\mathbf{k}} \gamma(\mathbf{k}) a_k^\dagger a_k \tag{3.3.23}$$

$$\sum_{\langle i,j \rangle} a_i^\dagger a_i = z \sum_{\mathbf{k}} a_k^\dagger a_k \tag{3.3.24}$$

$$\mathcal{H} = 2SJ \sum_{\mathbf{k}} [z - \gamma(\mathbf{k})] a_k^\dagger a_k \tag{3.3.25}$$

$$= \underline{\underline{\sum_{\mathbf{k}} \omega_k a_k^\dagger a_k}} \implies \text{Non-interacting Boson-gas} \tag{3.3.26}$$

$$\omega_k = \underline{\underline{2SJ(z - \gamma(\mathbf{k}))}} \quad \text{Determined by J and lattice structure} \tag{3.3.27}$$

$$z = \#\text{ vectors } \delta \text{ included in } \gamma(\mathbf{k}). \tag{3.3.28}$$

$$\gamma(\mathbf{k}) = \sum_{\delta} \mathrm{e}^{i\mathbf{k}\cdot\delta} \tag{3.3.29}$$

$$= \gamma(-\mathbf{k}) \tag{3.3.30}$$

$$\gamma(0) = z, \text{ since } \sum_{\delta} \cdot 1 = z \tag{3.3.31}$$

$$\gamma(\mathbf{k}) = z - \frac{1}{2}\sum_{\delta}(\mathbf{k}\cdot\delta)^2 + \ldots\ ; \quad |\mathbf{k}|\,|\delta| \ll 1 \tag{3.3.32}$$

Simple cubic lattice: $\delta_x = \delta_y = \delta_z = a$

$$\gamma(\mathbf{k}) = z - \frac{2a^2}{2}(k_x^2 + k_y^2 + k_z^2) + \ldots \tag{3.3.33}$$

$$= z - a^2k^2\ ; \quad k^2 = k_x^2 + k_y^2 + k_z^2 z - \gamma(\mathbf{k}) \qquad = a^2k^2 \tag{3.3.34}$$

Missing figure: ω_k as function of k

$$[a_k, a^\dagger_{k'}] = \delta_{k,k'} \tag{3.3.35}$$

$$[a_k, a_{k'}] = 0 \tag{3.3.36}$$

$$[a^\dagger_k, a^\dagger_{k'}] = 0 \tag{3.3.37}$$

Introduce thermal average
$\langle a^\dagger_k a_k\rangle$ = thermal average of bosons in state with q.n. k. This is the Bose-Einstein distribution function

$$\langle a^\dagger_k a_k\rangle = \frac{1}{\mathrm{e}^{\beta\omega_k} - 1}\ ; \quad \beta = \frac{1}{k_B T} \tag{3.3.38}$$

<u>Internal energy U</u>:

$$U = \langle\mathcal{H}\rangle = \sum_k \omega_k \langle a^\dagger_k a_k\rangle \tag{3.3.39}$$

$$= \sum_k \frac{\omega_k}{\mathrm{e}^{\beta\omega_k - 1}} \xrightarrow{\beta\to\infty} 0 \tag{3.3.40}$$

Zero corrections to the classical ground state energy when $T \to 0$.

Magnetization:

$$
\begin{aligned}
M = \langle S_{iz} \rangle = \frac{1}{N} \langle \sum_i S_{iz} \rangle & & (3.3.41)\\
= S - \frac{1}{N} \sum_i \langle a_i^\dagger a_i \rangle & & (3.3.42)\\
= S - \frac{1}{N} \sum_{\mathbf{k}} \langle a_k^\dagger a_k \rangle & & (3.3.43)\\
= S - \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\mathrm{e}^{\beta\omega_k - 1}} \xrightarrow{\beta\to\infty} \underline{\underline{S}} & & (3.3.44)
\end{aligned}
$$

Thus, there are zero corrections to the classical ground state magnetization when $T \to 0$.

Conclusion: There are no fluctuation effects at $T = 0$ in the isotropic Heisenberg quantum ferromagnet. Fluctuations at $T = 0$ are called quantum fluctuations.

> There are no quantum fluctuations in the isotropic Heisenberg ferromagnet, and the exact ground state is the fully polarized classical ground state. Quantum fluctuations may, however, be introduced by exchange interactions which are anisotropic in spin-space.

Physical interpretation of the operators

$$
\begin{aligned}
a_k &= \frac{1}{\sqrt{N}} \sum_{\mathbf{r}_i} a_i \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_i} & (3.3.45)\\
a_k^\dagger &= \frac{1}{\sqrt{N}} \sum_{\mathbf{r}_i} a_i \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_i} & (3.3.46)
\end{aligned}
$$

The first thing to note is that these operators involve excitations of spins on all lattice points! Therefore, they are collective excitations.
$a_k^\dagger a_k$ involve creation and destruction of long-lived excitations (free, non-scattering bosons) with wavenumber $\mathbf{k}$. These excitations are spin-waves.

Missing figure: spin-waves

$(a_k^\dagger, a_k)$ create and destroy quantized excitations of these spin-waves. These quanta are called magnons. In this case, they are ferromagnetic magnons.

3.3.2 Quantum antiferromagnets

Nearest neighbor interactions

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad ; \quad J < 0 \tag{3.3.47}$$

We consider the system on a biparticle lattice, i.e. a lattice that can be decomposed into two, and only two, sublattices. An example would be a 2D square lattice. Another example would be a 3D cubic lattice. A counterexample would be a 2D triangular lattice. On a 2D square lattice, the classical would be:

Missing figure: Bibartite lattice

We partition the lattice into the two sublattices associated with the "up" and "down" spins of the classical ground state. "Up"- lattice: A. "Down"-lattice: B. If (i, j) are nearest-neigbors, then if $(i \in A, j \in B)$; $(i \in B, j \in A)$. Hence, we may write

$$\mathcal{H} = -J \sum_{\substack{i \in A \\ j \in B}} \mathbf{S}_i \cdot \mathbf{S}_j - J \sum_{\substack{i \in B \\ j \in A}} \mathbf{S}_i \cdot \mathbf{S}_j \tag{3.3.48}$$

Spins on sublattice A : $\mathbf{S}_{iA}$
Spins on sublattice B : $\mathbf{S}_{iB}$
$\mathbf{S}_{iA}$: Assumed mostly "up", with small "down"-fluctuations.
$\mathbf{S}_{iB}$: Assumed mostly "down", with small "up"-fluctuations.

Now introduce Holstein-Primakoff transformation on each sublattice.

$$S_{iAz} = S - a_i^\dagger a_i \tag{3.3.49}$$

$$S_{iA+} = \sqrt{2S} \left(1 - \frac{a_i^\dagger a_i}{2S} \right)^{1/2} a_i \tag{3.3.50}$$

$$S_{iA-} = \sqrt{2S} \left(1 - \frac{a_i^\dagger a_i}{2S} \right)^{1/2} a_i^\dagger \tag{3.3.51}$$

$$S_{iBz} = S - b_i^\dagger b_i \tag{3.3.52}$$

$$S_{iB+} = \sqrt{2S} \left(1 - \frac{b_i^\dagger b_i}{2S} \right)^{1/2} b_i^\dagger \tag{3.3.53}$$

$$S_{iB-} = \sqrt{2S} \left(1 - \frac{b_i^\dagger b_i}{2S} \right)^{1/2} b_i \tag{3.3.54}$$

$$\tag{3.3.55}$$

$a_i^\dagger$: Creates a "down"-fluctuation on "up"-spins.
$b_i^\dagger$: Creates an "up"-fluctuation on "down"-spins.

The following identity is also useful:

$$\mathbf{S}_i \cdot \mathbf{S}_j = S_{iz}S_{jz} + S_{i+}S_{j-} \tag{3.3.56}$$

The Hamiltonian may now be written as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} [S_{iAz}S_{iBz} + S_{iA+}S_{jB-} + S_{iBz}S_{jAz} + S_{iB+}S_{jA-}]. \tag{3.3.57}$$

Here, we must remember that $\sum_i$ runs over either the A-sublattice or the B-sublattice, with j the corresponding nearest neighbor.

We now consider the case where the spin-system is nearly ordered, so that we again calculate to quadratic order in boson-operators

$$S_{iA+} \approx \sqrt{2S}a_i \tag{3.3.58}$$
$$S_{iA-} \approx \sqrt{2S}a_i^\dagger \tag{3.3.59}$$
$$S_{iB+} \approx \sqrt{2S}b_i^\dagger \tag{3.3.60}$$
$$S_{iB-} \approx \sqrt{2S}b_i \tag{3.3.61}$$

We now insert this into $\mathcal{H}$, retaining only terms that are quadratic in (a, b)-operators.

If the $a-$ and $b-$operators satisfy bosonic commutation relations, then we get correct commutation relations for the spin-operators.

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} [(S - a_i^\dagger a_i)(-S + b_j^\dagger b_j) + (-S + b_i^\dagger b_i)(S - a_j^\dagger a_j) + 2Sa_i b_j + 2Sb_i^\dagger a_j^\dagger] \tag{3.3.62}$$

$$= E_0 - J \sum_{\langle i,j \rangle} [S(a_i^\dagger a_i + b_j^\dagger b_j) + S(b_i^\dagger b_i + a_j^\dagger a_j) + 2S(a_i b_j + b_j^\dagger a_i^\dagger] \tag{3.3.63}$$

$$E_0 \equiv 2JS^2 \sum_{\langle i,j \rangle} \cdot 1 \quad ; \quad J < 0 \tag{3.3.64}$$

N : # lattice sites on one sublattice.

z : # nearest neighbors.

$$\underline{\underline{E_0 = 2NzJS^2}} \quad ; \quad J < 0 \tag{3.3.65}$$

This energy will simply serve as a zero-point of energy, and will be discarded in the following.

$$\boxed{\mathcal{H} = -2JSz\sum_i (a_i^\dagger a_i + b_i^\dagger b_i) - 2JS\sum_{\langle i,j\rangle}(a_i b_j + b_i^\dagger a_j^\dagger)} \tag{3.3.66}$$

This Hamiltonian contains terms of a type that we have not encountered previously; namely the two last terms which contain only destruction-operators or creation-operators, or only creation operators.

- $a_i^\dagger a_i$: Number of "down"-fluctuations on a lattice site i (of lattice A).

- $b_i^\dagger b_i$: Number of "up"-fluctuations on a lattice site i (of lattice B).

It is important to realize that in the Hamiltonian given above, i and j run over <u>one of the sublattices</u> of the total bipartite lattice! As in the ferromagnetic case, we introduce Fourier-transformed magnon operators

$$\left.\begin{aligned} a_{\boldsymbol{q}} &= \tfrac{1}{\sqrt{N}}\textstyle\sum_i a_i \mathrm{e}^{i\boldsymbol{q}\cdot\mathbf{r}_i} \\ a_{\boldsymbol{q}}^\dagger &= \tfrac{1}{\sqrt{N}}\textstyle\sum_i a_i^\dagger \mathrm{e}^{-i\boldsymbol{q}\cdot\mathbf{r}_i} \\ b_{\boldsymbol{q}} &= \tfrac{1}{\sqrt{N}}\textstyle\sum_i b_i \mathrm{e}^{-i\boldsymbol{q}\cdot\mathbf{r}_i} \\ b_{\boldsymbol{q}}^\dagger &= \tfrac{1}{\sqrt{N}}\textstyle\sum_i b_i^\dagger \mathrm{e}^{i\boldsymbol{q}\cdot\mathbf{r}_i} \end{aligned}\right\} \begin{array}{l}\text{One set of operators} \\ \text{for each sublattice.}\end{array} \tag{3.3.67}$$

We next insert these expressions in $\mathcal{H}$. <u>Note:</u> $\boldsymbol{q}$ runs over the Brillouin-zone of sublattice A or B (which are the same).

$$\sum_i a_i^\dagger a_i = \frac{1}{N}\sum_i \sum_{\boldsymbol{q}_1,\boldsymbol{q}_2} a_{\boldsymbol{q}_1}^\dagger a_{\boldsymbol{q}_2} \mathrm{e}^{i(\boldsymbol{q}_1-\boldsymbol{q}_2)\cdot\mathbf{r}_i} = \sum_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \tag{3.3.68}$$

$$\sum_i b_i^\dagger b_i = \sum_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}} \tag{3.3.69}$$

$$\begin{aligned}\sum_{\langle i,j\rangle} a_i b_j &= \frac{1}{N}\sum_i \sum_{\boldsymbol{\delta}} \sum_{\boldsymbol{q}_1,\boldsymbol{q}_2} a_{\boldsymbol{q}_1} \mathrm{e}^{-i\boldsymbol{q}_1\cdot\mathbf{r}_i} b_{\boldsymbol{q}_2} \mathrm{e}^{i\boldsymbol{q}_2\cdot(\mathbf{r}_i+\boldsymbol{\delta})} \\ &= \sum_{\boldsymbol{q}_1,\boldsymbol{q}_2} a_{\boldsymbol{q}_1} b_{\boldsymbol{q}_2} \underbrace{\sum_{\boldsymbol{\delta}} \mathrm{e}^{i\boldsymbol{q}_2\cdot\boldsymbol{\delta}}}_{\equiv\gamma(\boldsymbol{q}_2)} \delta_{\boldsymbol{q}_1\boldsymbol{q}_2} = \sum_{\boldsymbol{q}} \gamma(\boldsymbol{q}) a_{\boldsymbol{q}} b_{\boldsymbol{q}} \end{aligned} \tag{3.3.70}$$

$$\begin{aligned}\sum_{\langle i,j\rangle} b_i^\dagger a_j^\dagger &= \frac{1}{N}\sum_i \sum_{\boldsymbol{\delta}} \sum_{\boldsymbol{q}_1,\boldsymbol{q}_2} b_{\boldsymbol{q}_1}^\dagger \mathrm{e}^{-i\boldsymbol{q}_1\cdot\mathbf{r}_i} a_{\boldsymbol{q}_2}^\dagger \mathrm{e}^{i\boldsymbol{q}_2\cdot(\mathbf{r}_i+\boldsymbol{\delta})} \\ &= \sum_{\boldsymbol{q}} \gamma(\boldsymbol{q}) b_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}^\dagger \end{aligned} \tag{3.3.71}$$

with

$$\gamma(\boldsymbol{q}) \equiv \sum_{\boldsymbol{\delta}} \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{\delta}}. \tag{3.3.72}$$

From these results, we obtain the Hamiltonian

$$\boxed{\mathcal{H} = -2JSz\sum_{\boldsymbol{q}} \left(a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} + b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}}\right) - 2JS\sum_{\boldsymbol{q}} \gamma(\boldsymbol{q}) \left(a_{\boldsymbol{q}} b_{\boldsymbol{q}} + b_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}^\dagger\right). \quad (3.3.73)}$$

1. z in the first term $\to \gamma(\boldsymbol{q})$ in the second term.

2. The $a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}$ and $b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}}$ - terms are of the same form as the Hamiltonian of a non-interacting boson-gas.

3. The $a_{\boldsymbol{q}} b_{\boldsymbol{q}}$ and $b_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}^\dagger$-terms are not of the same form as a Hamiltonian of a non-interacting boson-gas. These two terms are a qualitatively new feature not present in the ferromagnetic case. It originates with magnon-couplings between different sublattices "up" and "down"- As we will now demonstrate, it leads to drastically altered ground-state properties of an antiferromagnet, compared to a ferromagnet.

In the ferromagnetic case, with $\mathcal{H} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}$, $a_{\boldsymbol{q}}$ and $a_{\boldsymbol{q}}^\dagger$ represent long-lived quantized spin-excitations. Since the antiferromagnetic case is not on this form, it implies that $(a_{\boldsymbol{q}}, a_{\boldsymbol{q}}^\dagger)$ and $(b_{\boldsymbol{q}}, b_{\boldsymbol{q}}^\dagger)$ do not represent long-lived quantized spin-excitations. Our next task is therefore to transform $\mathcal{H}$ in order to express it in new operators which do represent long-lived excitations. This is achieved using a so-called Bogoliubov-transformation, a widely used technique which we will return to also later. We write the new operators as linear combinations of $(a_{\boldsymbol{q}}, a_{\boldsymbol{q}}^\dagger, b_{\boldsymbol{q}}, b_{\boldsymbol{q}}^\dagger)$, and demand that the new operators also are boson-operators.

$q = \boldsymbol{q}$ (notasjon)

$$A_q = u_q a_q + v_q b_q^\dagger \qquad A_q^\dagger = u_q a_q^\dagger + v_q b_q \tag{3.3.74}$$
$$B_q = v_q a_q^\dagger + u_q b_q \qquad B_q^\dagger = v_q a_q + u_q b_q^\dagger. \tag{3.3.75}$$

$$[a_q, a_{q'}^\dagger] = [b_q, b_{q'}^\dagger] = \delta_{q,q'}. \tag{3.3.76}$$

Now demand that
$$[A_q, A_{q'}^\dagger] = [B_q, B_{q'}^\dagger] = \delta_{q,q'}. \tag{3.3.77}$$

Thus,

$$\begin{aligned}\left[u_q a_q + v_q b_q^\dagger, u_{q'} a_{q'}^\dagger + v_{q'} b_{q'}\right] &= u_q u_{q'} \delta_{qq'} + v_q v_{q'} \delta_{qq'}(-1)\\ &= \delta_{qq'} \implies\end{aligned}$$

$$\boxed{u_q^2 - v_q^2 = 1.} \tag{3.3.78}$$

This is a contraint on u_q, v_q to ensure that A_q, B_q represent bosons. Thus, we may write

$$u_q = \cosh\theta_q \tag{3.3.79}$$
$$v_q = \sinh\theta_q, \tag{3.3.80}$$

where θ_q is a "Squeezing"-parameter that must be determined by requiring that $\mathcal{H}$ only contains $A_q^\dagger A_q-$ and $B_q^\dagger B_q$-terms.

$$\begin{pmatrix} A_q \\ B_q^\dagger \end{pmatrix} = \begin{pmatrix} u_q & v_q \\ v_q & u_q \end{pmatrix} \begin{pmatrix} a_q \\ b_q^\dagger \end{pmatrix} = S \begin{pmatrix} a_q \\ b_q^\dagger \end{pmatrix} \tag{3.3.81}$$

$$\begin{pmatrix} a_q \\ b_q^\dagger \end{pmatrix} = S^{-1} \begin{pmatrix} A_q \\ B_q^\dagger \end{pmatrix} = \begin{pmatrix} u_q & -v_q \\ -v_q & u_q \end{pmatrix} \begin{pmatrix} A_q \\ B_q^\dagger \end{pmatrix} \tag{3.3.82}$$

$$a_q = u_q A_q - v_q B_q^\dagger \qquad a_q^\dagger = u_q A_q^\dagger - v_q B_q \tag{3.3.83}$$
$$b_q^\dagger = -v_q A_q + u_q B_q^\dagger \qquad b_q = -v_q A_q^\dagger + u_q B_q. \tag{3.3.84}$$

This is now inserted into $\mathcal{H}$ in eq. (3.3.73), and u_q, v_q (i.e. θ_q) are chosen such that only $A_q^\dagger A_q-$ and $B_q^\dagger B_q$-terms are present in $\mathcal{H}$.

$$\begin{aligned}\mathcal{H} = -2JS\sum_{\boldsymbol{q}} \big\{ z \big[&\left(u_q A_q^\dagger - v_q B_q\right)\left(u_q A_q - v_q B_q^\dagger\right) \\ &+ \left(-v_q A_q + u_q B_q^\dagger\right)\left(-v_q A_q^\dagger + u_q B_q\right)\big] \\ &+ \gamma(\boldsymbol{q}) \left[\left(u_q A_q - v_q B_q^\dagger a_q^\dagger\right)\left(-v_q A_q^\dagger + u_q B_q\right)\right. \\ &+ \left.\left(-v_q A_q + u_q B_q^\dagger\right)\left(u_q A_q^\dagger - v_q B_q\right)\right]\big\}.\end{aligned}$$

Let us sort out terms of different types;

$$\begin{aligned}
A_q^\dagger A_q &: & -2JS\left[z u_q^2 - u_q v_q \gamma(\boldsymbol{q})\right] \\
A_q A_q^\dagger &: & -2JS\left[z v_q^2 - u_q v_q \gamma(\boldsymbol{q})\right] \\
B_q^\dagger B_q &: & -2JS\left[z u_q^2 - u_q v_q \gamma(\boldsymbol{q})\right] \\
B_q B_q^\dagger &: & -2JS\left[z v_q^2 - u_q v_q \gamma(\boldsymbol{q})\right] \\
A_q^\dagger B_q^\dagger &: & -2JS\left[-2z u_q v_q + \gamma(\boldsymbol{q})(u_q^2 + v_q^2)\right] \\
A_q B_q &: & -2JS\left[-2z u_q v_q + \gamma(\boldsymbol{q})(u_q^2 + v_q^2)\right]
\end{aligned}$$

We choose u_q, v_q such that the coefficients of $A_q B_q, A_q^\dagger B_q^\dagger$ vanish. We also use that

$$A_q A_q^\dagger = A_q^\dagger A_q + 1 \tag{3.3.85}$$

$$B_q B_q^\dagger = B_q^\dagger B_q + 1. \tag{3.3.86}$$

Thus, the coefficient of $A_q^\dagger A_q$ and $B_q^\dagger B_q$ will be

$$\boxed{\omega_q = -2JS\left[z(u_q^2 + v_q^2) - 2\gamma(q) u_q v_q\right].} \tag{3.3.87}$$

The coefficient that must vanish:

$$-2JS\left[-2z u_q v_q + \gamma(q)(u_q^2 + v_q^2)\right]. \tag{3.3.88}$$

Furthermore, we had $E_0 = 2NzJS^2$. We now see that there will be a correction to E_0, absent in the ferromagnet, due to $A_q A_q^\dagger = 1 + A_q^\dagger A_q$, $B_q B_q^\dagger = 1 + B_q^\dagger B_q$. The correction is given by

$$-2JS\sum_q \left[z(v_q^2 + v_q^2) - 2\gamma(q) u_q v_q\right] = 2JSzN + \sum_q \omega_q. \tag{3.3.89}$$

Here, we have used

$$v_q^2 + v_q^2 = v_q^2 + u_q^2 - (u_q^2 - v_q^2) = v_q^2 + u_q^2 - 1, \tag{3.3.90}$$

and

$$\sum_q 1 = N. \tag{3.3.91}$$

Now, we define

$$\tilde{E}_0 = E_0 + 2NJzS = 2NJzS(S+1). \tag{3.3.92}$$

Note how the quantum nature of the spin stands out in $\tilde{E}_0$, unlike the FM case. Thus,

$$\mathcal{H} = \tilde{E}_0 + \sum_q \omega_q + \sum_q \omega_q (A_q^\dagger A_q + B_q^\dagger B_q) \tag{3.3.93}$$

$$= \tilde{E}_0 + \sum_q \hbar\omega_q \left(A_q^\dagger A_q + \frac{1}{2} \right) + \sum_q \hbar\omega_q \left(B_q^\dagger B_q + \frac{1}{2} \right), \tag{3.3.94}$$

Note also the factors $\frac{1}{2}$ in both terms, absent in the ferromagnet! The correction in $\tilde{E}_0$ to E_0 as well as the correction $\sum_q \omega_q$ hint at the presence of quantum fluctuations in the ground state of the quantum anti-ferromagnet.

> The correction $\sum_q \omega_q$ is analogous to the zero-point energy in a harmonic oscillator. Absent in ferromagnets.

The fact that there are corrections to the classical ground state energy E_0, clearly demonstrates that a quantum antiferromagnet is endowed with quantum fluctuations, absent in the ferromagnet. The operators $(A_q, A_q^\dagger)$, $(B_q, B_q^\dagger)$ now represent long-lived quantized spin-fluctuations on the bipartite lattice. Their excitation energies are ω_q.

> Har rokkert litt på rekkefølgen side 10-13 i forelesningsnotater (uke 5).

First, we determine u_q, v_q from the two equations

$$2JS \left[-2zu_q v_q + \gamma(q)(u_q^2 + v_q^2) \right] = 0 \tag{3.3.95}$$

$$u_q^2 - v_q^2 = 1. \tag{3.3.96}$$

$$2zu_q v_q = \gamma(q)(u_q^2 + v_q^2). \tag{3.3.97}$$

Introduce $x = u_q^2$ such that $v_q^2 = -1 + x$. Square eq. (3.3.97) and get

$$4z^2 x(-1+x) = \gamma^2 (2x-1)^2 \tag{3.3.98}$$

$$x = \frac{1}{2}\left(1 + \frac{z}{\sqrt{z^2-\gamma^2}}\right) = u_q^2 \tag{3.3.99}$$

$$v_q^2 = \frac{1}{2}\left(-1 + \frac{z}{\sqrt{z^2-\gamma^2}}\right) \tag{3.3.100}$$

$$\begin{aligned} u_q^2 v_q^2 &= \frac{1}{4}\left(\frac{z^2}{z^2-\gamma^2} - 1\right) = \frac{\gamma^2}{4(z^2-\gamma^2)} \\ u_q v_q &= \frac{1}{2}\frac{\gamma}{\sqrt{z^2-\gamma^2}}. \end{aligned}$$

Note that even though $u_q^2 - v_q^2 = 1$, u_q and v_q individually may become very large!

Next, with these expressions for u_q and v_q, work out ω_q as

$$\begin{aligned} \omega_q &= -2JS\left[z(u_q^2+v_q^2) - 2\gamma(q)u_q v_q\right] \\ &= -2JS\left[z\frac{2z}{\sqrt{z^2-\gamma^2}}\frac{1}{2} - \frac{2\gamma}{2}\frac{\gamma}{\sqrt{z^2-\gamma^2}}\right] \\ &= \frac{2JS}{\sqrt{z^2-\gamma^2}}\left(z^2-\gamma^2\right) = -2JS\sqrt{z^2-\gamma^2}, \end{aligned}$$

which implies ($J < 0$)

$$\omega_q = 2|J|S\sqrt{z^2-\gamma^2}. \tag{3.3.101}$$

Let us consider ω_q in some more detail.

$$\gamma(\boldsymbol{q}) = \sum_{\boldsymbol{\delta}} \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{\delta}} \tag{3.3.102}$$

Motsatt fortegn på fasen i eq. (3.3.72). Irrelevant for rektanglulært gitter.

The assumption is that we are working on a bipartite lattice. To be specific, let us consider simple "cubic" lattices in d dimensions. $\boldsymbol{\delta}$ runs over all vectors connecting a site to its z nearest neighbors (hence, there are z such vectors $\boldsymbol{\delta}$). This gives

$$\gamma(\boldsymbol{q}) = \sum_{\alpha=1}^{d} 2\cos(\boldsymbol{q}_\alpha). \tag{3.3.103}$$

We have chosen the lattice constant equal to unity. Consider now small $|q_\alpha| \ll 1$.

$$
\begin{aligned}
\gamma(\boldsymbol{q}) &= 2\sum_{\alpha=1}^{d}\left(1-\frac{1}{2}q_\alpha^2+\dots\right) \\
&= 2d-\boldsymbol{q}^2+\dots = z-\boldsymbol{q}^2.
\end{aligned} \tag{3.3.104}
$$

$$
\begin{aligned}
\omega &= 2|J|S\sqrt{z^2-(z-\boldsymbol{q}^2)^2} \\
&= 2|J|S\left(z^2-z^2+2z\boldsymbol{q}^2+\dots\right)^{\frac{1}{2}} \\
&\simeq 2\sqrt{2z}|J|S|\boldsymbol{q}|.
\end{aligned} \tag{3.3.105}
$$

Note that this low-energy spectrum is linear in wave-vector, unlike the ccase for ferromagnets, where $\omega_q \sim q^2$ for small $\boldsymbol{q}$. Since $q^2 \ll q$ for $q \ll 1$, the quantized spin-excitations at long wavelengths are much more energetically costly in an anti-ferromagnet than in a ferromagnet. In the ferromagnet, we saw that there were only thermal corrections to the magnetization, and no quantum fluctuations (Recall that there were no quantum corrections to the ground state energy (classical) either). Since we know that there are quantum corrections to the classical ground state energy in the antiferromagnet, let us investigate the quantum corrections to the magnetization. We will do this by computing the magnetization on one sublattice, the "up"-lattice, say.

$$
M = S - \frac{1}{N}\sum_i \langle a_i^\dagger a_i\rangle \tag{3.3.106}
$$

$$
= \frac{1}{N}\,\langle\sum_i S_{iz}\rangle_A\,, \tag{3.3.107}
$$

where N is the number of lattice sites on the A-sublattice.

$$
M = S - \frac{1}{N}\sum_{\boldsymbol{q}}\left\langle a_q^\dagger a_q\right\rangle. \tag{3.3.108}
$$

In the ferromagnet,

$$
\left\langle a_q^\dagger a_q\right\rangle = \frac{1}{\mathrm{e}^{\beta\omega_q}-1}, \tag{3.3.109}
$$

with $\omega_q \sim q^2$. Here,

$$
\left\langle A_q^\dagger A_q\right\rangle = \left\langle B_q^\dagger B_q\right\rangle = \frac{1}{\mathrm{e}^{\beta\omega_q}-1} \tag{3.3.110}
$$

with ω_q appropriate for AFM

$$\omega_q = 2|J|S\sqrt{z^2-\gamma^2}. \tag{3.3.111}$$

We had

$$\begin{aligned} a_q &= u_q A_q - v_q B_q^\dagger \\ a_q^\dagger &= u_q A_q^\dagger - v_q B_q \end{aligned}$$

$$\begin{aligned} \langle a_q^\dagger a_q \rangle = u_q^2 \langle A_q^\dagger A_q \rangle + v_q^2 \left(\langle B_q^\dagger B_q \rangle + 1 \right) \\ - u_q v_q \underbrace{\langle A_q^\dagger B_q^\dagger \rangle}_{=0} - u_q v_q \underbrace{\langle B_q A_q \rangle}_{=0} \end{aligned}$$

$$M = S - \underbrace{\frac{1}{N}\sum_{\boldsymbol{q}} v_q^2}_{\text{Quantum correction to ground state magnetization. No counterpart in a ferromagnet.}} - \frac{1}{N}\sum_{\boldsymbol{q}} \frac{u_q^2+v_q^2}{\mathrm{e}^{\beta\omega_q}-1}. \tag{3.3.112}$$

As we have previously noted, u_q and v_q could potentially become quite large, so the quantum correction to M could be considerable. Let us investigate what it is in more detail. $\sum_q$ runs over the Brillouin-zone of the sublattice. We found that

$$v_q^2 = \frac{1}{2}\left(-1 + \frac{z}{\sqrt{z^2-\gamma^2}}\right). \tag{3.3.113}$$

v_q^2 diverges as $q \to 0$, so the dominant contribution to the integral will come from small q, The magnetization is

$$\begin{aligned} M &= S + \frac{1}{2} - \frac{1}{N}\sum_{\boldsymbol{q}} \frac{z}{z^2-\gamma^2} \\ &\simeq S + \frac{1}{2} - \frac{\Omega_d}{(2\pi)^d}\int_{\frac{1}{L}}^{\frac{1}{a}} \mathrm{d}q\, \frac{q^{d-1}}{\sqrt{2z}q} \end{aligned} \tag{3.3.114}$$

Forslag: Legge inn skriftlig forklaring på integrasjonsteknikken

where, a is the lattice constant and L is the system size.

- If $d=1$: The integral goes as $\sim \ln\left(\frac{L}{a}\right)$, which is divergent as $L \to \infty$.
- If $d>1$: Integral $\sim \left(\frac{a}{L}\right)^\epsilon$ with $d = 1+\epsilon$. This is convergent as $L \to \infty$.
- If $d<1$: Integral $\sim \left(\frac{L}{a}\right)^\epsilon$ with $d = 1-\epsilon$, i.e. divergent as $L \to \infty$.

The $1d$ Heisenberg-chain has no long-range order in tha antiferromagnetic case, even at $T = 0$ (the ferromagnetic chain is ordered at $T = 0$). There are many interesting extensions of this model

- The model can be defined on non-bipartite lattices
- One can add longe-range interactions
- One can introduce anisotropy

All of these changes will alter ω_q. The first two are particularly interesting and can lead to destruction of long-range order at $T = 0$ even in higher dimensions than $d = 1$. Such non-ordered quantum spin systems are being intensively studied at present. One particular important issue is to what extent the many-spin ground state features entanglement of its one-spin constituent factors. Entangled, non-ordered ground states in quantum antiferromagnets are referred to as spin-liquids.

Problems

Problem 3.1. In class (lecture notes Week 4) we have seen how to compute the magnon-spectrum to lowest order in magnon-operators (spin-fluctuations around a fully ordered state) for the ferromagnetic Heisenberg model

$$\mathcal{H} = -J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j$$

In realistic situations, this may turn out to be a too simple model. Often, it is very useful to modify this model to account for crystalline anisotropies. One simple way of doing this is to augment the Hamiltonian slightly as follows

$$\mathcal{H} = -J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j - K \sum_i S_{iz}^2$$

where K is a so-called anisotropy parameter. It could be both positive and negative.

a) Explain qualitatively on physical grounds how you expect the ordered state we considered for $K = 0$ to be affected by $K \neq 0$. Consider the cases $K > 0$ and $K < 0$ separately.

b) Consider now in more detail the case $K > 0$. Use the same technique as introduced in lectures (Holstein-Primakoff transformation), to compute the magnon-sprectrum.

c) Compare the result with what we found in class for $K = 0$, and comment on the physics of the difference, paying particular attention to the qualitative discussion in point **a)**.

Problem 3.2. In class, we have seen how to compute the magnon spectrum of the isotropic ferromagnetic Heisenberg quantum spin model

$$\begin{aligned}\mathcal{H} &= -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\ &= -J \sum_{\langle i,j \rangle} \left[S_{iz} S_{jz} + \frac{1}{2} \left(S_{i+} S_{j-} + S_{j+} S_{i-} \right) \right]\end{aligned}$$

by using the Holstein-Primakoff transformation and calculating to quadratic order in magnon-operators.

a) Generalize the results of **a)** to the case with arbitrary-ranged *ferromagnetic*, but isotropic in spin-space, spin-interactions $J_{ij} > 0$, i.e. the Hamiltonian is given by

$$\mathcal{H} = -\sum_{i,j} J_{ij} \left[S_{iz}S_{jz} + \frac{1}{2}\left(S_{i+}S_{j-} + S_{j+}S_{i-}\right)\right]$$

You may assume that $J_{ij} = J(\mathbf{r}_i - \mathbf{r}_j)$, where $\mathbf{r}_i$ is the position of lattice site i. Find the expression for the magnon-spectrum in this case.

b) In class, we have seen that there are no quantum fluctuations in the isotropic ferromagnetic Heisenberg-model, while we do get quantum-fluctuations through squeezing of magnons in the ground state of isotropic antiferromagnetic case.

Consider now a generalization of the ferromagnetic Heisenberg-model with nearest-neighbor interactions to the case with spin-space anisotropy

$$\mathcal{H} = -\sum_{\langle i,j\rangle} \left[JS_{iz}S_{jz} + J_xS_{ix}S_{jx} + J_yS_{iy}S_{jy}\right].$$

(Such spin-space anisotropy could, for instance, originate with spin-orbit coupling in the system.) In this problem, we will assume that $(J, J_x, J_y) > 0$, $J > (J_x, J_y)$ and that $J_x \neq J_y$. Introduce the Holstein-Primakoff-transformation for the ferromagnet, calculate to quadratic order in boson-operators, and show that the Hamiltonian may be written on the form

$$\mathcal{H} = -JNS^2z + 2JSz\sum_i a_i^\dagger a_i - 2\bar{J}S\sum_{\langle i,j\rangle} a_i^\dagger a_j + \Delta JS\sum_{\langle i,j\rangle}\left[a_i^\dagger a_j^\dagger + a_ia_j\right]$$

with $2\bar{J} \equiv J_x + J_y$ and $2\Delta J \equiv J_x - J_y$. N is the total number of lattice sites. Note the appearance of the "anomalous" terms $a_i^\dagger a_j^\dagger$ and a_ia_j due to $J_x \neq J_y$. Hence, a symplectic Bogoliubov-transformation will be needed to obtain the magnon-spectrum of this system as well.

c) Introduce first a Fourier-transformed operators like we did in class, and show that

$$\mathcal{H} = -JNS^2z + \sum_q \left\{\gamma_1(q)\left[a_q^\dagger a_q + a_{-q}^\dagger a_{-q}\right] + \gamma_2(q)\left[a_qa_{-q} + a_q^\dagger a_{-q}^\dagger\right]\right\}$$

and give expressions for $\gamma_1(q)$ and $\gamma_2(q)$.

d) Introduce the Bogoliubov-transformation

$$A_q = u_qa_q + v_qa_{-q}^\dagger$$
$$A_{-q}^\dagger = u_qa_{-q}^\dagger + v_qa_q$$

and find expressions for u_q and v_q that diagonalize the Hamiltonian.

e) Explain what the main difference between the squeezing-factors u_q and v_q in the present case is, and the squeezing factors we found in the isotropic quantum antiferromagnet. Comment on the presence of quantum-fluctuations in the ground state of the anisotropic quantum ferromagnet, compared to those that are present in the isotropic quantum-antiferromagnet. (Hint: Consider the limit $q \to 0$ of u_q and v_q for both cases and compare).

f) Squeezing of magnons has potentially very useful applications. One possible application is in low-dissipation heterostructures where magnons may induce loss of dissipation (electrical resistance) in heterostrucure of magnetic insulators and normal metals. Electronic devices where electrical dissipation can be eliminated or strongly reduced, is of obvious practical importance. To facilitate such loss or reduction, it turns out that large squeezing is important. Given this, what would you suggest is the most efficient heterostructure to use: i) an NM/FM-structure or an NM/AFM-structure? Here, NM means normal metal, FM is anisotropic quantum ferromagnet, and AFM is isotropic quantum antiferromagnet.

Problem 3.3. Use the results we derived in class to compute the low-temperature thermal corrections to the sublattice magnetization in the isotropic Heisenberg quantum antiferromagnet, in arbitrary dimensions d. Low temperature here means that $T \ll J$.

Problem 3.4. In this problem, we will study the coupling between a system of itinerant electrons (i.e. electrons that can move around), modelled as a tight-binding model with hopping on a lattice and nearest neighbor hopping, and a system of localized spins (spin 1/2) $\mathbf{S}_i$ which are located on the same lattice as the electrons can hop. We denote the electron spins as

$$\mathbf{s}_i = \frac{1}{2} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta}$$

where $c_{i\sigma}^{\dagger}, c_{i\sigma}$ are creation and destruction operators for the electrons, a summation convention is implicit on α and β, and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli-matrices.

It is assumed that the electron-spins interact with the localized spins through an exchange coupling of the type $-J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i$. The subscript sd refers to the fact that this type of model is often used to describe itinerant electrons interacting with localized spins (a metallic magnet), where the dominant orbital content of the electron band is a Wannier-orbital with s-wave symmetry, while the dominant orbital content of the localized spins is a Wannier-orbital with d-wave symmetry.

The Hamiltonian of the system is given by

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_{\text{el}} + \mathcal{H}_{\text{spin}} + \mathcal{H}_{\text{el-spin}} \\
\mathcal{H}_{\text{el}} &= -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma} \\
\mathcal{H}_{\text{spin}} &= -J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\
\mathcal{H}_{\text{el-spin}} &= -J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i
\end{aligned}$$

You may assume that $(J, J_{sd}) > 0$, and that the localized spins are almost completely ferromagnetically magnetically ordered, such that a truncation of the Holstein-Primakoff transformation for $\mathbf{S}_i$ to lowest order in magnon-operators is justified. A spin-flip "up" operator for the electrons is given by $s_{i+} = c^\dagger_{i\uparrow} c_{i\downarrow}$, while a spin-flip "down" operator for the electrons is given by $s_{i-} = c^\dagger_{i\downarrow} c_{i\uparrow}$ (for details, see the lectures notes on the derivation of the Heisenberg model from the Hubbard-model).

a) Show that, to lowest order in the magnon-operators introduced in the Holstein-Primakoff-transformation, the Hamiltonian may be written on the form

$$\begin{aligned}
\mathcal{H} = E_0 + 2JS \sum_{\langle i,j,\rangle} \left[a^\dagger_i a_i - a^\dagger_i a_j\right] - t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma} - J_{sd} S \sum_{i,\sigma} \sigma\, c^\dagger_{i\sigma} c_{i\sigma} \\
+ J_{sd} \sum_{i,\sigma} \sigma\, a^\dagger_i a_i c^\dagger_{i,\sigma} c_{i,\sigma} - \frac{J_{sd}}{2} \sum_i \sqrt{2S} \left[a_i\, c^\dagger_{i\downarrow} c_{i\uparrow} + a^\dagger_i\, c^\dagger_{i\uparrow} c_{i\downarrow}\right]
\end{aligned}$$

b) Give a physical interpretation of the last term in the first line, and explain its presence.

c) Give a physical interpretation of the difference in spin-structure of the two terms in the second line.

c) Express the Hamiltonian in terms of Fourier-transformed magnon- and electron-operators.

d) Explain how the above Hamiltonian effectively may contain interactions between electrons. (Hint: It may be helpful to draw on an analogy with electron-phonon coupling, and consider diagrammatic representations of the electron-magnon coupling like we did in class for electron-phonon coupling).

e) In the above Hamiltonian, there is the nearest-neighbor spin-interaction term $-J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j$. Explain how the above Hamiltonian generates additional, longer-ranged, interactions between spins $\mathbf{S}_i$ on different lattice sites. (Hint: Try to give a pictorial representation of these interactions in the same way that we used pictures to represent interactions among electrons via phonons in class.)

CHAPTER 4

IONIC CRYSTALS AND PHONONS

4.1 Quantization of Lattice Vibrations

So far, we have studied electrons on rigid lattices. In reality, particularly at elevated temperatures, ions are thermally excited out of their classical equilibrium positions. As a result, the lattice vibrates. In addition, we might even have quantum vibrations of the lattice. These lattice vibrations will in turn affect the motion of electrons through the lattice. This impacts the transport properties of metals, such as resistivity, and also leads indirectly to new interactions between the electrons. It is therefore an important issue to study lattice vibrations, and their quantized version. Lattice vibrations give rise to sound waves, n the same way that spin-fluctuations give rise to spin-waves. Quantized spin-waves were dubbed magnons, whereas quantized sound-waves will be called phonons. To begin with, we focus exclusively on the ion-part of the problem. Later on, we will introduce the coupling to lattice vibrations.

The classical Hamiltonian for an ion vibrating at lattice site i, with mass M_i, is given by

$$\mathcal{H}_i = \frac{\boldsymbol{P}_i^2}{2M_i} + \sum_{j \neq i} V(\boldsymbol{R}_i - \boldsymbol{R}_j), \tag{4.1.1}$$

where V is a Coulomb-potential originating with the surrounding ions, $\boldsymbol{R}_l$ is the position of ion at lattice site l. Denote the classical equilibrium position of the ion at lattice site l by $\boldsymbol{R}_{0l}$. We now envisage that the ions execute small vibrations with amplitude $\boldsymbol{u}_l$ around $\boldsymbol{R}_{0l}$. Denote the lattice constant by a.

By small, we mean that for all l,

$$|\boldsymbol{u}_l| \ll a. \tag{4.1.2}$$

Under such circumstances, we may Taylor-expand $V(\boldsymbol{R}_i - \boldsymbol{R}_j)$ to low order around $\boldsymbol{R}_{0i} - \boldsymbol{R}_{0j}$, thus

$$\begin{aligned}\sum_{j\neq i} V(\boldsymbol{R}_i - \boldsymbol{R}_j) = \sum_{j\neq i} V(\boldsymbol{R}_{0i} - \boldsymbol{R}_{0j}) + \sum_{j\neq i} \left.\frac{\partial V}{\partial R_{i\mu}}\right|_{\boldsymbol{R}_{0i}} \Delta R_{i\mu} \\ + \frac{1}{2}\sum_{j\neq i} \left.\frac{\partial^2 V}{\partial R_{i\mu}\partial R_{j\nu}}\right|_{\boldsymbol{R}_0} \Delta R_{i\mu}\Delta R_{j\nu}\end{aligned} \tag{4.1.3}$$

Indeks på $\boldsymbol{R}_0$ i det siste leddet? Evt skrive $|_{\boldsymbol{R}_{0i},\boldsymbol{R}_{j0}}$?

(μ, ν) are cartesian coordinatex (x, y, z) and

$$\Delta R_{i\mu} \equiv u_{i\mu}. \tag{4.1.4}$$

The first term is just a constant which we will discard. The second term is the net force on the ion at site i from all the surrounding atoms, when ion at site i is exactly at its equilibrium position. This net force is zero. Thus, the lowest order remaining term will be the term involving quadratic fluctuations. Of course, if the deviations from equilibrium grow larger, then we need to expand further. In the following, we assume thatthe condition are such (e.g. low enough temperatures) that these higher order terms may be ignored. Hence, we obtain

$$\mathcal{H}_{\text{ion}} = \sum_i \frac{\boldsymbol{P}_i^2}{2M_i} + \frac{1}{2}\sum_{\substack{i,j\\ \mu,\nu}} u_{i\nu}\Phi^{ij}_{\mu\nu}u_{j\mu}, \tag{4.1.5}$$

with

$$\Phi^{ij}_{\mu\nu} \equiv \left.\frac{\partial^2 V}{\partial R_{i\mu}\partial R_{j\nu}}\right|_{\boldsymbol{R}_0}. \tag{4.1.6}$$

Φ is often called the dynamical matrix (a 3×3 matrix for a $3D$ lattice with one-atom basis). It plays the same role as a spring constant in a harmonic oscillator

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}kx^2. \tag{4.1.7}$$

Note that the dynamical matrix couples lattice vibrations on different lattice sites. We will now treat this problem of coupled harmonic vibrations of the lattice in the same way that one treats the single $1D$ harmonic oscillator:

i) Classical treatment to find eigenfrequencies ω.

ii) Quantization of p and x using bosonic ladder-operators.

4.1.1 Quantization of $1D$ harmonic oscillator

Hamilton's equations:

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial x} = -kx \tag{4.1.8}$$

$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m} \implies p = m\dot{x}. \tag{4.1.9}$$

$$\underline{m\ddot{x} = -kx} \quad ; \quad x = u_0 \mathrm{e}^{i\omega t} \tag{4.1.10}$$

$$-m\omega^2 u_0 \mathrm{e}^{i\omega t} = -k u_0 \mathrm{e}^{i\omega t} \tag{4.1.11}$$

$$\underline{m\omega^2 = k} \implies \omega = \sqrt{\frac{k}{m}}. \tag{4.1.12}$$

Note: ω obtained by classical methods. Next quantize:

$$x = \sqrt{\frac{\hbar}{2m\omega}} \left(a^\dagger + a\right) \tag{4.1.13}$$

$$p = i\sqrt{\frac{m\hbar\omega}{2}} \left(a^\dagger - a\right), \tag{4.1.14}$$

with $[a, a^\dagger] = 1$. This implies $[x, p] = i\hbar$ and

$$\mathcal{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2}\right), \tag{4.1.15}$$

where $a^\dagger a$ is the number operator satisfying

$$a^\dagger a \left|n\right\rangle = n \left|n\right\rangle \tag{4.1.16}$$

$$\mathcal{H} \left|n\right\rangle = \hbar\omega \left(n + \frac{1}{2}\right) \left|n\right\rangle = E_n \left|n\right\rangle. \tag{4.1.17}$$

Spectrum quantized in units of $\hbar\omega$, where ω is obtained from classical physics. We next proceed the same was for the lattice vibrations.

4.1.2 Quantization of lattice ion hamiltonian

Disse overskriftene er strengt tatt ikke nødvendig, men jeg tenkte det ble mer ryddig.

$$\mathcal{H}_{\text{ion}} = \sum_i \frac{\boldsymbol{P}_i^2}{2M_i} + \frac{1}{2} \sum_{\substack{i,j \\ \mu,\nu}} u_{i\nu} \Phi^{ij}_{\mu\nu} u_{j\mu}. \tag{4.1.18}$$

Assume translational invariance, such that $\Phi^{ij}_{\mu\nu} = \Phi_{\mu\nu}(\boldsymbol{\delta})$, where $\boldsymbol{\delta}$ is a vector that connects lattice i to j via the matrix $\Phi^{ij}_{\mu\nu}$. Define $p_i = \frac{P_i}{M_i}$ and introduce

Her er ikke tilde-notasjonen helt riktig i notatene. Skal det også være

Fourier-transform $\tilde{\boldsymbol{p}}_k$

$$\tilde{\boldsymbol{p}}_i = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \tilde{\boldsymbol{p}}_{\boldsymbol{k}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}_{0i}}. \tag{4.1.19}$$

Likewise:

$$\boldsymbol{u}_i = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \tilde{\boldsymbol{u}}_{\boldsymbol{k}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}_{0i}}. \tag{4.1.20}$$

$\tilde{u} = \sqrt{M}u$? For å bevare kommutasjonsrel.

The first term in $\mathcal{H}_{\text{ion}}$: $\sum_{\boldsymbol{k}} \frac{\tilde{\boldsymbol{p}}_{\boldsymbol{k}}\cdot\tilde{\boldsymbol{p}}_{-\boldsymbol{k}}}{2}$. The second term:

$$\frac{1}{2} \sum_{\substack{i,\boldsymbol{\delta} \\ \mu,\nu}} \Phi_{\mu\nu}(\boldsymbol{\delta}) \frac{1}{N} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \tilde{u}_{\boldsymbol{k}_1\nu}\tilde{u}_{\boldsymbol{k}_2\mu} \mathrm{e}^{i\boldsymbol{k}_1\cdot\boldsymbol{R}_{0i}} \mathrm{e}^{i\boldsymbol{k}_2\cdot(\boldsymbol{R}_{0i}+\boldsymbol{\delta})} \tag{4.1.21}$$

$$= \frac{1}{2} \sum_{\boldsymbol{k}} \underbrace{\left\{ \sum_{\boldsymbol{\delta}} \Phi_{\mu\nu}(\boldsymbol{\delta}) \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{\delta}} \right\}}_{\equiv \gamma_{\mu\nu}(\boldsymbol{k})} \tilde{u}_{\boldsymbol{k}\nu}\tilde{u}_{-\boldsymbol{k}\mu} \tag{4.1.22}$$

$$= \frac{1}{2} \sum_{\boldsymbol{k}} \tilde{\boldsymbol{u}}_{\boldsymbol{k}}^{\intercal} \gamma(\boldsymbol{k}) \tilde{\boldsymbol{u}}_{-\boldsymbol{k}} \tag{4.1.23}$$

On a lattice with a one-atom basis in d dimensions, $\boldsymbol{\gamma}$ is a $d \times d$-matrix. On a lattice with an r-atom basis in d dimensions, $\boldsymbol{\gamma}$ is a $dr \times dr$-matrix.

$u_{-k} \to u_k$ her. Hvorfor?

In the second term of the Hamiltonian, we may rotate to a new basis

$$\tilde{\boldsymbol{u}}_{\boldsymbol{k}}^{\intercal} \gamma(\boldsymbol{k}) \tilde{\boldsymbol{u}}_{\boldsymbol{k}} = (\tilde{\boldsymbol{u}}_{\boldsymbol{k}}^{\intercal} S) \underbrace{S^{-1}\gamma S}_{} (S^{-1}\tilde{\boldsymbol{u}}_{-\boldsymbol{k}}) \tag{4.1.24}$$

diagonal with the eigenvalues of $\boldsymbol{\gamma}$ on the diagonal. There are dr such eigenvalues. The corresponding eigenvectors are called the normal modes of the lattice.

Let λ be an index that identifies a normal mode. There are dr normal modes, z_λ, $\lambda \in (\lambda_1, \lambda_2, \ldots, \lambda_{dr})$. Let us consider $r = 1$ and $M_i = M$. The second term becomes

$$\frac{1}{2} \sum_{\boldsymbol{k}} \sum_{\lambda} M\omega_\lambda^2(\boldsymbol{k}) \tilde{\boldsymbol{z}}_{\boldsymbol{k},\lambda} \cdot \tilde{\boldsymbol{z}}_{\boldsymbol{k},\lambda}, \tag{4.1.25}$$

where we have denoted the eigenvalues of $\boldsymbol{\gamma}$ by $M\omega_\lambda^2(\boldsymbol{k})$.

$$\mathcal{H}_{\text{ion}} = \sum_{\boldsymbol{k}} \left[\frac{\tilde{\boldsymbol{P}}_{\boldsymbol{k}} \cdot \tilde{\boldsymbol{P}}_{-\boldsymbol{k}}}{2M} + \frac{1}{2} M \sum_{\lambda} \omega_\lambda^2(\boldsymbol{k}) \tilde{\boldsymbol{z}}_{\boldsymbol{k},\lambda} \cdot \tilde{\boldsymbol{z}}_{\boldsymbol{k},\lambda} \right]. \tag{4.1.26}$$

$\tilde{P}$ er ikke definert

Also the $\tilde{P}_{\boldsymbol{k}}$-vector has as many components as the normal modes $\tilde{\boldsymbol{z}}_{\boldsymbol{k},\lambda}$. We now quantize as for the single $1D$ harmonic oscillator,

$$\tilde{\boldsymbol{z}}_{\boldsymbol{k}\lambda} = \sqrt{\frac{\hbar}{2M\omega_{\boldsymbol{k}\lambda}}}\hat{e}_\lambda \left(a^\dagger_{-\boldsymbol{k},\lambda} + a_{+\boldsymbol{k},\lambda}\right) \tag{4.1.27}$$

$$\tilde{\boldsymbol{P}}_{\boldsymbol{k}\lambda} = i\sqrt{\frac{M\hbar\omega_{\boldsymbol{k}\lambda}}{2}}\hat{e}_\lambda \left(a^\dagger_{-\boldsymbol{k},\lambda} - a_{+\boldsymbol{k},\lambda}\right) \tag{4.1.28}$$

$\hat{e}_\lambda$: Unit vector of normal mode λ. Insert in $\mathcal{H}_{\text{ion}}$,

$$\mathcal{H}_{\text{ion}} = \sum_{\boldsymbol{k},\lambda} \hbar\omega_{k\lambda} \left(a^\dagger_{\boldsymbol{k}\lambda} a_{\boldsymbol{k}\lambda} + \frac{1}{2}\right) \tag{4.1.29}$$

$$[a_{\boldsymbol{k}\lambda}, a^\dagger_{\boldsymbol{k}'\lambda'}] = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'}. \tag{4.1.30}$$

$(a^\dagger_{\boldsymbol{k}\lambda}, a_{\boldsymbol{k}\lambda})$: Create a phonon with wavenumber $\boldsymbol{k}$ in normal mode λ.

Including higher-order terms in the lattice fluctuations will lead to interactions among the phonons. Usually, this interaction is very weak. Close to the melting point, larger lattice fluctuations are essential, but they cannot be treated reliably to any low-order expansion in deviations from equilibrium positions.

4.2 Electron-phonon coupling

The next step will be to consider the coupling of electrons and phonons

$$\mathcal{H}_{\text{phonon}} = \sum_{q,\lambda} \omega_{q\lambda} \left(a^\dagger_{q\lambda} a_{q\lambda} + \frac{1}{2}\right). \tag{4.2.1}$$

<u>Plane-wave basis for electrons:</u>

$$\begin{aligned}\mathcal{H}_{\text{el}} = &\sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \boxed{\sum_{k,q,\sigma} \tilde{U}(q) c^\dagger_{k+q} c_{k\sigma}} \\ &+ \sum_{k,k',q}\sum_{\sigma\sigma'} \tilde{V}(q) c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k'\sigma'} c_{k\sigma}\end{aligned} \tag{4.2.2}$$

In $\mathcal{H}_{\text{el}}$, the second term originates with the crystal potential that the electrons move through. In our earlier considerations, this crystal potential was assumed to come from a rigid lattice of ions. The coupling with electrons and lattice vibrations also originates with this term, when we allow the ions to vibrate around their equilibrium positions.

$$\mathcal{H}_{\text{el-ion}} = \sum_i U(\boldsymbol{r}_i) = \sum_{i,j} V_{\text{el-ion}}(\boldsymbol{r}_i - \boldsymbol{R}_j \tag{4.2.3}$$

Previously, we considered a rigid ionic crystal $\{\boldsymbol{R}_j\} = \{\boldsymbol{R}_{0j}\}$

$$U_0 \equiv \sum_j V_{\text{el-ion}}(\boldsymbol{r}_i - \boldsymbol{R}_{0j}) \tag{4.2.4}$$

$$\sum_i U_0(\boldsymbol{r}_i) \to \sum_{k,q,\sigma} \tilde{U}_0(\boldsymbol{q}) c^\dagger_{k+q,\sigma} c_{k,\sigma}, \tag{4.2.5}$$

as we have seen, where

$$\tilde{U}_0(\boldsymbol{q}) = \frac{1}{V} \sum_{\boldsymbol{r}} U_0(\boldsymbol{r}) \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}}. \tag{4.2.6}$$

We now allow $\{\boldsymbol{R}_j\}$ to deviate from the equilibrium positions $\{\boldsymbol{R}_{0j}\}$

$$\sum_i U(\boldsymbol{r}_i) \to \sum_{k,q,\sigma} \tilde{U}(\boldsymbol{q}) c^\dagger_{k+q,\sigma} c_{k,\sigma} \tag{4.2.7}$$

$$\tilde{U}(\boldsymbol{q}) = \frac{1}{V} \sum_{\boldsymbol{r}} U(\boldsymbol{r}) \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}}. \tag{4.2.8}$$

$$\begin{aligned} U(\boldsymbol{r}) &= \sum_j V\left(\boldsymbol{r} - \boldsymbol{R}_{0j} + \sum_\lambda \boldsymbol{u}_{j\lambda}\right) \\ &= U_0(\boldsymbol{r}) + \sum_j \sum_\lambda \boldsymbol{u}_{j\lambda} \cdot \boldsymbol{\nabla} V(\boldsymbol{r} - \boldsymbol{R}_{0j}) \\ &= U_0(\boldsymbol{r}) + F(\boldsymbol{r}) \end{aligned} \tag{4.2.9}$$

$$\boldsymbol{u}_{j\lambda} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \underbrace{\tilde{u}_{\boldsymbol{k}\lambda}}_{\text{normal modes}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}_{0j}} \tag{4.2.10}$$

$$V(\boldsymbol{R}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \tilde{V}(\boldsymbol{k}) \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}} \tag{4.2.11}$$

$$\tilde{F}(\boldsymbol{q}) = \frac{1}{V} \sum_{\boldsymbol{r}} F(\boldsymbol{r}) \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \tag{4.2.12}$$

$$\boldsymbol{\nabla} V = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} i\boldsymbol{k} \tilde{V}(\boldsymbol{k}) \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}}. \tag{4.2.13}$$

$$U(\boldsymbol{r}) = U_0(\boldsymbol{r}) + F(\boldsymbol{r}) \tag{4.2.14}$$

$$\sum_i U(\boldsymbol{r}_i) \to \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \tilde{U}_0(\boldsymbol{q}) c^\dagger_{k+q,\sigma} c_{k,\sigma} + \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \tilde{F}(\boldsymbol{q}) c^\dagger_{k+q,\sigma} c_{k,\sigma} \tag{4.2.15}$$

$$\tilde{F}(\boldsymbol{q}) = \frac{1}{V}\sum_{\boldsymbol{r}} \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F(\boldsymbol{r}) \tag{4.2.16}$$

$$= \frac{1}{V}\sum_{\boldsymbol{r}} \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \sum_{\boldsymbol{R}_{0j}}\sum_{\lambda} \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}_1} \tilde{\boldsymbol{u}}_{\boldsymbol{k}_1\lambda} \mathrm{e}^{i\boldsymbol{k}_1\cdot\boldsymbol{R}_{0j}} \tag{4.2.17}$$

$$\times \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}_2} i\boldsymbol{k}_2 \tilde{V}(\boldsymbol{k}_2) \mathrm{e}^{i\boldsymbol{k}_2\cdot(\boldsymbol{r}-\boldsymbol{R}_{0j})}. \tag{4.2.18}$$

$$\sum_{\boldsymbol{r}} \to V\delta_{\boldsymbol{k}_2,\boldsymbol{q}} \tag{4.2.19}$$

$$\sum_{\boldsymbol{R}_{0j}} \to N\delta_{\boldsymbol{k}_2,\boldsymbol{k}_1} \tag{4.2.20}$$

$$\tilde{F}(\boldsymbol{q}) = \sum_{\lambda} \tilde{\boldsymbol{u}}_{q\lambda} \cdot i\boldsymbol{q}\tilde{V}(\boldsymbol{q}), \tag{4.2.21}$$

I forrige seksjon brukes $\tilde{\boldsymbol{z}}_{q\lambda}$ for normalmodene.

where $\tilde{\boldsymbol{u}}_{q\lambda}$ us a normal mode given by

$$\tilde{\boldsymbol{u}}_{q\lambda} = \sqrt{\frac{\hbar}{2M\omega_{q\lambda}}} \left(a^\dagger_{-q,\lambda} + a_{+q,\lambda}\right) \hat{e}_{q\lambda}. \tag{4.2.22}$$

Thus, we obtain

$$\sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \tilde{F}(\boldsymbol{q}) c^\dagger_{k+q,\sigma} c_{k,\sigma} = \sum_{\boldsymbol{k},\boldsymbol{q},\sigma,\lambda} \sqrt{\frac{\hbar}{2M\omega_{q\lambda}}} \left(i\boldsymbol{q}\cdot\hat{e}_{q\lambda}\right) \tilde{V}_{\text{el-ion}}(\boldsymbol{q}) \tag{4.2.23}$$

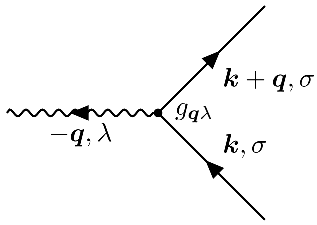
$$\times \left(a^\dagger_{-q,\lambda} + a_{+q,\lambda}\right) c^\dagger_{k+q,\sigma} c_{k,\sigma} \tag{4.2.24}$$

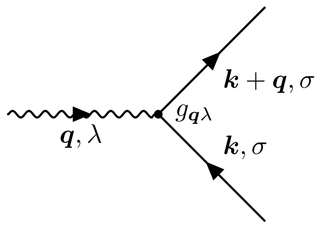
$$= \sum_{\boldsymbol{k},\boldsymbol{q},\sigma,\lambda} g_{\boldsymbol{q},\lambda} \left(a^\dagger_{-q,\lambda} + a_{+q,\lambda}\right) c^\dagger_{k+q,\sigma} c_{k,\sigma} \tag{4.2.25}$$

with

$$g_{\boldsymbol{q},\lambda} \equiv i\sqrt{\frac{\hbar}{2M\omega_{q\lambda}}} \left(\boldsymbol{q}\cdot\hat{e}_{q\lambda}\right) \tilde{V}_{\text{el-ion}}(\boldsymbol{q}). \tag{4.2.26}$$

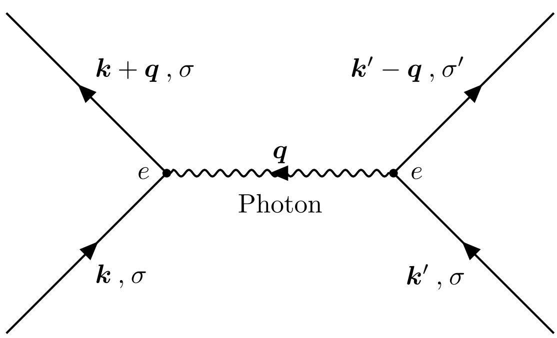
$g_{\boldsymbol{q},\lambda}$: Strength of electron-phonon coupling. The scattering of electrons by phonons is diagrammatically depicted as:



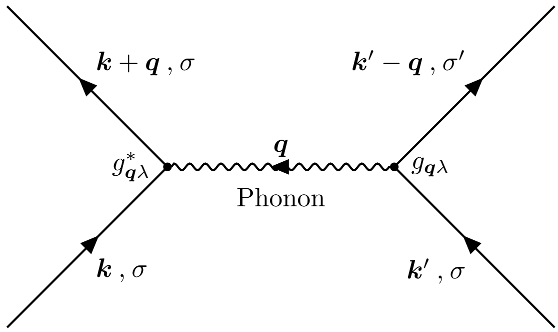


Note: $g_{q\lambda} \sim \frac{1}{\sqrt{M}}$ and $g_{q\lambda} \to 0; q \to 0$. The strongest el-ph coupling is via acoustical phonons ($\omega_{q\lambda} \to 0; q \to 0$), while optical phonons ($\omega_{q\lambda} \neq 0; q \to 0$) couple relatively weakly.

Notice how similar this looks like electron-photon coupling. The only difference lies in the coupling constant, which is e, the charge of the electron, in the electron-photon case. Coulomb-interactions between electrons are in fact mediated by photons. We may illustrate this as follows:



With phonons, we clearly can get the same effect:



In other words, in addition to Coulomb-interactions between electrons, we may have an additional electron-electron interaction mediated by phonons. This interaction is very weak, but as we will see later, it is responsible for driving a profound phase-transition in the electron gas which photons can never do: It can change a metal with ohmic resistance into a new state of matter with zero electrical resistance, a state called a superconductor.

Problems

CHAPTER 5

MANY-PARTICLE PERTURBATION THEORY

We assume that we are considering a system with a Hamiltonian $\mathcal{H}$, containing a part $\mathcal{H}_0$ that we can write the following way

$$\mathcal{H}_0 = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \qquad \text{(Fermions)} \tag{5.0.1}$$

$$\mathcal{H}_0 = \sum_{q,\lambda} \omega_{q\lambda} a^\dagger_{q\lambda} a_{q\lambda} \qquad \text{(Bosons)} \tag{5.0.2}$$

Suppose $\mathcal{H} = \mathcal{H}_0 + V$, and we want to describe the quantitative changes in observables when $\mathcal{H} = \mathcal{H}_0 \to \mathcal{H}_0 + V$, when we cannot solve the problem with $V \neq 0$ exactly. One then has to resort to more or less systematic approaches.

Examples of V:

i)
$$V = \sum_{k,q,\sigma} g_{q\lambda} \left(a^\dagger_{-q,\lambda} + a_{q,\lambda} \right) c^\dagger_{k+q,\sigma} c_{k,\sigma}$$

ii)
$$V = \sum_{\substack{k,k',q \\ \sigma,\sigma'}} \tilde{V}(q) c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k'\sigma'} c_{k\sigma}$$

iii) Hubbard-interaction

iv) etc

5.1 Time-evolution of states

i) Schrödinger-picture:

Operators are time-independent. States are time-dependent.

$$\begin{aligned} \hat{O}(t) &= \hat{O}(0) \\ i\frac{\mathrm{d}\left|\psi\right\rangle}{\mathrm{d}t} &= \mathcal{H}\left|\psi\right\rangle \\ \left|\psi(t)\right\rangle &= \mathrm{e}^{-\mathcal{H}t}\left|\psi(0)\right\rangle \end{aligned}$$

ii) Heisenberg-picture:

Operators are time-dependent. States are time-independent

$$\hat{O}(t) = \mathrm{e}^{i\mathcal{H}t}\hat{O}(0)\mathrm{e}^{-i\mathcal{H}t} \tag{5.1.1}$$

$$\left|\psi(t)\right\rangle = \left|\psi(0)\right\rangle \tag{5.1.2}$$

Notice that $\langle\psi(0)|\hat{O}(t)|\psi(0)\rangle = \langle\psi(t)|\hat{O}(0)|\psi(t)\rangle$, i.e Matrix-elements are the same in both the Heisenberg- and Schrödinger-picture. This suggests a considerable degree of freedom in choosing how to time-evolve operators and states, and the choice is to some extent dictated by convenience. For developing a (in principle!) systematic perturbation theory for observables in many-body systems, it turns out that a picture which is a hybrid of the Schrödinger- and Heisenberg picture, is convenient. In this picture "most of" the time-evolution the time-evolution is put in the operators, and "a little bit" of the time-evolution is put in the states;

$$\begin{aligned} O(t) &= \mathrm{e}^{i\mathcal{H}_0 t}\hat{O}(0)\mathrm{e}^{-i\mathcal{H}_0 t} \\ \left|\psi(t)\right\rangle &= \mathrm{e}^{i\mathcal{H}_0 t}\mathrm{e}^{-i\mathcal{H}t}\left|\psi(0)\right\rangle . \end{aligned} \tag{5.1.3}$$

The relations in eq. (5.1.3) give the same matrix-elements as in the Schrödinger and Heisenberg pictures. The non-trivial operator evolving $\left|\psi(t)\right\rangle$ is

$$U(t) = \mathrm{e}^{i\mathcal{H}_0 t}\mathrm{e}^{-i\mathcal{H}t} \tag{5.1.4}$$

$$\left|\psi(t)\right\rangle = U(t)\left|\psi(0)\right\rangle . \tag{5.1.5}$$

We would, ideally, like to establish a perturbation series in V in U. Note that in general, $[\mathcal{H}_0, V] \neq 0$ such that

$$\mathrm{e}^{-\mathcal{H}_0 t}\mathrm{e}^{i\mathcal{H}t} \neq \mathrm{e}^{-iVt}!$$

Proceed as follows:

$$\begin{aligned}
\frac{\mathrm{d}U(t)}{\mathrm{d}t} &= i\mathcal{H}_0 \mathrm{e}^{i\mathcal{H}_0 t}\mathrm{e}^{-i\mathcal{H}t} - i\mathrm{e}^{i\mathcal{H}_0 t}\mathrm{e}^{-i\mathcal{H}t}\mathcal{H} \\
&= i\mathrm{e}^{i\mathcal{H}_0 t}\underbrace{(\mathcal{H}_0 - \mathcal{H})}_{-V} e^{-i\mathcal{H}t} \\
&= -i\,\underbrace{\mathrm{e}^{i\mathcal{H}_0 t} V \mathrm{e}^{-i\mathcal{H}_0 t}}_{V(t)}\underbrace{\mathrm{e}^{i\mathcal{H}_0 t}\mathrm{e}^{-i\mathcal{H}t}}_{=U(t)} \\
&= -iV(t)U(t) \\
\int_{\tilde{t}}^{t} \mathrm{d}t'\,\frac{\mathrm{d}U(t')}{\mathrm{d}t'} &= -i\int_{\tilde{t}}^{t} \mathrm{d}t'\,V(t')U(t') \\
U(t) &= U(\tilde{t}) - i\int_{\tilde{t}}^{t} \mathrm{d}t'\,V(t')U(t') \\
U(0) &= 1, \quad \text{Choose } \tilde{t} = 0 \\
U(t) &= 1 - i\int_{0}^{t} \mathrm{d}t\,V(t')U(t')
\end{aligned}$$

This equation can be solved by iteration to generate a power seris in V. This is essentially what we will do, but before doing so, it will be convenient to introduce a slightly more general evolution-operator.

5.2 The S-matrix

The S-matrix is defined as follows:

$$\begin{aligned}
|\psi(t)\rangle &= S(t,t')\,|\psi(t')\rangle \\
S(t,0) &= U(t) \\
|\psi(t)\rangle &= S(t,t')U(t')\,|\psi(0)\rangle \\
U(t) &= S(t,t')U(t') \\
S(t,t') &= U(T)U^{-1}(t')
\end{aligned}$$

Using that $U^{\dagger} = U^{-1}$ (by the definition of U) we get

$$S(t,t') = U(t)U^{\dagger}(t') \tag{5.2.1}$$

Some properties of S:

i)
$$S(t,t') = 1$$

ii)
$$S^\dagger(t,t') = S(t',t) \tag{5.2.2}$$

iii)
$$\begin{aligned}
|\psi(t)\rangle &= S(t,t')\,|\psi(t')\rangle \\
&= S(t,t')S(t',t'')\,|\psi(t'')\rangle \\
&= S(t,t'')\,|\psi(t'')\rangle
\end{aligned}$$
$$S(t,t'') = S(t,t')S(t',t'') \tag{5.2.3}$$

The equation for S is

$$\begin{aligned}
\frac{\partial S(t,t')}{\partial t} &= \frac{\partial U}{\partial t} U^\dagger(t') \\
&= -V(t)U(t)U^\dagger(t') \\
&= -iV(t)S(t,t') \\
\int_{\tilde{t}}^{t} \mathrm{d}t''\, \frac{\partial S}{\partial t''} &= -i \int_{\tilde{t}}^{t} \mathrm{d}t''\, V(t'')S(t'',t') \\
S(t,t') &= S(\tilde{t},t') - i \int_{\tilde{t}}^{t} V(t'')S(t'',t')
\end{aligned}$$

Now choose $\tilde{t} = t'$ and use that $S(t',t') = 1$ to obtain

$$S(t,t'') = 1 - i \int_{t'}^{t} \mathrm{d}t''\, V(t'')S(t'',t') \tag{5.2.4}$$

This we will solve by iteration to produce a power series in V for S. This power-series for S will then generate a power-series in V for any observable.

Iteration:

0th order:
$$S_0('t,t') = 1$$

1st order:
$$\begin{aligned}
S_1(t,t') &= 1 - i \int_{t'}^{t} \mathrm{d}t''\, V(t'')S_0(t'',t') \\
&= 1 - i \int_{t'}^{t} \mathrm{d}t''\, V(t'')
\end{aligned}$$

2nd order:

$$S_2(t,t') = 1 - i\int_{t'}^{t} \mathrm{d}t''\, V(t'')S_1(t'',t')$$
$$= 1 + (-i)\int_{t'}^{t} \mathrm{d}t''\, V(t'') + (-i)^2 \int_{t'}^{t} \mathrm{d}t''\, V(t'') \int_{t'}^{t''} \mathrm{d}t'''\, V(t''')$$

Infinite order:

$$S(t,t') = 1 + \sum_{n=1}^{\infty} (-i)^n \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t_1} \mathrm{d}t_2 \cdots \int_{t'}^{t_{n-1}} \mathrm{d}t_n\, V(t_1)\cdots V(t_n) \tag{5.2.5}$$

Note: Lower integration limits are all the same, but the upper ones are different. We will now transform this integral into one where also all upper limits are the same, by introducing the time-ordering operator. $\tilde{T}$: time-ordering operator for fermions.

$$\tilde{T}\left[A(t_1)B^\dagger(t_2)\right] = \begin{cases} A(t_1)B^\dagger(t_2), & t_1 > t_2 \\ -B^\dagger(t_2)A(t_1), & t_2 > t_1 \end{cases} \tag{5.2.6}$$

Consider now the second-order in V-term in eq. (5.2.5), and work backwards, starting with

$$\frac{1}{2!}\int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t} \mathrm{d}t_2\, \tilde{T}[V(t_1)V(t_2)].$$

For $V(t)$, we assume that it is composed of fermion- or boson-operators in such a way that

$$\tilde{T}[V(t_1)V(t_2)] = \begin{cases} V(t_1)V(t_2), & t_1 > t_2 \\ V(t_2)V(t_1), & t_2 > t_1 \end{cases} \tag{5.2.7}$$

$$\frac{1}{2!}\int_{t'}^{t} \mathrm{d}t' \int_{t'}^{t_1} \mathrm{d}t_2\, V(t_1)V(t_2)$$
$$+ \frac{1}{2!}\int_{t'}^{t} \mathrm{d}t_1 \int_{t_1}^{t_2} \mathrm{d}t_2\, V(t_2)V(t_1)$$

Now let $t_1 \leftrightarrows t_2$ in the second term

$$\Longrightarrow \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t_1} \mathrm{d}t_2\, V(t_1)V(t_2) = \frac{1}{2!}\int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t} \mathrm{d}t_2\, \tilde{T}[V(t_1)V(t_2)] \tag{5.2.8}$$

In the same way,

$$
\begin{aligned}
&\frac{1}{n!}\int_{t'}^{t}\mathrm{d}t_1\int_{t'}^{t}\mathrm{d}t_2\cdots\int_{t'}^{t}\mathrm{d}t_n\,\tilde{T}[V(t_1)\cdots V(t_2)] \\
&\quad=\int_{t'}^{t}\mathrm{d}t_1\cdots\int_{t'}^{t_{n-1}}\mathrm{d}t_n\,V(t_1)\cdots V(t_n)
\end{aligned}
\tag{5.2.9}
$$

Thus, we have for $S(t,t')$

$$
\begin{aligned}
S(t,t') &= 1+\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int_{t'}^{t}\mathrm{d}t_1\cdots\int_{t'}^{t}\mathrm{d}t_n\,\tilde{T}[V(t_1)\cdots V(t_n)] \\
&= 1+\tilde{T}\left\{\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\left[\int_{t'}^{t}\mathrm{d}t''\,V(t'')\right]^n\right\} \\
\implies S(t,t') &= \tilde{T}\left[\exp\left\{-i\int_{t'}^{t}\mathrm{d}t''\,V(t'')\right\}\right].
\end{aligned}
\tag{5.2.10}
$$

Typically, what we want to compute is some matrix-element of the form

$$
\begin{aligned}
&\langle\psi(0)|\hat{O}(t)|\psi(0)\rangle && \text{Heisenberg-picture} \\
&=\langle\psi(t)|\hat{O}(0)|\psi(t)\rangle && \text{Schrödinger-picture} \\
&=\langle\psi(t)|O(t)|\psi(t)\rangle && \text{Interaction-picture}
\end{aligned}
\tag{5.2.11}
$$

where $\hat{O}$ is an operator representing som observable. The main problem is that $|\psi\rangle$ is unknown. What we know how to find, is Φ_0 by

$$
\mathcal{H}_0\,|\Phi_0\rangle = E_0\,|\Phi_0\rangle\,. \tag{5.2.12}
$$

$|\Phi_0\rangle$: Eigenstate of the non-interacting system. The idea now is to replace $\langle\psi|\hat{O}|\psi\rangle$ with $\langle\Phi_0|\hat{A}|\Phi_0\rangle$, where we at least can find a power series in V for $\hat{A}$. Since Φ_0 is known, the necessary matrix-elements can be computed. It is the S-matrix that will facilitate this replacement. So we need to relate ψ and Φ_0.

Imagine that at $t=-\infty$ (distant past, "way before the dinosaurs"), $V(t)=0$. Then $\mathcal{H}=\mathcal{H}_0$, $\mathcal{H}\,|\psi\rangle=\mathcal{H}_0\,|\psi\rangle=E_0\,|\Phi_0\rangle$.

$$
|\psi(-\infty)\rangle = |\Phi_0\rangle\,.
$$

Next, bring in perturbation adiabatically.

$$
\mathcal{H}=\mathcal{H}_0+V\mathrm{e}^{-\varepsilon|t|}
$$

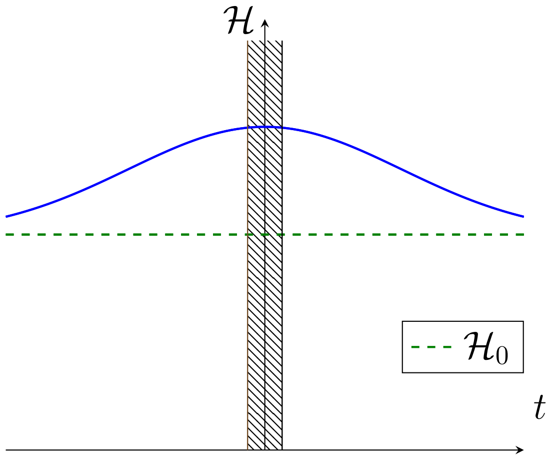


Figure 5.1: The shaded region represents the time interval of interest.

For $|t| << \varepsilon^{-1}, \mathcal{H} = \mathcal{H}_0 + V$, while for $|t| >> \varepsilon^{-1}, \mathcal{H} = \mathcal{H}_0$.

$$|\psi(t)\rangle = S(t, -\infty)\,|\Phi_0\rangle \tag{5.2.13}$$

What is $|\psi(+\infty)\rangle$? In the interaction picture, we have

$$\langle\psi(t)|O(t)|\psi(t)\rangle = \langle\Phi_0|S(-\infty, t)O(t)S(t, -\infty)|\Phi_0\rangle \tag{5.2.14}$$

If the leftmost factor of S had been $S(+\infty, t)$, then $SO(t)S$ would have been time-ordered. Therefore, we will try to bring in $S(+\infty, t)$ on the left, instead of $S(-\infty, t)$. We do this as follows:

$$\begin{aligned}
|\psi(\infty)\rangle &= S(\infty, -\infty)\,|\psi(-\infty)\rangle \\
&= S(\infty, -\infty)\,|\Phi_0\rangle \\
&= \mathrm{e}^{iL}\,|\Phi_0\rangle \\
\langle\Phi_0|\Phi_0\rangle &= 1 \\
\Longrightarrow\ \mathrm{e}^{iL} &= \langle\Phi_0|\psi(+\infty)\rangle \\
&= \langle\Phi_0|S(\infty, -\infty)|\Phi_0\rangle \\
|\psi(-\infty)\rangle &= S(-\infty, \infty)\,|\psi(+\infty)\rangle\,,
\end{aligned}$$

where eq. (5.2.2) was used in the last step.

NB:

$$|\Phi_0\rangle = \mathrm{e}^{iL} S(-\infty, \infty)\,|\Phi_0\rangle\,.$$

Now, we have what we need! By inserting $\langle\Phi_0| = \mathrm{e}^{-iL}\langle\Phi_0|\, S(\infty,-\infty)$ in eq. (5.2.14), we get

$$\langle\Phi_0|S(-\infty,t)O(t)S(t,-\infty)|\Phi_0\rangle = \mathrm{e}^{-iL}\langle\Phi_0|S(+\infty,t)O(t)S(t,-\infty)|\Phi_0\rangle$$

and finally

$$\langle\psi(t)|O(t)|\psi(t)\rangle = \frac{\langle\Phi_0|S(+\infty,t)O(t)S(t,-\infty)|\Phi_0\rangle}{\langle\Phi_0|S(\infty,-\infty)|\Phi_0\rangle} \tag{5.2.15}$$

with

$$O(t) = \mathrm{e}^{i\mathcal{H}_0 t}\hat{O}(0)\mathrm{e}^{-i\mathcal{H}_0 t}$$

(as in eq. (5.1.3)). Perturbation-expansion for $S \implies$ perturbation-expansion for matrix-element of $O(t)$. We also know the states with which to compute the matrix-elements. Notice that we may write

$$S(+\infty,t)O(t)S(t,-\infty)$$

as

$$\tilde{T}[O(t)S(+\infty,t)S(t,-\infty)] = \tilde{T}[O(t)S(\infty,-\infty)].$$

Therefore, we also have

$$\boxed{\langle\psi(t)|O(t)|\psi(t)\rangle = \frac{\langle\Phi_0|\tilde{T}[O(t)S(\infty,-\infty)]|\Phi_0\rangle}{\langle\Phi_0|S(\infty,-\infty)|\Phi_0\rangle}.} \tag{5.2.16}$$

Recall the relations for the different pictures eq. (5.2.11)

$$\begin{aligned}
&\langle\psi(0)|\hat{O}(t)|\psi(0)\rangle && \text{Heisenberg-picture}\\
&=\langle\psi(t)|\hat{O}(0)|\psi(t)\rangle && \text{Schrödinger-picture}\\
&=\langle\psi(t)|O(t)|\psi(t)\rangle && \text{Interaction-picture.}
\end{aligned}$$

The above was done for an operator $O(t)$ working at one time t. We need to generalize this to a product of operators working at different times t. To accomplish this, it is best to start in the Heisenberg-picture (otherwise, which times to use in $|\psi(t)\rangle$?

$$\begin{aligned}
\hat{O}(t_i) &= \mathrm{e}^{i\mathcal{H}t_i}\hat{O}(0)\mathrm{e}^{-i\mathcal{H}t_i}\\
&= \mathrm{e}^{i\mathcal{H}t_i}\mathrm{e}^{-i\mathcal{H}_0t_i}\mathrm{e}^{i\mathcal{H}_0t_i}\hat{O}(0)\mathrm{e}^{-i\mathcal{H}_0t_i}\mathrm{e}^{i\mathcal{H}_0t_i}\mathrm{e}^{-i\mathcal{H}t_i}\\
&= U^\dagger(t_i)O(t_i)O(t_i)\\
&= S^\dagger(t_i,0)O(t_i)S(t_i,0)\\
&= \underline{S(0,t_i)O(t_i)S(t_i,0)}
\end{aligned} \tag{5.2.17}$$

$$\begin{aligned}\hat{O}(t_1)\hat{O}(t_2) &= S(0,t_1)O(t_1)\underbrace{S(t_1,0)S(0,t_2)}_{=S(t_1,t_2)}O(t_2)S(t_2,0) \\ &= S(0,t_1)O(t_1)S(t_1,t_2)O(t_2)S(t_2,0)\end{aligned} \tag{5.2.18}$$

$$\begin{aligned}\tilde{T}[\hat{O}(t_1)\hat{O}(t_2)] &= \tilde{T}[O(t_1)O(t_2)\underbrace{S(0,t_1)S(t_1,t_2)S(t_2,0)}_{=S(0,0)=1}] \\ &= \tilde{T}[O(t_1)O(t_2)]\end{aligned} \tag{5.2.19}$$

This generalises to an arbitrary number of operators. Finally, we therefore have

$$\boxed{\langle\psi(0)|\tilde{T}[\hat{O}_1(t_1)\dots\hat{O}_n(t_n)]|\psi(0)\rangle = \frac{\langle\Phi_0|\tilde{T}[O_1(t_1)\dots O_n(t_n)S(\infty,-\infty)]|\Phi_0\rangle}{\langle\Phi_0|S(\infty,-\infty)|\Phi_0\rangle}} \tag{5.2.20}$$

So also the expectation values of such more complicated objects have a perturbation series generated by the perturbation series for S. **Equation (5.2.20) applies to bosons as well as fermions.** We are now set to compute expectation values of any observable in a systematic perturbation expansion. We will focus on a particularly important quantity, namely the **single-particle Green's function.** This quantity is extremely important, since it gives direct information about the exact excitation spectrum of for instance electrons or magnetic excitations, and can be measured with a number of well-established highly accurate and sophisticated techniques. Examples of such techniques are

1. Small-angle neutron scattering (SANS)
2. Angle-resolved photoemmision spectroscopy (ARPES)
3. Tunneling Electron Microscopy (TEM)
4. etc.

5.3 Single-particle Green's function

Let $(c_\lambda^\dagger, c_\lambda)$ be the creation or destruction operator for a fermion or boson in state λ. Define the single-particle Green's function $G(\lambda_1,t_1;\lambda_2,t_2)$ as follows

$$G(\lambda_1,t_1;\lambda_2,t_2) \equiv -i\,\langle\psi(0)|\tilde{T}[\hat{c}_{\lambda_2}(t_2)\hat{c}^\dagger_{\lambda_1}(t_1)]|\psi(0)\rangle \tag{5.3.1}$$

Notice that the basic formulation is in the Heisenberg-picture, since G involves a time-ordered product of operators (at different times). Using our general result in eq. (5.2.20), we immidiately formulate G as

$$G(\lambda_1, t_1; \lambda_2, t_2) = -i \frac{\langle \Phi_0 | \tilde{T}[c_{\lambda_2}(t_2) c^\dagger_{\lambda_1}(t_1) S(\infty, -\infty)] | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle}. \tag{5.3.2}$$

Physical interpretation of G: It is the probability amplitude that if a particle is created in state λ_1 at time t_1, it is found in state λ_2 at time t_2. Green's function for the **non-interacting case**: $G_0(\lambda_1, t_2; \lambda_2, t_2)$. To get some more intuition for what G means, let us compute G_0 explicitly.

$V = 0 \implies S(t, t') = 1 \implies$

$$G_0(\lambda_1, t_1; \lambda_2, t_2) = -i \langle \Phi_0 | \tilde{T}[c_{\lambda_2}(t_2) c^\dagger_{\lambda_1}(t_1)] | \Phi_0 \rangle \tag{5.3.3}$$

$$c_\lambda(t) = \mathrm{e}^{i\mathcal{H}_0 t} c_\lambda \mathrm{e}^{-i\mathcal{H}_0 t} \tag{5.3.4}$$

$$c^\dagger_\lambda(t) = \mathrm{e}^{i\mathcal{H}_0 t} c^\dagger_\lambda \mathrm{e}^{-i\mathcal{H}_0 t} \tag{5.3.5}$$

$$\mathcal{H}_0 |\Phi_0\rangle = E_0 |\Phi_0\rangle \tag{5.3.6}$$

To proceed further, we now have to treat fermions and bosons separately, both because of the different effects $\tilde{T}$has, but also because of the vast difference in $|\Phi_0\rangle$.

5.3.1 Fermions

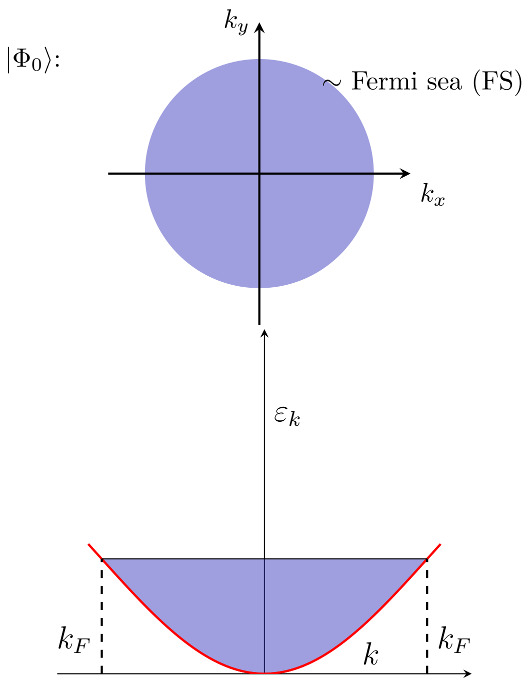
$\lambda = \mathbf{k}, \sigma$

$$\mathcal{H}_0 = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \tag{5.3.7}$$

i) Consider first $t_2 > t_1$:

$$\begin{aligned}
&G_0(\lambda_1, t_1, \lambda_2, t_2) \\
&= -i\theta(t_2 - t_1) \langle \Phi_0 | c_{k_2,\sigma_2}(t_2) c^\dagger_{k_1\sigma_1}(t_1) | \Phi_0 \rangle \\
&= -i\theta(t_2 - t_1) \langle \Phi_0 | \mathrm{e}^{i\mathcal{H}_0 t_2} c_{k_2\sigma_2} \mathrm{e}^{-i\mathcal{H}_0 t_2} \mathrm{e}^{i\mathcal{H}_0 t_1} c^\dagger_{k_1\sigma_1} \mathrm{e}^{-i\mathcal{H}_0 t_1} | \Phi_0 \rangle \\
&= -i\theta(t_2 - t_1) \langle \Phi_0 | \mathrm{e}^{i(E_0 + \varepsilon_{k_1} - \varepsilon_{k_2}) t_2} c_{k_2\sigma_2} \mathrm{e}^{-i(E_0 + \varepsilon_{k_1}) t_2} \mathrm{e}^{i(E_0 + \varepsilon_{k_1}) t_1} c^\dagger_{k_1\sigma_1} \mathrm{e}^{-E_0 t_1} | \Phi_0 \rangle \\
&= -i\theta(t_2 - t_1) \mathrm{e}^{i(\varepsilon_{k_1} - \varepsilon_{k_1}) t_2} \mathrm{e}^{-i\varepsilon_{k_1}(t_2 - t_1)} \underbrace{\langle \Phi_0 | c_{k_2\sigma_2} c^\dagger_{k_1\sigma_1} | \Phi_0 \rangle}_{\delta_{k_1k_2}\delta_{\sigma_1\sigma_2}\theta(\varepsilon_{k_1} - \varepsilon_{k_F})} \\
&= -i\theta(t_2 - t_1) \mathrm{e}^{-i\varepsilon_{k_1}(t_2 - t_1)} \delta_{k_1k_2} \delta_{\sigma_1\sigma_2} \theta(\varepsilon_{k_1} - \varepsilon_{k_F})
\end{aligned}$$

ii) $t_1 > t_2$:



(a) States are filled up to the energy ε_F at $k = k_F$ according to the Pauli-principle.

$$
\begin{aligned}
&G_0(\lambda_1, t_1, \lambda_2, t_2)\\
&= -i\theta(t_1 - t_2)(-1)\, \langle \Phi_0 | c^\dagger_{k_1\sigma_1}(t_1) c_{k_2,\sigma_2}(t_2) | \Phi_0 \rangle\\
&= i\theta(t_1 - t_2)\, \langle \Phi_0 | \mathrm{e}^{i\mathcal{H}_0 t_1} c^\dagger_{k_1\sigma_1} \mathrm{e}^{-i\mathcal{H}_0 t_1} \mathrm{e}^{i\mathcal{H}_0 t_2} c_{k_2\sigma_2} \mathrm{e}^{-i\mathcal{H}_0 t_2} | \Phi_0 \rangle\\
&= i\theta(t_1 - t_2)\, \langle \Phi_0 | \mathrm{e}^{i(E_0 + \varepsilon_{k_1} - \varepsilon_{k_2}) t_1} c^\dagger_{k_1\sigma_1} \mathrm{e}^{-i(E_0 - \varepsilon_{k_2}) t_1} \mathrm{e}^{i(E_0 - \varepsilon_{k_2}) t_2} c_{k_2\sigma_2} \mathrm{e}^{-E_0 t_2} | \Phi_0 \rangle\\
&= i\theta(t_1 - t_2) \mathrm{e}^{i\varepsilon_{k_1} t_1} \mathrm{e}^{-i\varepsilon_{k_2} t_2} \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \theta(\varepsilon_{k_F} - \varepsilon_{k_1})\\
&= i\theta(t_1 - t_2) \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \theta(\varepsilon_{k_F} - \varepsilon_{k_1}) \mathrm{e}^{-i\varepsilon_{k_1}(t_2 - t_1)}
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
G_0(k_1\sigma_1, t_1; k_2\sigma_2, t_2) = &- i\theta(t_2 - t_1)\theta(\varepsilon_{k_1} - \varepsilon_{k_F}) \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \mathrm{e}^{-i\varepsilon_{k_1}(t_2 - t_1)}\\
&+ i\theta(t_1 - t_2)\theta(\varepsilon_{k_F} - \varepsilon_{k_1}) \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \mathrm{e}^{-i\varepsilon_{k_1}(t_2 - t_1)}
\end{aligned}
\tag{5.3.8}
$$

This is a rather unwieldy expression, so to simplify a bit, we set $t_2 - t_1 = t$ and introduce Fourier-transformed G_0.

$$
\begin{aligned}
G_0(k_1\sigma_1; k_2\sigma_2; \omega) &= \int_{-\infty}^{\infty} \mathrm{d}t\, G_0(k_1\sigma_1; k_2\sigma_2; t) \mathrm{e}^{i\omega t}\\
&= -i\theta(\varepsilon_{k_1} - \varepsilon_{k_F}) \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \int_0^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\varepsilon_{k_1} t} \underbrace{\mathrm{e}^{-\delta t}}_{\delta = 0^+} \mathrm{e}^{i\omega t}\\
&+ i\theta(\varepsilon_{k_F} - \varepsilon_{k_1}) \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{-i\varepsilon_{k_1} t} \underbrace{\mathrm{e}^{\delta t}}_{\delta = 0^+} \mathrm{e}^{i\omega t}\\
&= -i\theta(\varepsilon_{k_1} - \varepsilon_{k_F}) \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \int_0^{\infty} \mathrm{d}t\, \mathrm{e}^{i(\omega - \varepsilon_{k_1} + i\delta) t}\\
&+ i\theta(\varepsilon_{k_F} - \varepsilon_{k_1}) \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{i(\omega - \varepsilon_{k_1} - i\delta) t}\\
&= \delta_{k_1 k_2} \delta_{\sigma_1\sigma_2} \left(\frac{\theta(\varepsilon_{k_1} - \varepsilon_{k_F})}{\omega - \varepsilon_{k_1} + i\delta} + \frac{\theta(\varepsilon_{k_F} - \varepsilon_{k_1})}{\omega - \varepsilon_{k_1} - i\delta} \right)
\end{aligned}
$$

- The first term in the Green's function involves excitations above the Fermi-surface (particles), depicted in fig. 5.3. Particle created first, then destroyed later. Particle moves forward in time. This is seen directly from the expression for G_0 in the time-domain, eq. (5.3.8), when $t_2 > t_1$ (particle created first at time t_1, then destroyed later at time t_2).
- The second term in the Green's function involves excitations below the Fermi-surface (holes), depicted in fig. 5.4. Particle destroyed first, then created later. Particle moves backwards in time. This is again seen directly in eq. (5.3.8).

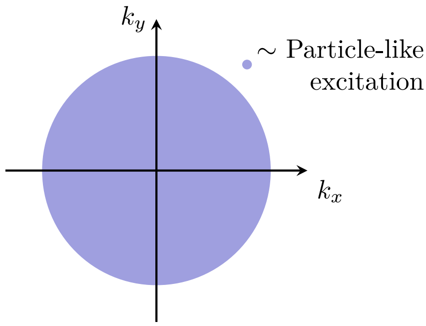


Figure 5.3: Particle excitation above the Fermi-surface.

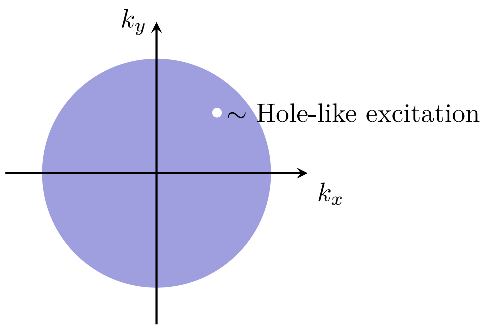


Figure 5.4: Hole excitation below the Fermi-surface.

- The part of G_0 that moves a particle forward in time is often referred to as a retarded Green's function G_0^R.
- The part of G_0 that moves a particle backwards in time is often referred to as a advanced Green's function G_0^A.

$$G_0^R(k_1,\sigma_1;k_2,\sigma_2;\omega) = \frac{\theta(\varepsilon_{k_1}-\varepsilon_F)}{\omega_-\varepsilon_{k_1}+i\delta}\delta_{k_1k_2}\delta_{\sigma_1\sigma_2} \tag{5.3.9}$$

$$G_0^A(k_1,\sigma_1;k_2,\sigma_2;\omega) = \frac{\theta(\varepsilon_F-\varepsilon_{k_1})}{\omega_-\varepsilon_{k_1}-i\delta}\delta_{k_1k_2}\delta_{\sigma_1\sigma_2} \tag{5.3.10}$$

With the understanding that in G_0, we must have $k_1 = k_2$; $\sigma_1 = \sigma_2$ and $\varepsilon_{k_1} > \varepsilon_F$ in G^R, $\varepsilon_{k_!} < \varepsilon_F$ in G^A, we may write

$$G_0^R(k,\omega) = \frac{1}{\omega-\varepsilon_k+i\delta} \tag{5.3.11}$$

$$G_0^A(k,\omega) = \frac{1}{\omega-\varepsilon_k-i\delta}, \tag{5.3.12}$$

which is summarized by

$$G_0(k,\omega) = \frac{1}{\omega-\varepsilon_k+i\delta_k}, \tag{5.3.13}$$

where $\delta_k = \delta\mathrm{sign}(\varepsilon_k-\varepsilon_F)$.

> Note that the single-particle excitation energies appear as simple poles in the Green's function!

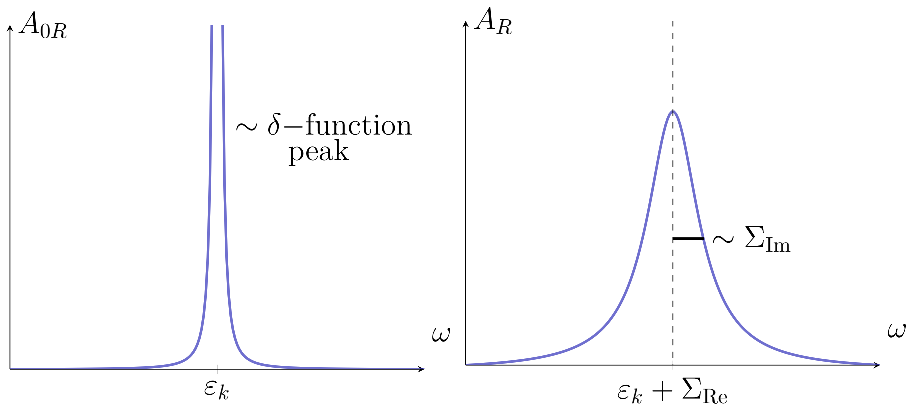
To aget a bit more perspective on things, consider $G_0^R(k,\omega)$ a bit further. $G_{0,R}^{-1} = \omega - \varepsilon_k + i\delta$ Imagine that we now introduce $V \neq 0$. What will happen is that the excitation spectrum ε_k will change, due to the perturbation $G_{0R}^{-1} \to G_R^{-1}(k,\omega)$.

$$G_R^{-1}(k,\omega) = \omega - \varepsilon_k - \Sigma(k,\omega), \tag{5.3.14}$$

$\Sigma(k,\omega) = \Sigma_{\mathrm{Re}}(k,\omega) + i\Sigma_{\mathrm{Im}}(k,\omega)$.

Σ_{Re} :	Real part of Σ
Σ_{Im} :	Imaginary part of Σ

Physicall interpretation og G_R: Create a particle in (k,σ) at $t=0$. What is the probability amplitude of finding the particle in the same state at $t>0$?



(a) Non-interacting system.

(b) Interacting system.

Figure 5.5: Spectral weights for both interacting and non-interacting system.

Answer: G_R. $\Sigma(k,\omega)$ is the single particle self-energy. Note: $G_R^{-1} = G_{0R}^{-1} - \Sigma$

$$
\begin{aligned}
G_R &= \frac{1}{G_{0R}^{-1} - \Sigma} = \frac{G_{0R}}{1 - G_{0R}\Sigma} \\
&= G_{0R} + G_{0R}\Sigma G_{0R} + G_{0R}\Sigma G_{0R}\Sigma G_{0R} + \dots
\end{aligned}
$$

We can generate a perturbation expansion for G_R by a much simpler perturbation expansion for Σ! Define the spectral weight $A_R(k,\omega)$

$$A_R(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\{G_R(k,\omega)\} \tag{5.3.15}$$

This is the quantity one measures in ARPES

$$A_R(k,\omega) = -\frac{1}{\pi}\frac{\Sigma_{\mathrm{Im}}}{(\omega - \varepsilon_k - \Sigma_{\mathrm{Re}})^2 - \Sigma_{\mathrm{Im}}^2} \tag{5.3.16}$$

In the non-interacting case: $\Sigma_{\mathrm{Im}} = 0, \Sigma_{\mathrm{Im}} = -\delta; \delta = 0^+$

$$A_{0R}(k,\omega) = -\frac{1}{\pi}\frac{-\delta}{(\omega - \varepsilon_k)^2 + \delta^2} = \delta(\omega - \varepsilon_k), \tag{5.3.17}$$

which is a Dirac δ-function, shown in fig. 5.5a. Send in photons of different energies and momenta to map out ε_k. For $V \neq 0$: Peak position is shifted, narrow peak is broadened, as shown in fig. 5.5b. From maximum in peak:

$\varepsilon_k + \Sigma_{\text{Re}} = \tilde{\varepsilon}_k$. From width of peak: Σ_{Im}. $\Sigma = \Sigma_{\text{Re}} + i\Sigma_{\text{Im}}$. Σ_{Re} and Σ_{Im} are related via the Kramers-Kronig relations

$$\Sigma_R(k,\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\Sigma_{\text{Im}}(k,\omega')}{\omega'-\omega}. \tag{5.3.18}$$

Therefore, from width of peak $\rightarrow \Sigma_{\text{Im}}$. From Kramers-Kronig: Σ_{Re}. This allows an ARPES experiment to uniquely determine both Σ_{Im} and Σ_{Re} from one measurement, and thus to back out the many-body effect in $\tilde{\varepsilon}_k$, the quasi-particle excitation spectrum. Note: For Kramers-Kronig to hold, $\Sigma(k,\omega)$ need to be analytic in the upper half-plane when ω is viewed as a complex variable. Moreover, Σ must fall off faster than $\frac{1}{|\omega|}$ when $|\omega| \rightarrow \infty$. For the perturbations we will consider, this will be the case.

> Our goal will therefore be to compute Σ in many-body perturbation theory.

Before we go into this, it will be turn out to be necessary to also consider bosonic Green's functions, and we start with the non-interacting case

5.3.2 Bosons

$$\begin{aligned} D(q,t-t') &= -i \langle \Psi(0)|\tilde{T}[\hat{A}_q(t)\hat{A}_q^\dagger(t')]|\Psi(0)\rangle \\ &= -i\frac{\langle \Phi_0|\tilde{T}[\hat{A}_q(t)\hat{A}_q^\dagger(t')S(\infty,-\infty)]|\Phi_0\rangle}{\langle \Phi_0|S(\infty,-\infty)|\Phi_0\rangle}. \end{aligned}$$

$|\Phi_0\rangle$: Unperturbed ground state of bosonic system.

$$D_0(q,t-t') = -i \langle \Phi_0|\tilde{T}[\hat{A}_q(t)\hat{A}_q^\dagger(t')]|\Phi_0\rangle . \tag{5.3.19}$$

Retarded boson-propagator: $t' < t$. Advanced boson-propagator: $t' > t$. At $T = 0$, the lowest energy state is occupied by all bosons (material particles), or there are no bosons present at all (phonons, magnons). Let us focus in the following focus on <u>phonons</u>.

$$\begin{aligned} A_q &= a_q + a_{-q}^\dagger \\ A_q(t) &= \mathrm{e}^{i\mathcal{H}_0 t}A_q\mathrm{e}^{-i\mathcal{H}_0 t} \\ \mathcal{H}_0 &= \sum_{q,\lambda}\omega_{q,\lambda}a_{q,\lambda}^\dagger a_{q,\lambda} \\ \mathcal{H}_0 |\Phi_0\rangle &= 0 = E_0 |\Phi_0\rangle, E_0 = 0 \end{aligned}$$

$t' = 0$, since D_0 will only be a function of $t - t'$ anyway. This is no loss of generality.

$t > 0$:

$$\begin{aligned} D_0(q,\lambda,t) &= -i\theta(t)\,\langle\Phi_0|\mathrm{e}^{i\mathcal{H}_0 t}A_{q\lambda}\mathrm{e}^{-i\mathcal{H}_0 t}A^\dagger_{q\lambda}|\Phi_0\rangle \\ &= -i\theta(t)\,\langle\Phi_0|A_{q\lambda}A^\dagger_{q\lambda}|\Phi_0\rangle\,\mathrm{e}^{-i\omega_{q,\lambda}t} \\ &= -i\theta(t)\mathrm{e}^{-i\omega_{q,\lambda}t} \end{aligned} \tag{5.3.20}$$

$t < 0$:

$$\begin{aligned} D_0(q,\lambda,t) &= -i\theta(-t)\,\langle\Phi_0|A^\dagger_{q\lambda}\mathrm{e}^{i\mathcal{H}_0 t}A_{q\lambda}\mathrm{e}^{-i\mathcal{H}_0 t}|\Phi_0\rangle \\ &= -i\theta(-t)\,\langle\Phi_0|A^\dagger_{q\lambda}A_{q\lambda}|\Phi_0\rangle\,\mathrm{e}^{i\omega_{q,\lambda}t} \\ &= -i\theta(-t)\mathrm{e}^{i\omega_{q,\lambda}t}. \end{aligned} \tag{5.3.21}$$

In total we have

$$D_0(q,\lambda,t) = -\theta(t)\mathrm{e}^{-i\omega_{q,\lambda}t} - i\theta(-i)\mathrm{e}^{i\omega_{q,\lambda}t}. \tag{5.3.22}$$

Note the sign change in the phase factor due to $A_q = a_q + a^\dagger_{-q}$. As for the fermionic case, let us Fourier-transform this, using shorthand notation $q = (q, \lambda)$.

$$\begin{aligned} D_0(q,\omega) &= \int_{-\infty}^{\infty} \mathrm{d}t\,\mathrm{e}^{i\omega t}D_0(q,t) \\ &= -i\int_0^\infty \mathrm{d}t\,\mathrm{e}^{i(\omega-\omega_q+i\delta)t} - i\int_{-\infty}^0 \mathrm{d}t\,\mathrm{e}^{i(\omega+\omega_q-i\delta)t} \\ &= \frac{1}{\omega-\omega_q+i\delta} - \frac{1}{\omega+\omega_q-i\delta} \\ &= \frac{2\omega_q}{\omega^2-\omega_q^2+i\eta}. \end{aligned} \tag{5.3.23}$$

Here, it does not make sense to consider retarded and advanced parts as for the fermions, since $A_q = a_q + a^\dagger_{-q}$

$$D_0^{-1} = \frac{\omega^2-\omega_q^2}{2\omega_q} + i\eta \tag{5.3.24}$$

Imagine now that we turn on interactions (between phonons and electrons, for example)

$$\boxed{D_0^{-1} \to D^{-1} = D_0^{-1} - \Pi} \tag{5.3.25}$$

Π : Phonon self-energy.

$$D = \frac{1}{D_0^{-1} - \Pi} = \frac{D_0}{1 - \Pi D_0}$$
$$= D_0 + D_0 \Pi D_0 + D_0 \Pi D_0 \Pi D_0 + \ldots$$

Again; Perturbation series for D by much simpler perturbation series for Π!

The equations

$$G_R^{-1} = G_{0R}^{-1} - \Sigma \tag{5.3.26}$$
$$D^{-1} = D_0^{-1} - \Pi \tag{5.3.27}$$

are usually referred to as the **Dyson's equations** for single-particle Green's functions. The physicall interpretations for G and D are the same (but of course applies to two different sorts of particles.) In the following, we will consider electron- phonon coupling as a perturbation. The phonons will lead to a Σ, and the electrons in turn will lead to a Π.

5.4 Perturbation theory for the single-particle Green's function

Denote this Green's function by $G(\lambda, t - t')$. We have previously argued that in the presence of interactions it may be expressed as follows

$$G^{-1} = G_0^{-1} - \Sigma \tag{5.4.1}$$

where G_0 is the single-particle Green's function in the non-interacting case, and Σ is the self-energy. Thus, our perturbation theory for G may be found by a perturbation expansion for Σ, which we may hope is easier to compute than a perturbation theory for G directly. The basic mathematical expression for G is, starting in the Heisenberg-picture

$$G(\lambda, t - t') = -i \langle \psi(0) | \tilde{T}[\hat{c}_\lambda(t) \hat{c}_\lambda^\dagger(t')] | \psi(0) \rangle \tag{5.4.2}$$

where $|\psi(0)\rangle$ are exact eigenstates and

$$\hat{c}_\lambda(t) = \mathrm{e}^{i\mathcal{H}t} c_\lambda \mathrm{e}^{-i\mathcal{H}t}. \tag{5.4.3}$$

Translated into interaction picture, we have

$$G(\lambda, t - t') = -i \frac{\langle \Phi_0 | \tilde{T}[c_\lambda(t) c_\lambda^\dagger(t') S(\infty, -\infty)] | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle}, \tag{5.4.4}$$

where S is the S-matrix,

$$c_\lambda(t) = \mathrm{e}^{i\mathcal{H}_0 t} c_\lambda \mathrm{e}^{-i\mathcal{H}_0 t}, \tag{5.4.5}$$

and $|\Phi_0\rangle$ is the eigenstate of $\mathcal{H}_0$, assumed to be known to us. Both of these expressions are formally exact, while the second one allows a systematic expansion in powers of $V(t)$, where

$$V(t) = \mathrm{e}^{i\mathcal{H}_0 t} V \mathrm{e}^{-i\mathcal{H}_0 t} \tag{5.4.6}$$

and $\mathcal{H} = \mathcal{H}_0 + V$. For $S(\infty, -\infty)$, we have (remember eq. (5.2.10))

$$S(t,t') = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} \mathrm{d}t_1 \cdots \int_{t'}^{t} \mathrm{d}t_n \, \tilde{T}[V(t_1)\cdots V(t_n)] \tag{5.4.7}$$

where the $n = 0$-term is 1. In these notes, we will focus on V taken to be the electron-phonon coupling. Another obvious choice would be the Coulomb-interaction.

$$V = \sum_{k,q,\sigma,\lambda} g_{q\lambda} A_{q\lambda} c^\dagger_{k+q,\sigma} c_{k,\sigma}, \tag{5.4.8}$$

$A_{q\lambda} = a^\dagger_{-q,\lambda} + a_{q\lambda}$.

$$\begin{aligned} V(t) &= \mathrm{e}^{i\mathcal{H}_0 t} V \mathrm{e}^{-i\mathcal{H}_0 t} \\ &= \sum_{k,q,\sigma,\lambda} g_{q\lambda} \mathrm{e}^{i\mathcal{H}_0 t} A_{q\lambda} c^\dagger_{k+q,\sigma} c_{k,\sigma} \mathrm{e}^{-i\mathcal{H}_0 t} \\ &= \sum_{k,q,\sigma,\lambda} g_{q\lambda} \left(\mathrm{e}^{i\mathcal{H}_0 t} A_{q\lambda} \mathrm{e}^{-i\mathcal{H}_0 t}\right) \left(\mathrm{e}^{i\mathcal{H}_0 t} c^\dagger_{k+q,\sigma} \mathrm{e}^{-i\mathcal{H}_0 t}\right) \left(\mathrm{e}^{i\mathcal{H}_0 t} c_{k,\sigma} \mathrm{e}^{-i\mathcal{H}_0 t}\right) \end{aligned}$$

$$\boxed{V(t) = \sum_{k,q,\sigma,\lambda} g_{q\lambda} A_{q\lambda}(t) c^\dagger_{k+q,\sigma}(t) c_{k,\sigma}(t)} \tag{5.4.9}$$

Compare $V(t)$ in eq. (5.4.9) to V in eq. (5.4.8). All time-dependence of operators is in the interaction picture. $V(t)$ is the perturbation we will use in $S(\infty, -\infty)$ and thus $G(\lambda, t - t')$. The expectation values we will have to compute will then consist of a product of $(c^\dagger, c)$-operators multiplied by a product of A-operators. Each V will give a factor $Ac^\dagger c$. Thus, n factors of V will give

$$\left.\begin{array}{cc} n+1 & c^\dagger\text{-factors} \\ n+1 & c\text{-factors} \\ n & A\text{ -factors} \end{array}\right\} \text{ in } G \tag{5.4.10}$$

The extra 1 in $n+1$ comes from $c^\dagger_\lambda(t'), c_\lambda(t)$ in the definition of G. Now, we factorize $|\Phi_0\rangle$ in a **boson-part** and a **fermion-part**.

$$\left.\begin{array}{cc} \text{Boson-part:} & |\Phi_0\rangle_B \\ \text{Fermion-part:} & |\Phi_0\rangle_F \end{array}\right\} \Longrightarrow |\Phi_0\rangle = |\Phi_0\rangle_B \otimes |\Phi_0\rangle_F \,. \tag{5.4.11}$$

$$\begin{aligned} G(\lambda, t-t') = & \frac{-i}{\langle\Phi_0|S(\infty,-\infty)|\Phi_0\rangle} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} \mathrm{d}t_1 \cdots \int_{-\infty}^{\infty} \mathrm{d}t_n \\ & \cdot \langle\Phi_0|\tilde{T}[c_\lambda(t)c^\dagger_\lambda(t')V(t_1)\ldots V(t_n)]|\Phi_0\rangle \,. \end{aligned} \tag{5.4.12}$$

$[\,\cdot\,]$: A product of $n+1$ $c^\dagger, c$-operators and n $A(t_i)$-operators. The expectation value of the fermion-operators are taken in $|\Phi_0\rangle_F$, while the expectation value of the boson-operators are taken in $|\Phi_0\rangle_B$. The expectation value may thus be written

$$\begin{aligned} & {}_B\langle\Phi_0|\tilde{T}[A_{q_1}(t_1)\ldots A_{q_n}(t_n)]|\Phi_0\rangle_B \\ & \cdot {}_F\langle\Phi_0|\tilde{T}[c_\lambda(t)c^\dagger_\lambda(t')c^\dagger_{k_1+q,\sigma_1}(t_1)c_{k_1\sigma_1}(t_1)\ldots c^\dagger_{k_n+q,\sigma_n}(t_n)c_{k_n\sigma_n}(t_n)]|\Phi_0\rangle_F \end{aligned}$$

NB! Be careful with the ordering of operators! We see that as n increases, the number of operators rapidly becomes sizeable, particularly in the fermionic part. One thing we immediately note, is that for these expectation values to be non-zero, we must have an even number of A-operators. Thus, for the electron-phonon coupling, only even powers of V contribute to the perturbation-series for G. (This is not the case if V were taken to be the Coulomb-interaction, which contains $c^\dagger c^\dagger cc$ and no boson-operators.) The lowest order term we need to consider, is therefore $n=2$, which contains 2 A-operators and 6 fermion-operators. For $n=2$, the boson-part is easy. Recall that

$$\begin{aligned} D_0(q,t) = & -i\,{}_B\langle\Phi_0|\tilde{T}[A_q(t)A_q(0)]|\Phi_0\rangle_B \\ & \Longrightarrow \\ & \quad {}_B\langle\Phi_0|\tilde{T}[A_q(t_1)A_q(t_2)]|\Phi_0\rangle_0 = iD_0(q,t_1-t_2), \end{aligned}$$

the free phonon Green's function we already computed. Next, we need to deal with the expectation value of a string of a fairly large number of fermion-operators (6 of them for $n=2$. $3c^\dagger$ and $3c$). To do this, we use a theorem which we give here without proof.

Wicks theorem

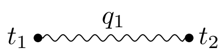
To compute the $|\Phi_0\rangle_F$-expectation value of a product of equally many $c^\dagger$ and c-operators, we pair in all possible ways and compute the expectation value as products of expectation values of one $c^\dagger$ and one c.

NB! When pairing up non-adjacent $c^\dagger$ and c, use anti-commutation relations to bring them side by side to compute an expectation value. Suppose we have a product of N creation operators and N destruction operators (bosonic of fermionic). The number of terms we then get by applying Wick's theorem is N! Thus for $n = 2$ with 3 $c^\dagger$ and 3 c, the number of terms is $3! = 6$. To fourth order, the number of bosonic terms will be $6 \cdot 2! = 12$ (since when expanding $A_q = a^\dagger_{-q} + a_q$ to fourth order there are 6 terms with 2 $a^\dagger$ and 2 a, and Wick's theorem applied to each of them gives another factor 2. The number of fermionic terms is given by $N = n + 1 = 5 \to 5! = 120$. Altogether $12 \cdot 120 = 1440$ terms. This rapidly gets out of hand, if we don't think a little and organize the calculations in a smart way. Recall the definitions of the non-interacting Green's functions of eqs. (5.3.3) and (5.3.19);

$$D_0(q_1, t_1 - t_2)\delta_{q_1,q_2} = -i \langle\Phi_0|\tilde{T}[A_{q_1}(t)A^\dagger_{q_2}(t')]|\Phi_0\rangle_B \tag{5.4.13}$$

$$G_0(k_1, t_1 - t_2)\delta_{k_1k_2}\delta_{\sigma_1\sigma_2} = -i \langle\Phi_0|\tilde{T}[c^\dagger_{k_1\sigma_1}(t_1)c_{k_2\sigma_2}(t_2)]|\Phi_0\rangle_F \tag{5.4.14}$$

We will give these the following pictorial representation:

$D_0(q_1, t_1 - t_2)$: 

(5.4.15)

$G_0(k_1, t_1 - t_2)$: 

(5.4.16)

These will turn out to be very helpful later on.

Start with $\langle\Phi_0|S(\infty, -\infty)|\Phi_0\rangle$:

$$\begin{aligned}&\langle\Phi_0|S(\infty, -\infty)|\Phi_0\rangle\\ &= 1 + \frac{(-i)^2}{2!}\int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \ \langle\Phi_0|\tilde{T}[V(t_1)V(t_2)]|\Phi_0\rangle + \mathcal{O}(V^4)\end{aligned}$$

Consider now in detail the second term

$$\frac{(-i)^2}{2!}\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{\infty}\mathrm{d}t_2\sum_{k_1,q_1,\sigma_1}\sum_{k_2,q_2,\sigma_2}g_{g_1}g_{q_2}$$
$$\cdot\,{}_B\langle\Phi_0|\tilde{T}[A_{q_1}(t_1)\underbrace{A_{q_2}(t_2)}_{=A^\dagger_{-q_2}(t_2)}]|\Phi_0\rangle_B$$
$$\cdot\,{}_F\langle\Phi_0|\tilde{T}[c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2\sigma_2}(t_2)]|\Phi_0\rangle_F$$

The bosonic expectation value $= iD_0(q_1, t_1-t_2)\delta_{q_1,-q_2}$. In the fermionic part, use Wick's theorem. There are 2 ways to pair the $c^\dagger$'s with the c's.

i)

$$c^\dagger_{k_1+q_1,\sigma_1}c_{k_1\sigma_1}c^\dagger_{k_2+q_2,\sigma_2}c_{k_2\sigma_2} \tag{5.4.17}$$

ii)

$$c^\dagger_{k_1+q_1,\sigma_1}c_{k_1\sigma_1}c^\dagger_{k_2+q_2,\sigma_2}c_{k_2\sigma_2} \tag{5.4.18}$$

with the corresponding equations

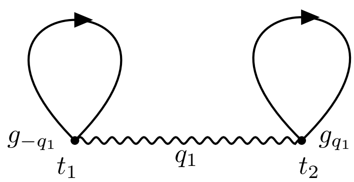
i)

$$\begin{aligned}&(+i)G_0(k_1+q_1,t_1-t_1)\delta_{k_1+q_1,k_1}\cdot(-1)\\ \cdot&(+i)G_0(k_2+q_2,t_2-t_2)\delta_{k_2+q_2,k_2}\cdot(-1)\end{aligned} \tag{5.4.19}$$

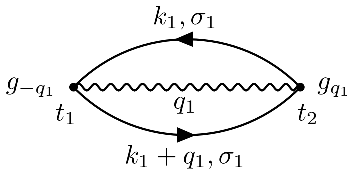
ii)

$$\begin{aligned}&(+i)G_0(k_1+q_1,t_2-t_1)\delta_{k_1+q_1,k_2}\delta_{\sigma_1\sigma_2}\cdot(-1)^3\\ \cdot&(+i)G_0(k_2+q_2,t_1-t_2)\delta_{k_2+q_2,k_1}\delta_{\sigma_1\sigma_2}\cdot(-1)\end{aligned} \tag{5.4.20}$$

In i), note that the δ-functions in k from the fermionic part forces $q_1 = 0, q_2 = 0$. Multiplying all the factors of i):

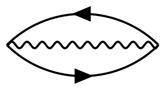


But $q_1 = q_2 = 0$. Since $g_q = 0$ when $q = 0$, this contribution to S vanishes. Consider next ii), which has the following representation:



Here, q_1 is not restricted to zero, so this contribution is nonzero. We must integrate over t_1, t_2, sum over k_1, q_1, σ_1. Note $g_{q_1} g_{-q_1} = g_{q_1} g^*_{q_1} = |g_{q_1}|^2$. So to $\mathcal{O}(V^2)$, we have

$$\langle \Phi_0 | S | \Phi_0 \rangle = 1 + \tag{5.4.21}$$



The first term is simply the normalization of $|\Phi_0\rangle$. The second contribution is a quantum fluctuation effect in $|\Phi_0\rangle$ due to the presence of phonons. These phonons "disturb" the inert state $|\Phi_0\rangle$. This is often called a vacuum-fluctuation. and is a quantum fluctuation effect, which is present even when the system is left all by itself. Note that this contribution enters into the denominator of the Green's function we are in the process of computing.

Consider next the numerator in G. The only difference between the numerator and $\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle$ is the extra $c_{k\sigma}(t) c^\dagger_{k\sigma}(t')$. The bosonic part is therefore exactly as in $\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle$, but the fermionic part now have 3 $c^\dagger$'s and 3 c's, instead of 2 $c^\dagger$'s and 2 c's. We therefore consider only this fermionic expectation value, remembering that the result must be multiplied with

$$iD_0(q_1, t_1 - t_2) \delta_{q_1, -q_2} g_{q_1} g_{q_2}. \tag{5.4.22}$$

The fermionic expectation value is

$${}_F \langle \Phi_0 | \tilde{T}[c_{k\sigma}(t) c^\dagger_{k\sigma}(t') c^\dagger_{k_1+q_1,\sigma_1}(t_1) c_{k_1\sigma_1}(t_1) c^\dagger_{k_2+q_2,\sigma_2}(t_2) c_{k_2\sigma_2}(t_2)] | \Phi_0 \rangle_F \,. \tag{5.4.23}$$

Using Wicks theorem, the terms are

1)

$$c_{k\sigma} c^\dagger_{k\sigma} c^\dagger_{k_1+q_1,\sigma_1} c_{k_1\sigma_1} c^\dagger_{k_2+q_2,\sigma_2} c_{k_2\sigma_2} \tag{5.4.24}$$

$$\Longrightarrow \delta_{k_1+q_1,k_1} \delta_{k_2+q_2,k_2} \delta_{\sigma_1\sigma_2} \Longrightarrow q_1 = q_2 = 0 \Longrightarrow \underline{1) = 0}.$$

2)

$$c_{k\sigma} c^\dagger_{k\sigma} c^\dagger_{k_1+q_1,\sigma_1} c_{k_1\sigma_1} c^\dagger_{k_2+q_2,\sigma_2} c_{k_2\sigma_2} \tag{5.4.25}$$

$$\implies \delta_{k,k_1+q_1}\delta_{\sigma,\sigma_1}\delta_{k,k_1}\delta_{k_2+q_2,k_2} \implies q_2 = 0 \implies \underline{2) = 0}.$$[1]

3)

$$c_{k\sigma}c^\dagger_{k\sigma}c^\dagger_{k_1+q_1,\sigma_1}c_{k_1\sigma_1}c^\dagger_{k_2+q_2,\sigma_2}c_{k_2\sigma_2} \tag{5.4.26}$$

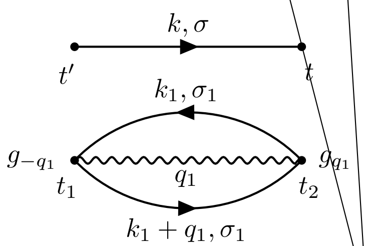
$$\implies \delta_{k,k_2+q_2}\delta_{\sigma,\sigma_2}\delta_{k,k_2}\delta_{k_1+q_1,k_1} \implies q_1 = 0 \implies \underline{3) = 0}.$$

4)

$$c_{k\sigma}c^\dagger_{k\sigma}c^\dagger_{k_1+q_1,\sigma_1}c_{k_1\sigma_1}c^\dagger_{k_2+q_2,\sigma_2}c_{k_2\sigma_2} \tag{5.4.27}$$

$$\begin{aligned} &= iG_0(k,t-t')(-i)G_0(k_1+q_1,t_2-t_1)\delta_{k_1+q_1,k_2}\delta_{\sigma_1,\sigma_2} \\ &\quad \cdot(+i)G_0(k_1,t_1-t_2)\delta_{k_2+q_2,k_1}\delta_{\sigma_1,\sigma_2} \end{aligned}$$

Let us give a pictorial representation of this:



This is a disconnected diagram. The interpretation of this is that the electron is disturbed by a quantum fluctuation in $|\Phi_0\rangle$, namely a vacuum-fluctuation. This vacuum-fluctuation is present even if we do not try to inject and extract an electron into the system. This is why the diagram comes out disconnected.

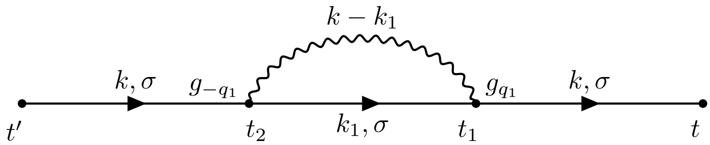
5)

$$c_{k\sigma}c^\dagger_{k\sigma}c^\dagger_{k_1+q_1,\sigma_1}c_{k_1\sigma_1}c^\dagger_{k_2+q_2,\sigma_2}c_{k_2\sigma_2} \tag{5.4.28}$$

$$\begin{aligned} = &(+i)G_0(k,t-t_1)\delta_{k,k_1+q_1}\delta_{\sigma,\sigma_1} \\ &(+i)G_0(k,t_2-t')\delta_{k,k_2}\delta_{\sigma,\sigma_2} \\ &(+i)G_0(k_1,t_1-t_2)\delta_{k_1,k_2+q_2}\delta_{\sigma_1,\sigma_2}(-1)^3 \end{aligned}$$

We may give the following pictorial representation of this:

[1] I think there is an error in the notes here for both 2) and 3) in the delta-functions, but the conclusions of zero contribution remains.



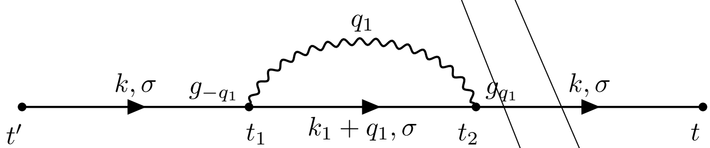
This is a connected diagram. The Green's function of the electron is disturbed by a quantum fluctuation, but in this case the quantum fluctuation is a direct result of injecting the electron into the system.

6)

$$c_{k\sigma}c^{\dagger}_{k\sigma}c^{\dagger}_{k_1+q_1,\sigma_1}c_{k_1\sigma_1}c^{\dagger}_{k_2+q_2,\sigma_2}c_{k_2\sigma_2} \tag{5.4.29}$$

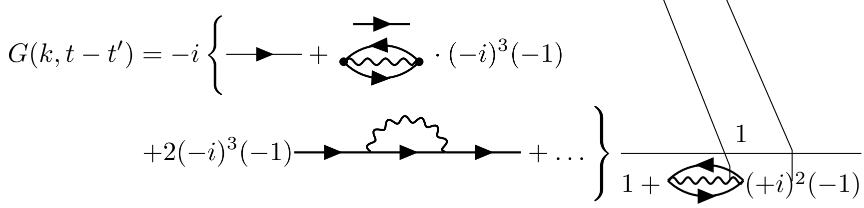
$$\begin{aligned}
&= (+i)G_0(k,t-t_2)\delta_{k,k_2+q_2}\delta_{\sigma,\sigma_2}\\
&\quad(-i)G_0(k,t_1-t')\delta_{k,k_1+q_1}\delta_{\sigma,\sigma_1}\\
&\quad(-i)G_0(k_1+q_1,t_2-t_1)\delta_{k_1+q_1,k_2}\delta_{\sigma_1,\sigma_2}(-1)^4
\end{aligned}$$

We may give the following pictorial description of this:

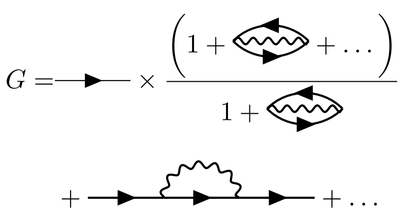


Same as 5).

Thus, we get to second order in g:



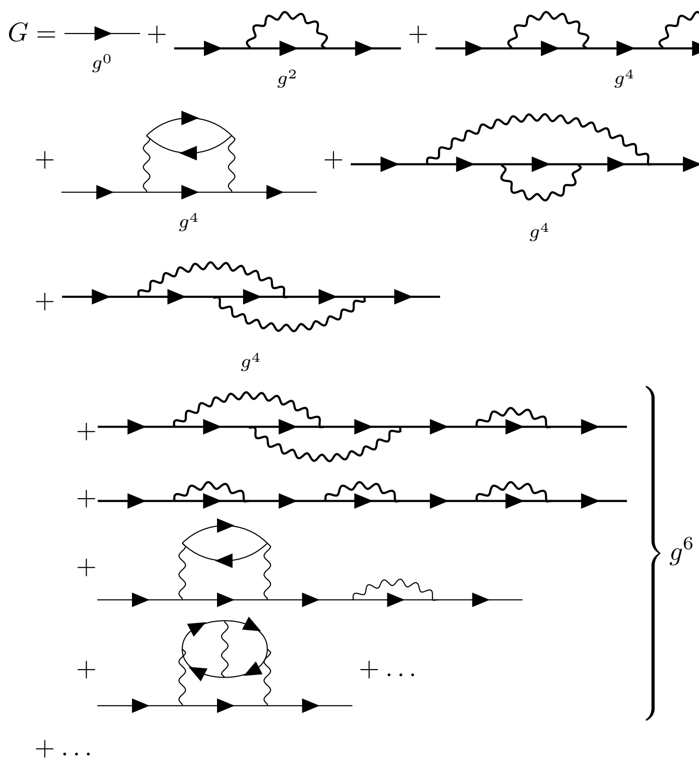
Schematically; to second order in g:



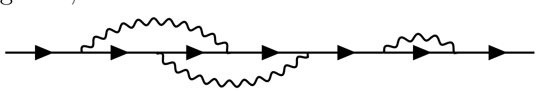
Disconnected diagrams cancel out. This will happen, order by order in g, to all orders.

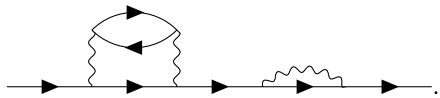
> G is the sum of connected diagrams.

Thus, we are computing corrections to G_0 which come about as a direct result of quantum fluctuations that arise **because** we injected an electron into the system. The vacuum fluctuations cancel out. Imagine now that we compute corrections to higher order in g, $g^4, g^6, \ldots$ etc. Schematically, we find

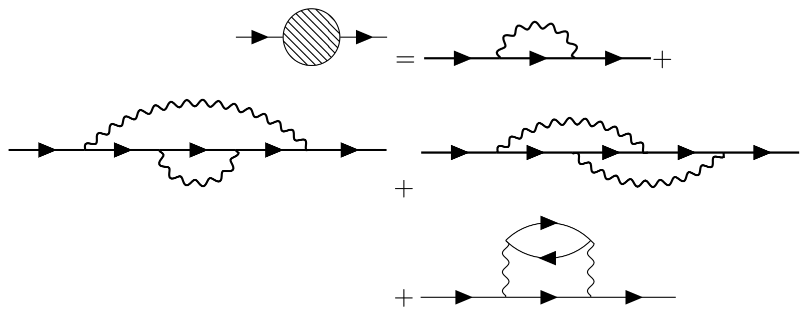


Note that some of these diagrams are just simple "products" of lower order diagrams, for instance ,

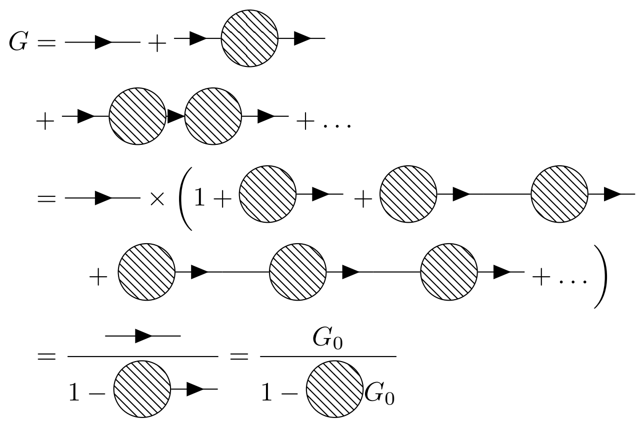
 and

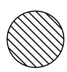


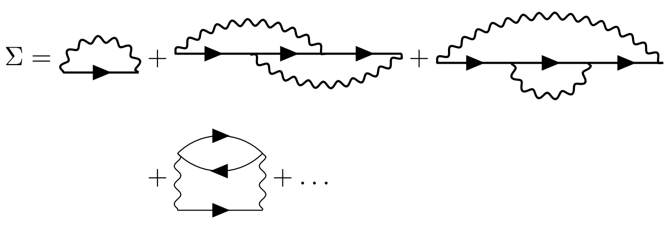
Imagine that we collect all non-repeated diagrams into one block:



Then



$$G^{-1} = G_0^{-1} -$$

$$= G_0^{-1} - \Sigma \tag{5.4.30}$$



Note: None of the diagrams that contribute to Σ will "fall apart" if we **cut one electron line**. Such diagrams are called **one particle irreducible**. There are infinitely fewer such diagrams than connected diagrams. As a counterexample: The diagram

"falls apart" into two pieces if we cut the middle electron line. This is therefore a **one particle reducible diagram**.

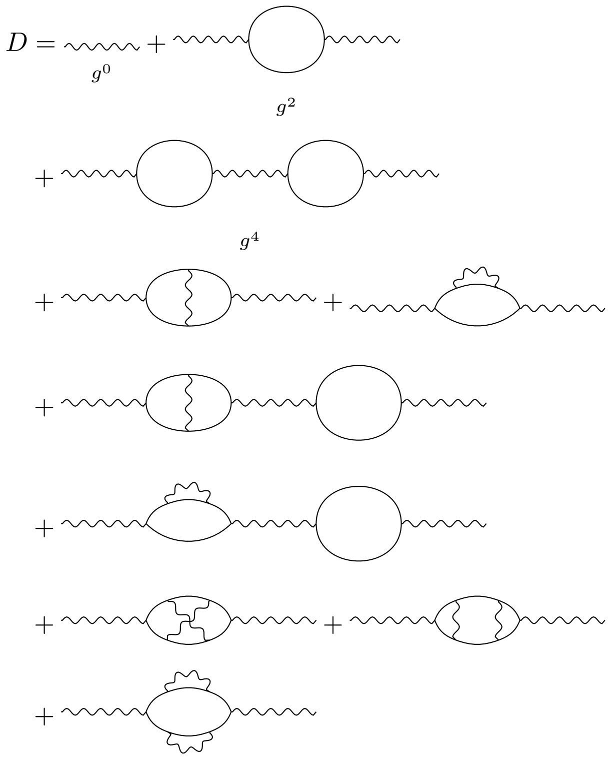
> Only **one-particle irreducible** diagrams contribute to Σ.

To calculate corrections to D_0, the free phonon-propagator, we proceed in a similar way.

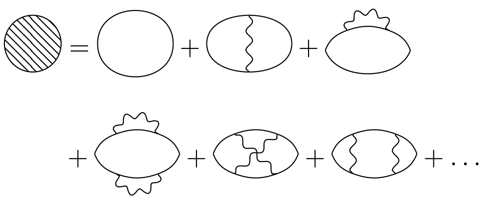
$$
\begin{aligned}
D(q, t-t') &= -i \langle \Psi(0) | \tilde{T}[A_q(t) A_q^\dagger(t')] | \Psi(0) \rangle \\
&= -i \frac{\langle \Phi_0 | \tilde{T}[A_q(t) A_q^\dagger(t') S(\infty, -\infty)] | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle}
\end{aligned}
$$

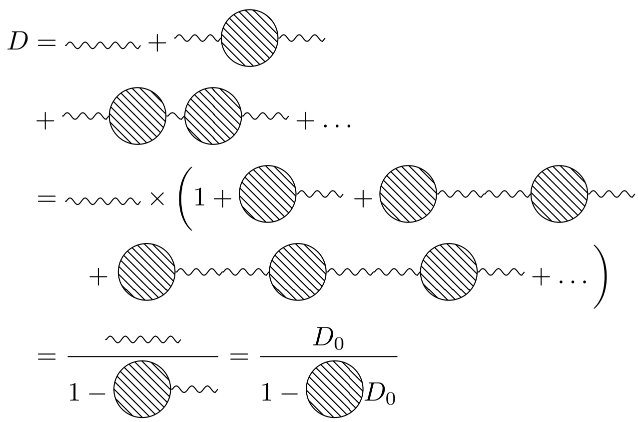
Again, the effect of the denominator is to cancel all disconnected diagrams. Only connected diagrams contribute to G.

D_0 :



Again, we see that the connected diagrams consists of two types: One which falls apart if we cut one phonon-line and one which does not. Again, denote the sum of the latter type by .





And we end up with Dyson's equation

$$D^{-1} = D_0^{-1} - \Pi, \tag{5.4.31}$$

where Π is the blob given above. Only one-phonon irreducible diagrams contribute to Π. The most convenient way of computing these corrections, is to introduce Fourier-transformed Green's functions

$$G(k,\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{i\omega t} G(k,t) \tag{5.4.32}$$

$$G(k,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t} G(k,\omega). \tag{5.4.33}$$

and correspondingly for $D(q,t), D(q,\omega)$. To second order in g, we found

$$\begin{aligned} G(k,t) = {} & G_0(k,t) \\ & - i^3 \int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \sum_q |g_q|^2 D_0(q, t_1 - t_2) \\ & \cdot G_0(k, t-t_1) G_0(k+q, t_1 - t_2) G_0(k, t_2) \end{aligned} \tag{5.4.34}$$

Fourier-transform:

$$
\begin{aligned}
G(k,\omega) = G_0(k,\omega) + i\cdot i\cdot(-i)\sum_q |g_q|^2 \\
\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{i\omega t} \int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \\
\cdot \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega_1\, \mathrm{e}^{-i\omega_1(t_1-t_2)} D_0(q,\omega_1) \\
\cdot \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega_2\, \mathrm{e}^{-i\omega_2(t-t_1)} G_0(k,\omega_2) \\
\cdot \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega_3\, \mathrm{e}^{-i\omega_3(t_1-t_2)} G_0(k+q,\omega_3) \\
\cdot \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega_4\, \mathrm{e}^{-i\omega_4(t_2)} G_0(k,\omega_4)
\end{aligned}
$$

First, focus on performing all the t-integration and use the identity

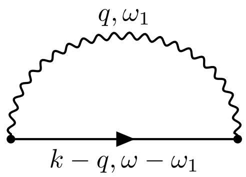
$$
\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{i\omega t} = 2\pi\delta(\omega). \tag{5.4.35}
$$

$$
\begin{aligned}
\int_{-\infty}^{\infty} \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \mathrm{e}^{i\omega t}\mathrm{e}^{-i\omega_1(t_1-t_2)} \\
\cdot\, \mathrm{e}^{-i\omega_2(t-t_1)}\mathrm{e}^{-i\omega_3(t_1-t_2)}\mathrm{e}^{-i\omega_4 t_2} \\
= \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{i(\omega-\omega_2)t} \int_{-\infty}^{\infty} \mathrm{d}t_1\, \mathrm{e}^{i(\omega_2-\omega_1-\omega_3)t_1} \\
\cdot \int_{-\infty}^{\infty} \mathrm{d}t_2\, \mathrm{e}^{i(\omega_1+\omega_3-\omega_4)t_2} \\
= (2\pi)^3\delta(\omega-\omega_2)\delta(\omega_2-\omega_1-\omega_3)\delta(\omega_1+\omega_3-\omega_4)
\end{aligned}
$$

$$
\begin{aligned}
\omega_2 &= \omega \\
\omega_3 &= \omega_2 - \omega_1 = \omega - \omega_1 \\
\omega_4 &= \omega_1 + \omega_3 = \omega_1 + \omega - \omega_1 = \omega
\end{aligned}
$$

Hence, to second order in g, we have

$$
\begin{aligned}
G(k,\omega) &= G_0(k,\omega) \\
&\quad - i^3 \sum_q |g_q|^2 \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega_1\, D_0(q,\omega_1) G_0(k,\omega) G_0(k+q,\omega-\omega_1) G_0(k,\omega) \\
&= G_0(k,\omega) + G_0(k,\omega)\Sigma^{(2)}(k,\omega) G_0(k,\omega) \\
\Sigma^{(2)}(k,\omega) &= -i^3 \sum_q |g_q|^2 \int_{-\infty}^{\infty} \mathrm{d}\omega_1\, D_0(q,\omega_1) G_0(k+q,\omega-\omega_1)
\end{aligned}
$$

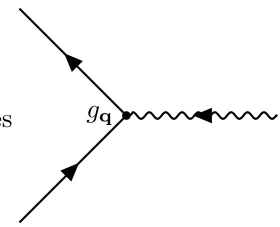
$=$ 

Note the conservation of energy (frequency) and momentum in each scattering vertex (elastic electron-phonon coupling).

5.5 Feynman rules for diagrams

(electron-phonon coupling)

1. Draw all topologically distinct diagrams with $2m$ vertices



   To each vertex: Associate a factor g_q.

2. To each electron-line, associate a factor

$$G_0(k,\omega) = \quad \alpha \xrightarrow{k,\omega} \beta \quad = \frac{\delta_{\alpha\beta}}{\omega - \varepsilon_k + i\delta_k} \tag{5.5.1}$$

   where $\delta_k = \delta \mathrm{sign}(\varepsilon_k - \varepsilon_F)$. Combined particle/hole Green's function.

3. To each phonon-line, associate a factor

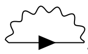
$$D_0(q,\omega) = \underset{q,\omega}{\sim\!\sim\!\sim} = \frac{2\omega_q}{\omega^2 - \omega_q^2 + i\delta} \tag{5.5.2}$$

4. Momentum and energy conservation in each vertex

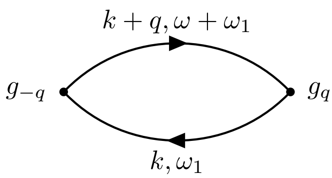
5. Prefactor $i^m(-1)^F(2s+1)^F$. s : spin ($= \frac{1}{2}$ for electrons). F : the number of closed fermion-loops in a diagram.

6. Integrate over internal frequencies and momenta in a diagram, with a factor $\frac{1}{2\pi}$ for each frequency-integration.

Examples:

1. Using these rules in , we recover our previous result for $\Sigma^{(2)}(k,\omega)$

2.



$$= \Pi^{(2)}(q,\omega) \tag{5.5.3}$$

$$\Pi^{(2)}(q,\omega) = |g_q|^2 i(-1) \sum_k \int_{-\infty}^{\infty} \mathrm{d}\omega_1 \, G_0(k+q,\omega+\omega_1) G_0(k,\omega_1) \tag{5.5.4}$$

The Feynman rules are the same for a V different from the electron-phonon coupling, with the modification that the vertex will differ, so rule 1) must be adopted to each case. This would for instance be the case if we were to consider Coulomb-interactions among electrons.

Problems

Problem 5.1. In this problem, we will consider a system defined by a Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + V = \sum_{k,\sigma} \varepsilon_k \; c^\dagger_{k,\sigma} c_{k,\sigma} + V$$

where V is a two-body interaction term that renders the problem not exactly solvable. In class, we have seen how we can express the single-particle electron Green's function for such a system as

$$\begin{aligned} G(k, t-t') &= -i\langle\Psi(0)|T\left[\hat{c}_k(t)\hat{c}^\dagger_k(t')\right]|\Psi(0)\rangle \\ &= -i\frac{\langle\phi_0|T\left[c_k(t)c^\dagger_k(t')S(\infty,-\infty)\right]|\phi_0\rangle}{\langle\phi_0|S(\infty,-\infty)|\phi_0\rangle} \end{aligned}$$

where $S(\infty, -\infty)$ is given by

$$S(\infty,-\infty) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n T\left[V(t_1)\cdots V(t_n)\right]$$

and T is the time-ordering operator. The notation is otherwise the same as we have used in class. Assume now that the perturbation is given by the Hubbard-interaction

$$V = U\sum_i n_{i\uparrow}n_{i\downarrow} = \frac{U}{2}\sum_{i,\sigma} n_{i\sigma}n_{i-\sigma}$$

a) Write the Hubbard-interaction on the form

$$V = \sum_{k,k',q,\sigma,\sigma'} \tilde{V}(q,\sigma,\sigma') \; c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}c_{k',\sigma'}c_{k,\sigma}$$

thereby specifying $\tilde{V}(q,\sigma,\sigma')$. (Note: this interaction is spin-dependent, contrary to what the case is for the standard density-density Coulomb-interaction or the effective electron-electron interaction mediated by phonons.)

b) Use the resulting interaction and calculate the leading order correction of the denominator in the second expression for $G(k, t-t')$, and give a diagrammatic representation for it along the same lines that we used for the electron-phonon coupling in class.

c) Calculate the leading order correction of the numerator in the second expression for $G(k, t-t')$, and give a diagrammatic representation for it along the same lines that we used for the electron-phonon coupling in class.

d) Show that, to leading order in V, the denominator cancels the disconnected diagrams appearing in the numerator.

Problem 5.2. In class, we have computed the polarizability $\Pi(\mathbf{q}, \omega)$

$$\Pi(q,\omega) = -2i \sum_k \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} G_0(k+q, \omega+\omega') G_0(k,\omega)$$

in the static long-wavelength limit $\omega = 0, q \to 0$. Here, G_0 is the free fermion propagator

$$G_0(k,\omega) = \frac{\Theta(\varepsilon_k - \varepsilon_F)}{\omega - \varepsilon_k + i\delta} + \frac{\Theta(\varepsilon_F - \varepsilon_k)}{\omega - \varepsilon_k - i\delta},$$

in the notation that was used in class.

a) Compute $\Pi(\mathbf{q}, 0)$ for all q for $d = 1$ and $d = 2$, for the case of a parabolic band

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}.$$

(Hint: When you consider the $d = 2$ case, it will be necesssary at some point in the calculation to consider separately the two cases $q < 2k_F$ and $q > 2k_F$).

b) Use this zero-frequency (but finite-q) expression to give an expression for a renormalized phonon-spectrum as a function of q, paying special attention to what happens at $q = 2k_F$, using the above expression for Π in the Dyson-equation for the phonon-propagator. (Hint: Consider the poles of the phonon-propagator).

c) Focusing now on what happens at $q = 2k_F$, try to give a physical interpretation of the special features that might arise in the renormalized phonon-spectrum at $q = 2k_F$.

Useful integral for the case $d = 2$:

$$\int_0^{2\pi} \frac{d\phi}{q^2 - k^2 \cos^2 \phi} = \frac{2\pi}{|q|} \frac{1}{\sqrt{q^2 - k^2}} \Theta(|q| - k)$$

where $\Theta(x)$ is the Heaviside step-function. (Can for instance be shown by using calculus of residues).

CHAPTER 6

INTERACTING FERMIONS. FERMI LIQUIDS AND QUASIPARTICLES

6.1 Fermi-liquids

In a non-interacting electron-system, we have seen that the Green's function (also often called the **propagator**) has the form

$$G_0(k,\omega) = \frac{1}{\omega - \varepsilon_k + \delta_k}, \tag{6.1.1}$$

where we have defined

$$\delta_k = \delta \text{sign}(\varepsilon_k - \varepsilon_F). \tag{6.1.2}$$

The simple poles mean that the system has well-defined and long-lived single-particle excitations, since $\delta = 0^+$. The excitation energy is determined by $\omega - \varepsilon_k$, and the lifetime, τ, of the excitation is given by

$$\tau_k = \frac{1}{\delta} \to \infty; \quad \delta \to 0^+. \tag{6.1.3}$$

In the interacting case, we have Dyson's equation

$$G^{-1}(k,\omega) = G_0^{-1}(k,\omega) - \Sigma(k,\omega), \tag{6.1.4}$$

or equivalently

$$G(k,\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k,\omega)} \tag{6.1.5}$$

$$G_0(k,\omega) = \frac{1}{\omega - \varepsilon_k + \frac{i}{\tau_k}}. \tag{6.1.6}$$

Note that for $G_0(k,\omega)$, the **residue** at $\omega = \varepsilon_k - i\delta_k$ is $\mathrm{Res}[G_0] = 1$. We will now write $G(k,\omega)$ on a similar form

$$G(k,\omega) = \frac{z_k}{\omega - \tilde{\varepsilon}_k + \frac{i}{\tau_k}} \tag{6.1.7}$$

and find expressions for $z_k, \tilde{\varepsilon}_k, \frac{1}{\tau_k}$ in terms of $\Sigma(k,\omega)$.

- z_k: **Quasiparticle residue**. Physically: How much of the original electron in the non-interacting case remains in the interacting case?
- τ_k: **Quasiparticle lifetime**.
- $\tilde{\varepsilon}_k$: New excitation spectrum of the interacting system.

Let us define more precisely what we mean by a **quasi-particle**. In the non-interacting case, we have well-defined single-particle excitations specified by a set of quantum numbers (k,σ), and with an excitation energy ε_k. For instance, we could have

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} \tag{6.1.8}$$

where m would be the mass of the electron. As we turn on interactions, things will change. The concept of a quasiparticle now assures that there is a **one-to-one** correspondence between the quantum numbers of the non-interacting case, and the quantum numbers of the interacting case. .

Insert figure depicting this 1-1 correspondence.

The dots represent quantum states. Thus, we may follow the state of an electron into a state with a new set of quantum numbers, and vice versa, as the interactions are turned on and off. The quantum states on the right are quasi-particle states. The renormalization $\varepsilon_k \to \tilde{\varepsilon}_k$ could for instance be of the form

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} \to \tilde{\varepsilon}_k = \frac{\hbar^2 k^2}{2m^*}, \tag{6.1.9}$$

where m^* is some effective quasiparticle mass different from the mass of the electron. As long as $z_k > 0$, we may talk about **quasiparticles**. In particular, the crucial issue is what z_k is on the Fermi-surface $k = k_F$, i.e. z_{k_F}. So we will

NB!

focus our attention on what is going on in the vicinity of the Fermi-surface. The self-energy is given by

$$\Sigma(k,\omega) = \Sigma_{\mathrm{Re}}(k,\omega) + i\Sigma_{\mathrm{Im}}(k,\omega). \tag{6.1.10}$$

We assume that the imaginary part is much less than the real part

$$\frac{|\Sigma_{\mathrm{Im}}|}{|\Sigma_{\mathrm{Re}}|} \ll 1. \tag{6.1.11}$$

The quasi-particle poles are found from the zeroes in $G^{-1}(k,\omega)$, i.e.

$$\boxed{\omega - \varepsilon_k - \Sigma_{\mathrm{Re}} - i\Sigma_{\mathrm{Im}} = 0 \qquad (6.1.12)}$$

To a first approximation, ignore Σ_{Im}.

$$\omega - \varepsilon_k - \Sigma_{\mathrm{Re}}(k, \omega) = 0 = \omega - \tilde{\varepsilon}_k. \tag{6.1.13}$$

This is a complicated equation, due to the frequency-dependence of the self-energy.

$$\omega = \tilde{\varepsilon}_k = \varepsilon + \Sigma_{\mathrm{Re}}(k,\omega) = \varepsilon_k + \Sigma_{\mathrm{Re}}(k,\tilde{\varepsilon}_k) \tag{6.1.14}$$

If the renormalization of $\varepsilon_k \to \tilde{\varepsilon}_k$ is weak, we may expand the self energy in ω around $\tilde{\varepsilon}_k$. Anticipating that ω will change away from $\tilde{\varepsilon}_k$ when Σ_{Im} is introduced:

$$\Sigma_{\mathrm{Re}}(k,\omega) = \Sigma_{\mathrm{Re}}(k,\tilde{\varepsilon}_k) + (\omega - \tilde{\varepsilon}_k)\underbrace{\left.\frac{\partial \Sigma_{\mathrm{Re}}}{\partial \omega}\right|_{\omega=\tilde{\varepsilon}_k}}_{\equiv \Sigma'_{\mathrm{Re}}} + \ldots \tag{6.1.15}$$

Set $\omega = \tilde{\varepsilon}_k + \omega_1$, where $\tilde{\varepsilon}_k$ is a solution to

$$\tilde{\varepsilon}_k = \varepsilon_k + \Sigma_{\mathrm{Re}}(k,\tilde{\varepsilon}_k) \tag{6.1.16}$$

$$\begin{gathered}
\omega - \varepsilon_k - \Sigma_{\mathrm{Re}}(k,\omega) - i\Sigma_{\mathrm{Im}}(k,\omega) = 0 \implies \\
\tilde{\varepsilon}_k + \omega_1 - \varepsilon_k - \Sigma_{\mathrm{Re}}(k,\tilde{\varepsilon}_k) - \omega_1\Sigma'_{\mathrm{Re}} - i\Sigma_{\mathrm{Im}}(k,\tilde{\varepsilon}_k) = 0
\end{gathered}$$

Using eq. (6.1.16), we have

$$\begin{aligned}
\omega_1 - \omega_1\Sigma'_{\mathrm{Re}} - i\Sigma_{\mathrm{Im}}(k,\tilde{\varepsilon}_k) &= 0 \\
\omega_1 &= i\frac{\Sigma_{\mathrm{Im}}(k,\tilde{\varepsilon}_k)}{1-\Sigma'_{\mathrm{Re}}} \\
\omega = \tilde{\varepsilon}_k - \frac{i}{\tau_k} &= \varepsilon_k + \omega_1 \implies \\
\frac{1}{\tau_k} &= -\frac{\Sigma_{\mathrm{Im}}(k,\tilde{\varepsilon}_k)}{1-\Sigma'_{\mathrm{Re}}}
\end{aligned}$$

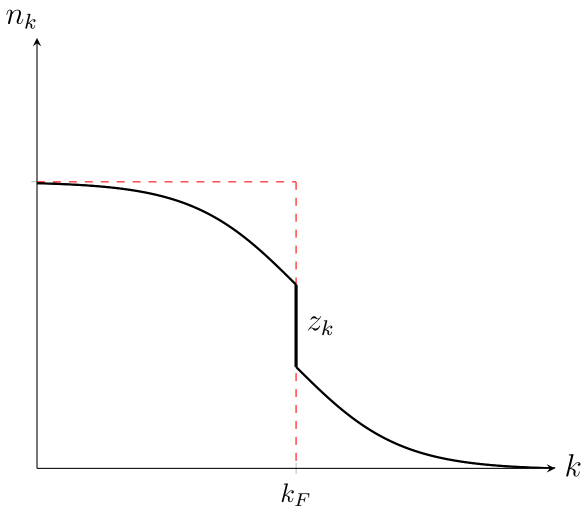
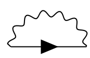


Figure 6.1: Momentum distribution for a non-interacting system (red dashed line) and a Fermi liquid.

This is the quasi-particle lifetime expressed in terms of the self-energy Σ. Let us also investigate the quasi-particle residue z_k.

$$\begin{aligned} G(k,\omega) &= \frac{1}{\omega - \varepsilon_k - \Sigma_{\text{Re}}(k,\omega) - i\Sigma_{\text{Im}}(ki,\omega)} \\ &= \frac{1}{\omega - \tilde{\varepsilon}_k - (\omega - \tilde{\varepsilon}_k \Sigma'_{\text{Re}}) - i\left(\frac{1-\Sigma'_{\text{Re}}}{\tau_k}\right)} \\ &= \frac{(1-\Sigma'_{\text{Re}})^{-1}}{\omega - \tilde{\varepsilon}_k + \frac{i}{\tau_k}} = \frac{z_k}{\omega - \tilde{\varepsilon}_k + \frac{i}{\tau_k}}. \end{aligned}$$

$$z_k = \frac{1}{1-\Sigma'_{\text{Re}}}. \tag{6.1.17}$$



$$\Sigma = \quad \Longrightarrow \quad \Sigma'_{\text{Re}} < 0 \implies z_k < 1. \tag{6.1.18}$$

An interacting fermion-system with $z_{k_F} > 0$ is called a Fermi-liquid.

At $T = 0$, the momentum distribution in the non-interacting case follow $n_k = 1 - \theta(\varepsilon_k - \varepsilon_F) = \theta(\varepsilon_F - \varepsilon_k)$. This is shown, together with the momentum-distribution for a Fermi-liquid in fig. 6.1

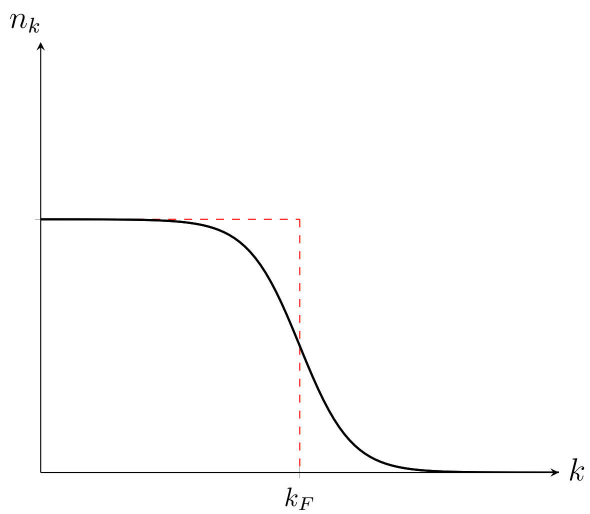
As long as a discontinuity in n_k exists on the Fermi-surface, we have remnants of **well defined** single-particle excitations in a one-to-one correspondence with the single-particle states of the non-interacting case

> A Fermi-liquid has $z_{k_F} > 0$ at $T = 0$.

Note that this statement is a $T = 0$-statement, since only at $T = 0$ is there a discontinuity in n_k at $k = k_F$ At non-zero T, $1 - \theta(\varepsilon_k - \varepsilon_F) = \theta(\varepsilon_F - \varepsilon_k)$ is replaced by the Fermi-distribution

$$n_k = \frac{1}{\mathrm{e}^{\beta(\varepsilon_k - \mu)}}; \quad \beta = \frac{1}{k_B T} \tag{6.1.19}$$

which is an analytic function of k at $k = k_F$. There are cases where Fermi-liquids are destroyed. A well understood example of this is the on-dimensional interacting electron gas. In one-dimension, any amount of interacting between electrons destroys z_{k_F}. **For example, the 1-d Hubbard model is not a Fermi-liquid for any $U > 0$.** Computing the momentum distribution of the 1-d Hubbard model is difficult, but the result is



not Fermi-liquid. $z_{k_F} = 0$.

$$n_k = \frac{1}{2}\left(1 - \mathrm{sign}\,(k - k_F)\,|k - k_F|^{1/\delta}\right). \tag{6.1.20}$$

Note, however,m that n_k still is non-analytic at $k = k_F$. Thus, we still have a well-defined Fermi-surface! In this case, the long-lived low-energy excitations around the Fermi-surface is not in a ne-to-one correspondence with the quantum states of the non-interacting case. This quantum liquid is called a Luttinger-liquid and its single-electron Green's function does not have simple poles, but rather branch-cuts. In three dimensions, however, the Fermi-liquid us extremely robust to Coulomb-interactions among electrons.

6.2 Screening of the Coulomb-interaction

$$V(r) = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}, \tag{6.2.1}$$

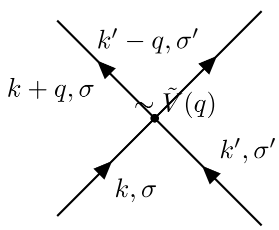
unscreened Coulomb interaction. Fourier-transform

$$\tilde{V}(q) = \frac{1}{V_0}\int \mathrm{d}r\, \mathrm{e}^{iq\cdot r} \tag{6.2.2}$$

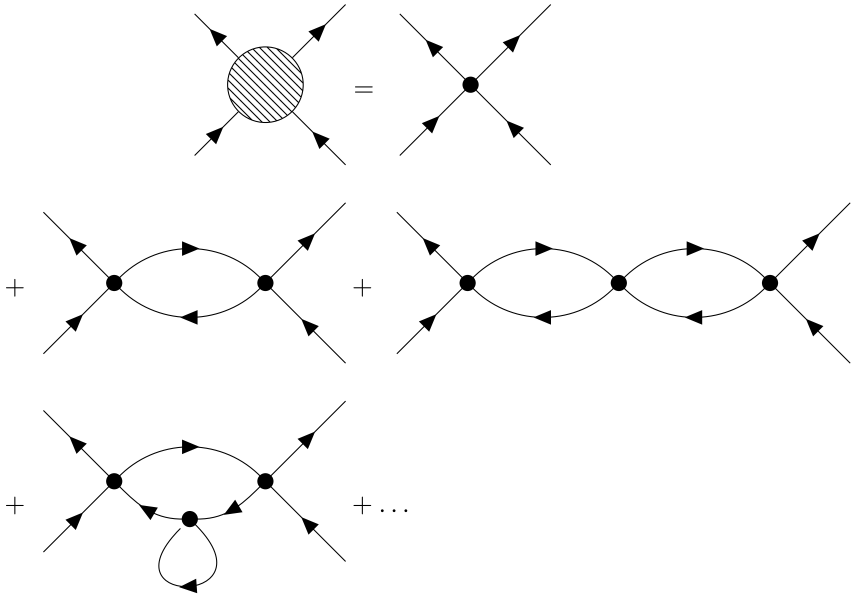
where V_0 is the volume of the system. Performing the Fourier-transform, we have

$$\tilde{V} = \frac{1}{V_0\epsilon_0}\frac{e^2}{q^2} = \frac{K}{q^2} \quad ; \quad K = \frac{e^2}{V_0\epsilon_0}. \tag{6.2.3}$$

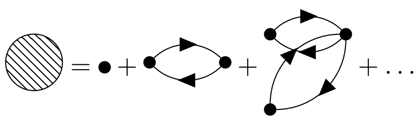
Diagrammatically:



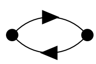
A scattering of two electrons off one another. More generally, the interaction may be presented as follows:



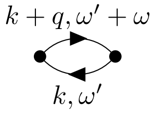
We now focus on a resummation of the simplest bubble-diagrams. This is an approximation, but it will give the qualitative correct result. The diagram which we would neglect above would be the last one. Then the effective screened interaction $\tilde{V}_{\mathrm{SC}}(q)$ would be



$$\begin{aligned}
\tilde{V}_{\mathrm{SC}}(q) &= \tilde{V}(q) + \tilde{V}(q)\Pi\tilde{V}(q) + \tilde{V}(q)\Pi\tilde{V}(q)\Pi\tilde{V}(q) + \dots \\
&= \tilde{V}(q)\left(1 + \tilde{V}(q)\Pi + \tilde{V}(q)\Pi\tilde{V}(q)\Pi + \dots\right) \\
&= \frac{\tilde{V}(q)}{1 - \tilde{V}(q)\Pi}
\end{aligned} \tag{6.2.4}$$

$\Pi(q) =$ 

We will now use the Feynman-rules to compute this bubble, using free electron Green's functions found previously. This means that we will compute a quantity tat a priori depends on both q and ω. At the end of the calculation, we let $\omega \to 0$ (static screening). Thus, consider

$\Pi(q,\omega) =$ 

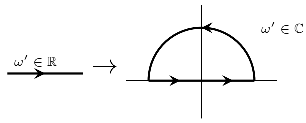
Here, k and ω' are to be integrated over (Feynman rules, see section 5.5) Number of vertices: $2 \implies m = 1$. Number of fermion loops: $F = 1$

$$\Pi(q,\omega) = i(-1)^1(2\cdot\frac{1}{2}+1)^1 \cdot \sum_k \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} G_0(k+q,\omega+\omega')G_0(k,\omega')$$

$$G_0(k,\omega) = \frac{\theta(\varepsilon_k - \varepsilon_F)}{\omega - \varepsilon_k + i\delta} + \frac{\theta(\varepsilon_F - \varepsilon_k)}{\omega - \varepsilon_k - i\delta}$$

Let us first perform the frequency-integration by the calculus of residues. Analytic continuation of ω from the real axis to the complex plane

$$\int_{-\infty}^{\infty} \mathrm{d}\omega' \to \int_C \mathrm{d}z$$



Close contour in upper half plane (we could equally well have close in lower half plane). Consider an integral of the following form

$$\begin{aligned}
&\int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{1}{\omega - A + i\delta} \cdot \frac{1}{\omega - B + i\delta} \\
\Rightarrow &\int_C \mathrm{d}z \, \frac{1}{z - A + i\delta} \cdot \frac{1}{z - B + i\delta} \\
= &\frac{1}{A-B} \int_C \mathrm{d}z \left(\frac{1}{z - A + i\delta} - \frac{1}{z - B + i\delta} \right)
\end{aligned}$$

The simple poles of both terms are in the lower half z-plane, outside the integration contour. This integral is therefore 0.

Consider next an integral of the form

$$\begin{aligned}
&\int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{1}{\omega - A - i\delta} \cdot \frac{1}{\omega - B - i\delta} \\
= &\frac{1}{A-B} \int_C \mathrm{d}z \left(\frac{1}{z - A - i\delta} - \frac{1}{z - B - i\delta} \right)
\end{aligned}$$

Both poles now contribute, since they both lie in the upper half plane. Thus, the integral will be given by

$$I = \frac{1}{A-B}\,(2\pi i - 2\pi i) = 0. \tag{6.2.5}$$

Here we have used the Cauchy integral formula

$$\oint_C \mathrm{d}z\,\frac{1}{z-a} = 2\pi i, \tag{6.2.6}$$

whenever a lie within the contour. Thus,

$$\int_{-\infty}^{\infty} \mathrm{d}\omega\,\frac{1}{\omega - A - i\delta}\cdot\frac{1}{\omega - B - i\delta} = 0. \tag{6.2.7}$$

Consider next an integral of the form

$$\begin{aligned}&\int_{-\infty}^{\infty} \mathrm{d}\omega\,\frac{1}{\omega - A + i\delta}\cdot\frac{1}{\omega - B - i\delta}\\ &= \frac{1}{A-B-2i\delta}\int_C \mathrm{d}z\left(\frac{1}{z-A+i\delta} - \frac{1}{z-B-i\delta}\right)\end{aligned}$$

In this case, the pole in the first term is in the lower half-plan and does not contribute. The pole in the second term does contribute, since it is in the upper half-plane. This the integral is

$$I = \frac{1}{A-B-2i\delta}\cdot(-2\pi i) \tag{6.2.8}$$

Finally, wee consider the integral

$$\begin{aligned}&\int_{-\infty}^{\infty} \mathrm{d}\omega\,\frac{1}{\omega - A - i\delta}\cdot\frac{1}{\omega - B + i\delta}\\ &= \frac{1}{A-B+2i\delta}\cdot(+2\pi i).\end{aligned}$$

We now use these results to compute

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} G_0(k+q,,\omega+\omega')G_0(k,\omega'). \tag{6.2.9}$$

G_0's consist of two parts: one part wit a pole in the upper half plane, the other part with a pole in the lower half-plane. The product of two G_0's will therefore have four contributions; all of the same form as we have considered above:

1. One contribution with both poles in upper half-plane (two hole-like factors). Gives 0.

2. One contribution with poles in lower half-plane (two particle-like factors). Gives 0.

3. Two contributions with one pole in lower and one pole in upper half-plane.

This gives the following contribution:

$$\begin{aligned} I = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \Bigg[& \frac{\theta(\varepsilon_{k+q} - \varepsilon_F)}{\omega + \omega' - \varepsilon_{k+q} + i\delta} \cdot \frac{\theta(\varepsilon_F - \varepsilon_k)}{\omega' - \varepsilon_k - i\delta} \\ & + \frac{\theta(\varepsilon_F - \varepsilon_{k+q})}{\omega + \omega' - \varepsilon_{k+q} - i\delta} \cdot \frac{\theta(\varepsilon_k - \varepsilon_F)}{\omega' - \varepsilon_k + i\delta} \Bigg] \end{aligned}$$

In these two contributions, we use the formulas we derived above, to obtain

$$\begin{aligned} I = & \frac{1}{2\pi} \frac{\theta(\varepsilon_{k+q} - \varepsilon_F)\theta(\varepsilon_F - \varepsilon_k) \cdot (-2\pi i)}{\varepsilon_{k+q} - \varepsilon_k - \omega + 2i\delta} \\ & + \frac{1}{2\pi} \frac{\theta(\varepsilon_F - \varepsilon_{k+q})\theta(\varepsilon_k - \varepsilon_F) \cdot (2\pi i)}{\varepsilon_{k+q} - \varepsilon_k - \omega - 2i\delta} \end{aligned} \tag{6.2.10}$$

Thus, we have for the “bubble´´-diagram

$$\Pi(q,\omega) = -2i \frac{2\pi i}{2\pi} \cdot \sum_k \left\{ \frac{\theta(\varepsilon_{k+q} - \varepsilon_F)\theta(\varepsilon_F - \varepsilon_k)}{\omega + \varepsilon_k - \varepsilon_{k+q} - 2i\delta} - \frac{\theta(\varepsilon_F - \varepsilon_{k+q})\theta(\varepsilon_k - \varepsilon_F)}{\omega + \varepsilon_k - \varepsilon_{k+q} + 2i\delta} \right\}. \tag{6.2.11}$$

In general this k-sum is difficult to perform analytically. However, we are interested in the limit of static screening, $\omega = 0$. Introduce the notation $n(\varepsilon_-k) = \theta(ep_F - \varepsilon_k)$. This is the Fermi-distribution at zero temperature.

$$\Pi(q,\omega = 0) = 2 \sum_k \left\{ \frac{n(\varepsilon_k)(1 - n(\varepsilon_{k+q}))}{\varepsilon_k - \varepsilon_{k+q} - 2i\delta} - \frac{n(\varepsilon_{k+q})(1 - n(\varepsilon_k))}{\varepsilon_k - \varepsilon_{k+q} + 2i\delta} \right\} \tag{6.2.12}$$

It is immediately seen that the imaginary part of $\Pi(q,0))$ is 0, since the imaginary part will include a $\delta(\varepsilon_k - \varepsilon_{k+q})$-factor in both terms

$$\begin{aligned} \delta(\varepsilon_{k+q} - \varepsilon_k) & \left[n(\varepsilon_k)(1 - n(\varepsilon_{k+q}))) + n(\varepsilon_{k+q})(1 - n(\varepsilon_k)) \right] \\ & = 2\delta(\varepsilon_{k+q} - \varepsilon_k) n(\varepsilon_k)(1 - n(\varepsilon_k)) \\ & = 0 \end{aligned}$$

The real part is given by

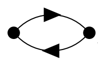
$$\mathrm{Re}\{\Pi(q,0)\} = 2\sum_k \left(\frac{n(\varepsilon_k) - n(\varepsilon_{k+q})}{\varepsilon_k - \varepsilon_{k+q}}\right) = \Pi(q,0).$$

Consider now screening in the $q \to 0$-limit:

$$\begin{aligned}
\Pi(q,0) &\overset{q\to 0}{=} 2\sum_k \frac{\partial n(\varepsilon_k)}{\partial k} \\
&= -2\sum_k \delta(\varepsilon_k - \varepsilon_F) \\
&= -2N(\varepsilon_F)
\end{aligned}$$

$N(\varepsilon_F)$ = Density of states on the Fermi-surface pr. spin. The factor 2 is a spin-summation factor.

$$\boxed{\Pi(q,\omega=0) = -2N(\varepsilon_F) \qquad (6.2.13)}$$

Firstly, this completes our first calculation of a Feynman-diagram, . Secondly, the result is extremely important, since it tells us precisely which quantity it is that determines the screening properties of a metal: the density of states on the the Fermi-surface. Inserting the result in eq. (6.2.4), we calculate

$$\begin{aligned}
\tilde{V}_{\mathrm{SC}}(q) &= \frac{\frac{K}{q^2}}{1 - \frac{K}{q^2}(-2N(\varepsilon_F))} \\
&= \frac{K}{q^2 + \lambda^{-2}}
\end{aligned}$$

Taking the inverse Fourier transform, we get

$$V_{\mathrm{SC}}(r) = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}\mathrm{e}^{-r/\lambda} \qquad (6.2.14)$$

$$\lambda = \left(\frac{1}{2KN(\varepsilon_F)}\right)^{\frac{1}{2}}, \qquad (6.2.15)$$

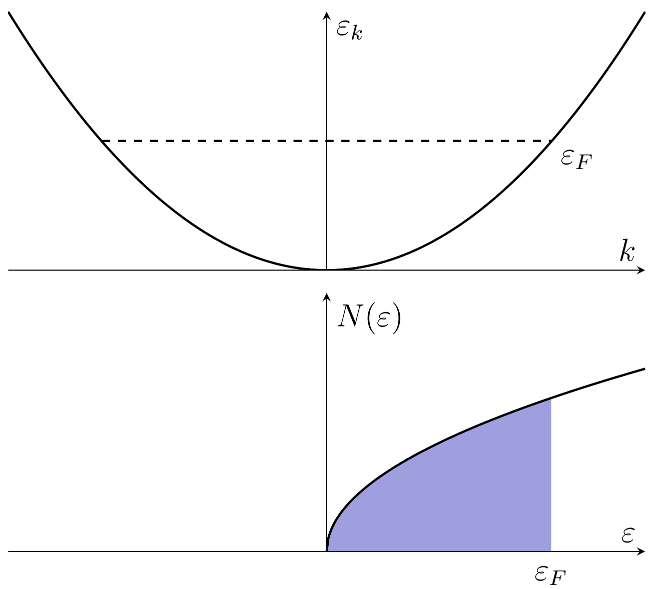
here, λ is the Screening length. Notice that $N(\varepsilon_F) \to 0 \implies \lambda \to \infty$, which gives

$$V_{\mathrm{SC}}(r) \to \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}, \qquad (6.2.16)$$

i.e. unscreened Coulomb-potential. Screening requires $N(\varepsilon_F) \neq 0$, which means that we need to have gapless excitations on the Fermi surface.

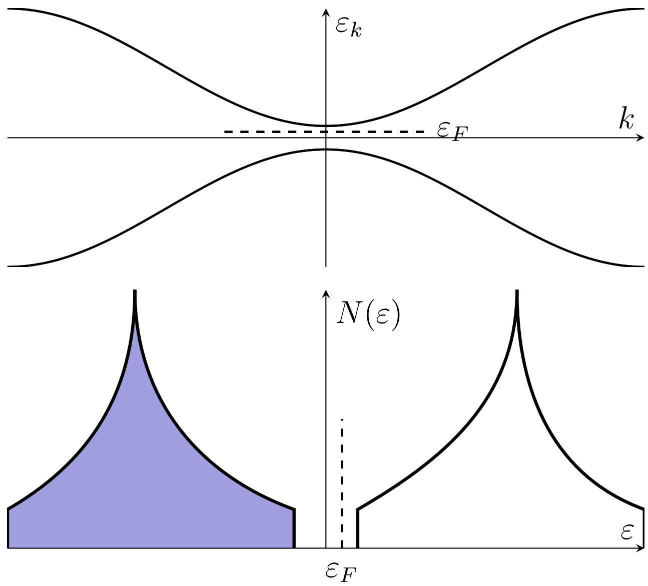
Examples:

i A good metal



Here $N(\varepsilon_F) \neq 0$ and the system screens well.

ii A band insulator



$N(\varepsilon_F) = 0$ and the system has no screening.

Let us give a physical picture for what is going on. The system is assumed to be overall charge-neutral, so there are equally many positive and negative charges in the problem. When we insert an extra electron into this system (a "test-charge") then positive charges are attracted to this negative charge, "dressing" it so that it appears to be less visible, particularly far away from the test-charge. This adjustment of charge around the "test-charge" requires gapless excitations to exist on the Fermi-surface.

> Screening is a long-distance phenomenon determined by the density of states on the Fermi-surface.

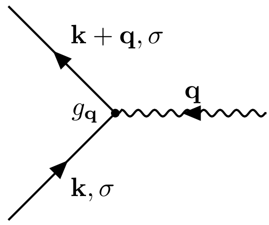


Figure 6.2: Diagram of electron-phonon vertex

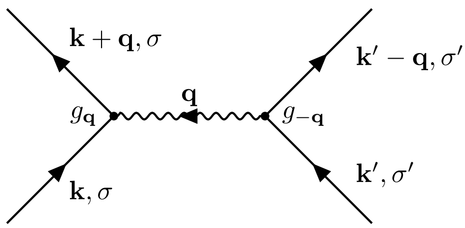
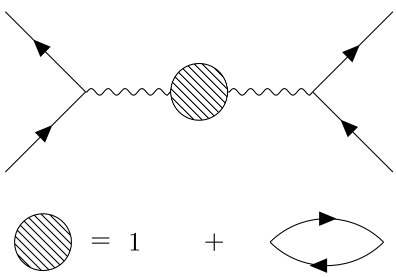


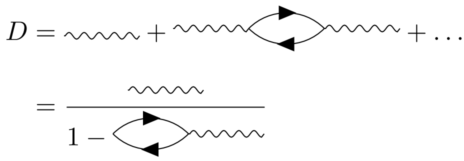
Figure 6.3: Diagram of the effective electron-phonon interaction

6.3 Phonon mediated electron-electron interaction

Due to the electron-phonon coupling depicted in fig. 6.2, we will get an effective phonon-mediated interaction between electrons, depicted in fig. 6.3 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 correctly 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



Here, we have resummed a <u>subset</u> 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 $\mathcal{O}(g^2)$.

$$V_{\text{eff}}(q,\omega) = |g_q^2| \frac{2\omega_q}{\omega^2 - \omega_q^2} \tag{6.3.1}$$

Thus, the interaction part of the Hamiltonian becomes

$$\mathcal{H} = \sum_{\substack{k,k',q \\ \sigma,\sigma'}} V_{\text{tot}}(q,\omega) c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma} \tag{6.3.2}$$

$$V_{\text{tot}}(q,\omega) = \frac{e^2}{4\pi\varepsilon q^2} + V_{\text{eff}}(q,\omega), \tag{6.3.3}$$

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

$$\omega = \varepsilon_{k+q} - \varepsilon_k \tag{6.3.4}$$

Insert figure

Note the singularities in V_{tot} when $|\omega| \to \omega_q$. In particular, note the <u>negative</u> 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 <u>attractive</u>.

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 electron 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 $\omega_{\text{min}} < \omega < \omega_{\text{masx}}$, as depicted in We may view the effective electron-electron attraction 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.

Insert figure

Disclaimer: The above two analogues 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.

6.4 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 insulator. (FMI) The question is if the spin-fluctuations of the FMI can give rise to an attractive interaction among electrons. We therefore consider a system of itinerant electrons with Hamiltonian

$$\mathcal{H}_{\text{el}} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma}. \tag{6.4.1}$$

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

$$\mathcal{H}_{\text{spin}} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{6.4.2}$$

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

$$\mathcal{H}_{\text{el-spin}} = -J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i. \tag{6.4.3}$$

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

$$\mathcal{H}_{\text{spin}} = \sum_q \omega_q a_q^\dagger a_q \tag{6.4.4}$$

$$\omega_q = 2JS(z - \gamma(\mathbf{q}))) \tag{6.4.5}$$

$$\gamma(\mathbf{q}) = \sum_\delta \mathrm{e}^{i\mathbf{q}\cdot\delta}, \tag{6.4.6}$$

where δ connects site i to all its nearest neighbours. One important fact to 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:

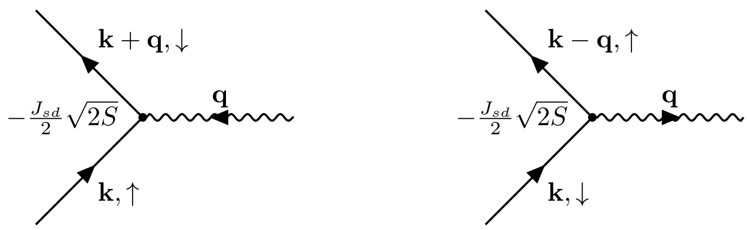
$$\mathcal{H}_{\text{el-spin}} = -J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i \tag{6.4.7}$$

$$= -J_{sd} \sum_i (S_{iz}s_{iz} + S_{ix}s_{ix} + S_{iy}s_{iy}) \tag{6.4.8}$$

$$= -J_{sd} \sum_i \left(S_{iz}s_{iz} + \frac{1}{2}\left(S_{i+}s_{i-} + S_{i-}s_{i+}\right) \right), \tag{6.4.9}$$

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.

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



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

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

Figure 6.4: The two interaction vertices of interest

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

Thus, we have

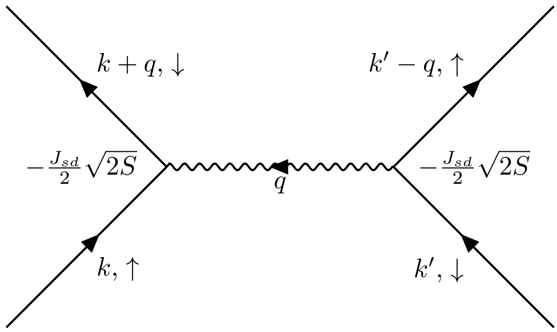
$$\begin{aligned} \mathcal{H}_{\text{el-spin}} = -J_{sd}S\sum_{i,\sigma}\sigma c^\dagger_{i\sigma}c_{i\sigma} + J_{sd}\sum_{i,\sigma}\sigma a^\dagger_i a_i c^\dagger_{i\sigma}c_{i\sigma} \\ - \frac{J_{sd}\sqrt{2S}}{2}\sum_i \left(a_i c^\dagger_{i\downarrow}c_{i\uparrow} + a^\dagger_i c^\dagger_{i\uparrow}c_{i\downarrow}\right) \end{aligned} \tag{6.4.10}$$

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. 6.4.

The Hamiltonian is then

$$H = \sum_{k,\sigma}(\varepsilon_k - \mu - JS\sigma)c^\dagger_{k\sigma}c_{k\sigma} + \sum_q \omega_q a^\dagger_q a_q - \frac{J_{sd}}{2}\sqrt{2S}\sum_{k,q}\left(a_q c^\dagger_{k+q,\downarrow}c_{k\uparrow} + a^\dagger_q c^\dagger_{k-q,\uparrow}c_{k,\downarrow}\right).$$

The effective interaction mediated by this coupling, will be to second order in J_{sd}:



$$V_{eff}(q,\omega) = \left(-\frac{J_{sd}}{2}\sqrt{2S}\right)^2 D_0(q,\omega) \tag{6.4.11}$$

$D_0(q,\omega)$: Free magnon Green's function. Note that $\omega = \varepsilon_{k+q\downarrow} - \varepsilon_{k\uparrow} = \varepsilon_{k'\downarrow} - \varepsilon_{k'-q\uparrow}$, where $\varepsilon_{k\sigma} = \varepsilon_k - \mu - JS\sigma$. Thus

$$\omega = \varepsilon_{k+q} - \varepsilon_k + 2JS = \varepsilon_{k'} - \varepsilon_{k'-q} + 2JS. \tag{6.4.12}$$

$2JS$ acts like a magnetic field, $q \to 0 \to |\omega| \to 2JS$. This fact also suppresses attractive interactions, since it increases the denominator of V_{eff}.

$$\begin{aligned}
D_0(q,\omega) &= -i \langle\varphi_0| T[a_q(t)a^\dagger(t')] |\varphi_0\rangle \\
a_q(t) &= \mathrm{e}^{i\mathcal{H}_0 t} a_q \mathrm{e}^{-i\mathcal{H}_0 t} \\
a_q^\dagger &= \mathrm{e}^{i\mathcal{H}_0 t'} a_q^\dagger \mathrm{e}^{-i\mathcal{H}_0 t'} \\
\mathcal{H}_0 &= \sum_q \omega_q a_q^\dagger a_q
\end{aligned}$$

where time-evolution is expressed in the interaction picture. Formally, this is exactly the same as for the phonon Green's function, and hence

$$V_{eff}(q,\omega) = \left(-\frac{J_{sd}}{2}\sqrt{2S}\right)^2 \frac{2\omega_q^2}{\omega^2 - \omega_q^2}, \tag{6.4.13}$$

which is an attractive interaction if $|\omega| < |\omega_q|$.

Recall what we found with phonons: phonon-mediated el-el interactions was found to be

$$V_{eff}(q,\omega) = |g_q|^2 \frac{2\omega_q^2}{\omega^2 - \omega_q^2}. \tag{6.4.14}$$

There are a couple of notable differences between these two results:

- The coupling constant $-\frac{J_{sd}}{2}\sqrt{2S}$ for magnons is constant for $q \to 0$. The coupling constant g_q for phonons go to 0 as $q \to 0$. For optical phonons, it vanishes $\sim q$. For acoustical phonons it vanishes $\sim \sqrt{q}$. The acoustical phonons are thus more important for creating a phonon mediated el-el interaction.

- Acoustical phonons: $\omega_q \sim |q| \quad (\sim 1THz)$
Magnons: $\omega_q \sim q^2 \quad (\sim 1GHz)$
Thus, for small q, $\omega_q^{mag} \ll \omega_q^{ph}$.

In total, we thus have

$$\begin{aligned}
V_{eff}^{\text{mag}} &\sim \frac{q^4}{\omega^2 - c_1 q^4} && \text{Ferromagnetic magnons} \\
V_{eff}^{\text{ph}} &\sim \frac{q^3}{\omega^2 - c_2 q^4} && \text{Acoustic phonons}
\end{aligned}$$

Thus, while ferromagnetic magnons will be able to create an attractive interaction between electrons, this attraction will be much weaker (due to smallness of the coupling constant and argument above) than the attraction created by phonons.

A good strategy for finding strong electron-electron attractions mediated by some boson, would be to look for bosons giving rise to a

$$V_{eff}(q,\omega) = |\lambda_q|^2 \frac{2\omega_q^2}{\omega^2 - \omega_q^2}, \tag{6.4.15}$$

with $\omega_q \sim |q|$ and $\lim_{q\to 0}\lambda_q = \lambda_0 \neq 0$. Candidate: Anti-ferromagnetic magnons!

Next, we will consider a very simple problem to illustrate the dramatic effect that an attractive interaction among electron has. The problem is so simple that it can be solved exactly. An important point to note, is that the solution to the problem will demonstrate that the answer could not have been found to any finite order in perturbation theory, no matter how weak the interaction is. Attractive interactions in the electron-system is a singular perturbation!

Problems

Problem 6.1. This problems draws on some of the techniques we developed for finding the excitation spectrum of the quantum antiferromagnet, but now for fermions. It will serve as an introduction to the techniques we will later use when we treat the problem of superconductivity.

The Hubbard model on a $2D$ quadratic lattice is defined by the Hamiltonian

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i \left(n_{i,\uparrow} - \frac{1}{2} \right) \left(n_{i,\downarrow} - \frac{1}{2} \right)$$

Introduce

$$c_{j,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k},\sigma} e^{-i\mathbf{k}\cdot\mathbf{r}_j}$$

where N is the number of lattice sites. We set the lattice constant $a = 1$. The Hamiltonian may then be written on the form

$$\begin{aligned}
\mathcal{H} &= \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{U}{4N} \sum_{\mathbf{k}} \left[n_{\mathbf{k}} n_{-\mathbf{k}} - \sigma^z_{\mathbf{k}} \sigma^z_{-\mathbf{k}} \right] - \frac{U n_{\mathbf{k}=0}}{2} + \frac{UN}{4} \\
\varepsilon_{\mathbf{k}} &= -2t \left(\cos(k_x) + \cos(k_y) \right) \\
n_{\mathbf{k}} &= \sum_{\mathbf{q},\sigma} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{q},\sigma} \\
\sigma^z_{\mathbf{k}} &= \sum_{\mathbf{q},\sigma} \sigma c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{q},\sigma}
\end{aligned}$$

Previously, we have considered this model in the limit $t/U \ll 1$ at half-filling, where it maps onto an insulating antiferromagnetic Heisenberg quantum spin model. We will now study this model also away from the limit $t/U \ll 1$, where we may have *itinerant* electrons. This is a problem which is too difficult to handle rigorously at the same level that we treated the half-filled case $t/U \ll 1$, so we will treat it approximately using a techniques which turns out to be quite powerful in many cases. We will treat the problem by using what is called a *mean-field theory.* We do this by introducing

$$\begin{aligned}
n_{\mathbf{k}} &= \langle n_{\mathbf{k}} \rangle + \delta n_{\mathbf{k}}; \quad \delta n_{\mathbf{k}} \equiv n_{\mathbf{k}} - \langle n_{\mathbf{k}} \rangle \\
\sigma^z_{\mathbf{k}} &= \langle \sigma^z_{\mathbf{k}} \rangle + \delta \sigma^z_{\mathbf{k}}; \quad \delta \sigma_{\mathbf{k}} \equiv \sigma^z_{\mathbf{k}} - \langle \sigma^z_{\mathbf{k}} \rangle
\end{aligned}$$

and neglecting terms of $\mathcal{O}(\delta n^2_{\mathbf{k}})$ and $\mathcal{O}((\delta \sigma^z_{\mathbf{k}})^2)$. $\langle n_{\mathbf{k}} \rangle$ and $\langle \sigma^z_{\mathbf{k}} \rangle$ are averages that need to be determined. We consider the case where we on average have one fermion per lattice point, i.e. half-filling.

a) Show that the Hamiltonian may be written

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{U}{2N} \sum_{\mathbf{k}} \left[n_{\mathbf{k}} \langle n_{-\mathbf{k}} \rangle - \sigma^z_{\mathbf{k}} \langle \sigma^z_{-\mathbf{k}} \rangle \right] \tag{6.4.16}$$
$$- \frac{U}{4N} \sum_{\mathbf{k}} \left[\langle n_{\mathbf{k}} \rangle \langle n_{-\mathbf{k}} \rangle - \langle \sigma^z_{\mathbf{k}} \rangle \langle \sigma^z_{-\mathbf{k}} \rangle \right] - \frac{U}{2} n_0 + \frac{UN}{4}$$

b) Assume that $\langle n_{\mathbf{k}} \rangle = N\delta_{\mathbf{k},0}$ and $\langle \sigma^z_{\mathbf{k}} \rangle = NS\delta_{\mathbf{k},\mathbf{Q}}$. Here, S must be determined. This describes a magnetically ordered system with a characteristic wavelength $\mathbf{Q}$, where the charge-distribution is uniform. In real-space, we have

$$\langle \sigma^z_{\mathbf{r}} \rangle = e^{i\mathbf{Q}\cdot\mathbf{r}}$$

where we will set $\mathbf{Q} = (\pi, \pi)$ describing a magnetization which varies periodically in space with a characteristic wavevector $\mathbf{Q}$. With this particular choice of $\mathbf{Q}$ we are describing an antiferromagnet. Note also that $2\mathbf{Q}$ is a reciprocal lattice vector, so that $\langle \sigma^z_{-\mathbf{Q}} \rangle = \langle \sigma^z_{\mathbf{Q}} \rangle$, since momenta are only defined modulo a reciprocal lattice vector.

Show that the Hamiltonian may be written on form

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{N\Delta^2}{U} - \Delta \sum_{\mathbf{k},\sigma} \sigma \; c^{\dagger}_{\mathbf{k}+\mathbf{Q},\sigma} c_{\mathbf{k},\sigma}$$

and give expression for Δ.

c) Introduce new fermion operators

$$\begin{aligned} c_{\mathbf{k},\sigma} &= \cos(\theta)\gamma^{(+)}_{\mathbf{k},\sigma} - \sigma \sin(\theta)\gamma^{(-)}_{\mathbf{k},\sigma} \\ c_{\mathbf{k}+\mathbf{Q},\sigma} &= \sin(\theta)\gamma^{(+)}_{\mathbf{k},\sigma} + \sigma \cos(\theta)\gamma^{(-)}_{\mathbf{k},\sigma} \end{aligned}$$

Use these operators and determine the angle θ such that the Hamiltonian is brought on form

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} \left[\gamma^{\dagger(+)}_{\mathbf{k},\sigma} \gamma^{(+)}_{\mathbf{k},\sigma} - \gamma^{\dagger(-)}_{\mathbf{k},\sigma} \gamma^{(-)}_{\mathbf{k},\sigma} \right] + \frac{N\Delta^2}{U}$$

Give an expression for $E_{\mathbf{k}}$.

c) With one fermion per lattice site, what is the ground state energy?

d) Minimize this ground state energy with respect to Δ, and find the equation determining Δ.

e) Try to solve this equation and find how Δ varies with U as $U \to 0$. (Hint: Convert the $\mathbf{k}$-sum in the equation to an energy integral which may be computed analytically under suitable approximations).

CHAPTER 7

SUPERCONDUCTIVITY

7.1 The Cooper problem

We consider a non-interacting Fermi-sea $|\Phi_0\rangle$, and two additional electrons. These two electrons do not interact with the Fermi-sea. They do however interact with each other. Let us now specify the way in which they interact. The initial states of the two electrons are taken to be $|k,\uparrow\rangle$ and $|-k,\downarrow\rangle$, such that a non-interacting two-particle state can be denoted by $|k,\uparrow;-k,\downarrow\rangle$. Short hand notation for this will be $|k,-k\rangle$, with the understanding that the electrons have opposite spins. While this choice of initial states may look a bit wierd, this is what we will work with, its justification will be made clear later. (Hint: go back and study the physical explanation for attractive phonon-mediated electron-electron interaction). The situation may be illustrated as in fig. 7.1.

The interaction among the electrons is now such that it scatters them into a new two-particle state $|k',-k'\rangle$, see illustration above. The interaction that causes such a scattering is denoted V. This interaction is assumed to be operative within a thin shell of width ω_0 around the Fermi-surface.

$$\mathcal{H}_0 |k,-k\rangle = \varepsilon_k |k,-k\rangle \tag{7.1.1}$$

ε_k: Kinetic energy of the two added electrons. $\mathcal{H}_0$: Hamiltonian with no $V_{kk'}$.

Exact two-particle state with interactions: $|1,2\rangle$.

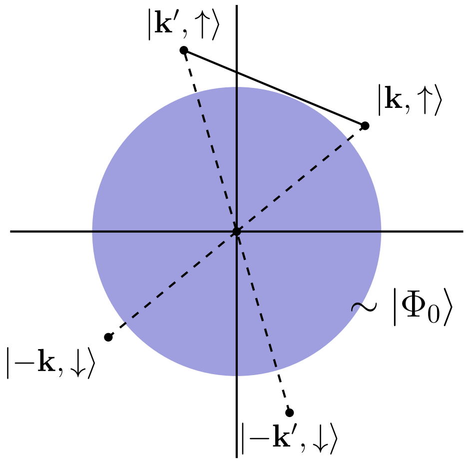


Figure 7.1: The scattering situation.

$$|1,2\rangle = \sum_{k'} a_{k'} |k', -k'\rangle, \tag{7.1.2}$$

where $a_{k'}$ must be determined.

$$(\mathcal{H}_0 + V_{eff}) |1,2\rangle = E |1,2\rangle \tag{7.1.3}$$

E: Exact two-particle energy for this problem.

$$(\mathcal{H}_0 + V_{eff}) \sum_{k'} a_{k'} |k', -k'\rangle = \sum_{k'} a_{k'} (\varepsilon_{k'} + V_{eff}) |k', -k'\rangle = \sum_{k'} a_{k'} E |k', -k'\rangle .$$

Multiplying with $\langle k, -k|$ and use orthonormality $\delta_{k,k'} = \langle k, -k|k', -k'\rangle$.

$$a_k \varepsilon_k + \sum_{k'} \langle k, -k| V_{eff} |k', -k'\rangle = a_k \varepsilon_k + \sum_{k'} V_{k,k'} = a_k E$$

$$V_{k,k'} = \begin{cases} -V & k, k' \in \Omega \\ 0 & k, k' \notin \Omega \end{cases}$$

where Ω denotes a region in k-space in the close vicinity of the Fermi-surface ("thin shell´´). The Schrödinger equation now reads

$$a_k(\varepsilon_k - E) = -\sum_{k' \in \Omega} a_{k'} V_{k,k'} = \sum_{k' \in \Omega} V a_{k'}$$

where we have inserted the expression for $V_{k,k'}$ in the Ω-region in k-space. We make this summation explicit by including Heaviside step-functions.

$$a_k(\varepsilon_k - E)\Theta(2\omega_0 - |\varepsilon_k - 2\varepsilon_F|) = V\sum_{k'} a_{k'}\Theta(2\omega_0 - |\varepsilon_k' - 2\varepsilon_F|)\Theta(2\omega_0 - |\varepsilon_k - 2\varepsilon_F|).$$

The two step-functions on the r.h.s originate with the fact that both k and k' in $V_{k,k'}$ must be within this energy shell around the Fermi-surface. The step-functions that depend on k cancel on both sides of the equation. Thus, we have

$$\sum_{k'} a_{k'}\Theta(2\omega_0 - |\varepsilon_k' - 2\varepsilon_F|) = K_1,$$

constant and independent of k.

$$a_k = \frac{K_1}{\varepsilon_k - E}$$

a_k depends on k only via ε_k, so we can convert the k-sum into an energy sum:

$$\sum_{k'} f(\varepsilon_{k'}) = \sum_{k'}\int_{-\infty}^{\infty} \mathrm{d}\varepsilon\delta(\varepsilon - \varepsilon_{k'})f(\varepsilon) = \int \mathrm{d}\varepsilon N(\varepsilon)f(\varepsilon)$$

NB: recall that ε is a two-particle kinetic energy.

$$a(\varepsilon)(\varepsilon - E) = V\int_{|\varepsilon' - 2\varepsilon_F| < 2\omega_0} \mathrm{d}\varepsilon' a(\varepsilon')N(\varepsilon')$$

$$a(\varepsilon) = \frac{K_1}{\varepsilon - E} \implies K_1 = V\int_{|\varepsilon' - 2\varepsilon_F| < 2\omega_0} \mathrm{d}\varepsilon' \frac{K_1}{\varepsilon' - E}N(\varepsilon')$$

Thus, the unknown factor K_1 drops out. Furthermore, the energy shell is thin, and we assume $N(\varepsilon)$ is a slowly varying function of ε around the , $\varepsilon \approx 2\varepsilon_F$.

$$1 \approx \overbrace{VN(\varepsilon_F)}^{\equiv\lambda}\int_{2\varepsilon_F}^{2\varepsilon_F + 2\omega_0} \mathrm{d}\varepsilon' \frac{1}{\varepsilon' - E}$$

$\lambda > 0$, by definition.

$$\frac{1}{\lambda} = \ln\left|\frac{2\varepsilon_F + 2\omega_0 - E}{2\varepsilon_F - E}\right|$$

Now define the two particle binding-energy $\Delta \equiv 2\varepsilon_F - E$
Then,

$$\frac{1}{\lambda} = \ln\left(1 + \frac{2\omega_0}{\Delta}\right)$$

$\lambda > 0$: Solution requires that $\Delta > 0 \implies E < 2\varepsilon_F$!
Solve for Δ:

$$\frac{2\omega_0}{\Delta} = \mathrm{e}^{\frac{1}{\lambda}} - 1$$
$$\Delta = 2\omega_0 \frac{1}{\mathrm{e}^{\frac{1}{\lambda}} - 1}$$
$$\lambda \ll 1 : \Delta \approx 2\omega_0 \mathrm{e}^{-\frac{1}{\lambda}}.$$

Had we cept $\hbar$ explicitly in the calculations, we would have found

$$\Delta = 2\hbar\omega_0 \mathrm{e}^{-\frac{1}{\lambda}}. \tag{7.1.4}$$

We next comment on $E < 2\varepsilon_F$. At first glance, this would seem to violate the Pauli-principle, since it looks like we have the two added electrons now residing inside the Fermi-sea. In fact, there is no violation of the Pauli-principle, for the following reason. The bound state must be viewed as an entity, not as two individual electrons. We may think about this as a state created by a creation operator

$$b_k^\dagger = c_{k\uparrow}^\dagger c_{-k\downarrow} \tag{7.1.5}$$

and corresponding destruction operator

$$b_k = c_{-k\downarrow}^\dagger c_{k\uparrow}. \tag{7.1.6}$$

These operators do not obey fermionic anti-commutation relations. Therefore, this composite particle is not a fermion. Note that by forming this pair, called a Cooper-pair, the electrons have gotten rid of the severe limitations posed by the Pauli-principle, and this composite state is allowed to reside inside the Fermi-sea. A few remarks are in order:

- The bound state energy
  $\Delta = 2\hbar\omega_0 \mathrm{e}^{-\frac{1}{\lambda}}$
  This means that $\Delta > 0$ is a quantum effect, since it requires $\hbar \neq 0$.

- Δ is exponentially sensitive to $\lambda = VN(\varepsilon_F)$. Note that, in addition to V, we must have a non-zero density of states on the Fermi-surface. Thus, a Fermi-surface is requried to get Cooper-pairs.

- These electron-pairs are bound states in momentum-space, not in real space!

- Note how Δ depends on λ . As $\lambda \to 0$, Δ features an essential singularity. Such a result could not have been obtained in perturbation theory to any finite order. An attractive electron-electron interaction is a singular perturbation.

- Thermal effects: It stands to reason that the bound state we have found will be dissocated at some temperature. This temperature will be $k_B T_0 \sim \Delta$. Above this temperature, no Cooper-pairs will exist.

- Note also the important fact that the binding of two electrons into a Cooper-pair (a composite non-fermionic entity) does not rely on a spesific mechanism for producing an attractive electron-electron interaction. Thus, the consept is quite general in any fermionic system with a non-zero density of states on the Fermi-surface.

- Note also that we are careful in not saying that Cooper-pairs are bosons, they are in fact not! Elementary particles are either bosons or fermions, but Cooper-pairs is not an elementary particle, obviously.

- The problem just considered is admittedly quite artificially, only two electrons in a thin shell around the Fermi-surface interact. What if we include interactions also among all electrons within a thin shell around the Fermi-surface?

In that case, we would have a real many-body problem to solve, with an interaction that cannot be treated in perturbation theory (lesson from Cooper-problem). This is the problem we will next, and it leads to a microscopic theory of superconductivity, the phenomena that a metal looses all electrical resistance below a certain temperature. The binding energy Δ of a Cooper-pair turns into a gap in the excitation spectrum of electrons close to the Fermi-surface. This protects electrons from scattering, leading to zero resistivity. This happens at a temperature $\sim$ gap at zero temperature.

7.2 The Bardeen-Cooper-Scheiffer theory of superconductivity

This is essentially the many-particle version of the Cooper-problem. Superconductivity:

Insert figure depicting resistivity

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

$$\rho(T) = \begin{cases} 0 & \text{if } T < T_C \\ \text{nonzero} & \text{if } T > T_C \end{cases} \tag{7.2.1}$$

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 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

$$\Delta = 2\hbar\omega_0 \mathrm{e}^{-\frac{1}{\lambda}} \tag{7.2.2}$$

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, $\tilde{V}_{\text{eff}}$.

$$\begin{aligned} \mathcal{H} = &\sum_{k,\sigma} (\varepsilon_k - \mu)\, c^\dagger_{k\sigma} c_{k\sigma} \\ &+ \sum_{\substack{k,k',q \\ \sigma,\sigma'}} \tilde{V}_{\text{eff}} c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma} \end{aligned} \tag{7.2.3}$$

[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.

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

$$\tilde{V}_{\text{eff}} = \frac{2|g_q|^2\omega_q}{\omega^2 - \omega_q^2} + V_{\text{Coulomb}}(q) \tag{7.2.4}$$

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

$$\tilde{V}_{\text{eff}} = \frac{2|g_q|^2\omega_q}{\omega^2 - \omega_q^2}. \tag{7.2.5}$$

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. 7.2. We see that in general, the state with 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

$$\mathcal{H} = \sum_{k,\sigma}(\varepsilon_k - \mu)c^\dagger_{k\sigma}c_{k\sigma} + \sum_{k,q,\sigma}\tilde{V}_{\text{eff}}c^\dagger_{k+q,\sigma}c^\dagger_{-(k+q),-\sigma}c_{-k,-\sigma}c_{k\sigma}. \tag{7.2.6}$$

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. (7.2.6) as

$$\mathcal{H} = \sum_{k,\sigma}(\varepsilon_k - \mu)c^\dagger_{k\sigma}c_{k\sigma} + \sum_{k,k'}V_{k,k'}c^\dagger_{k,\uparrow}c^\dagger_{-k,\downarrow}c_{-k',\downarrow}c_{k,\uparrow}, \tag{7.2.7}$$

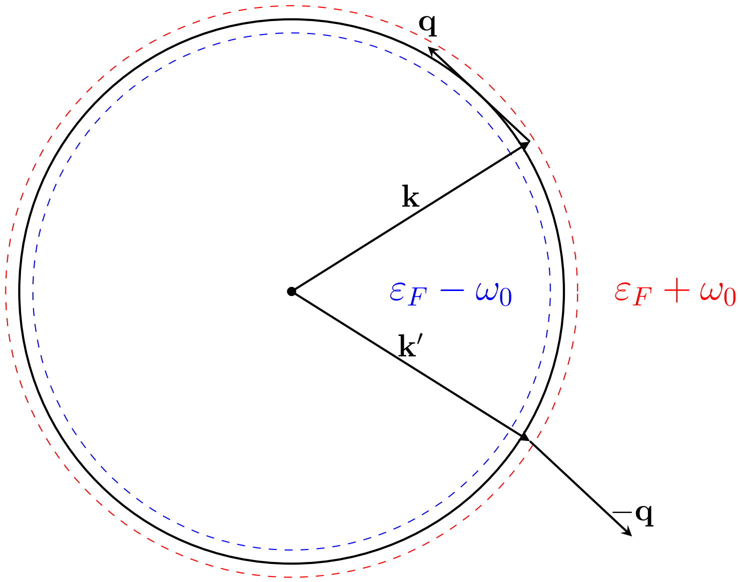


Figure 7.2: Thin shell around the Fermi surface.

with $V_{k,k'}$ being attractive if k, k' lie in a small vicinity of the Fermi-surface, and zero otherwise. eq. (7.2.7) 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:

$$\begin{aligned} c_{-k\downarrow}c_{k\uparrow} &= \underbrace{\langle c_{-k\downarrow}c_{k\uparrow}\rangle}_{\equiv b_k} + \underbrace{c_{-k\downarrow}c_{k\uparrow} - \langle c_{-k\downarrow}c_{k\uparrow}\rangle}_{\delta b_k} \\ &= b_k + \delta b_k. \end{aligned} \tag{7.2.8}$$

Here, b_k is a statistical average [2]. Note that 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. Note also that these expectations values are <u>not</u> on the usual $\langle c^\dagger c \rangle$-form, and the question now is to answer whether such expectation values can exist or not. Now insert the definitions in eq. (7.2.8) and the Hermitian conjugate into eq. (7.2.7) and ignore terms $\mathcal{O}((\delta b)^2)$ Consider the interaction term:

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

Next, define

$$\Delta_k \equiv -\sum_{k'} V_{kk'} b_{k'} \tag{7.2.9a}$$

$$\Delta^\dagger_k \equiv -\sum_{k} V_{kk'} b^\dagger_k. \tag{7.2.9b}$$

Inserting these in definitions into the Hamiltonian gives

$$\begin{aligned}\mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} - \sum_k \left[\Delta_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + \Delta^\dagger_k c_{-k\downarrow c_{k\uparrow}}\right] \\ + \sum_k \Delta_k b^\dagger_k.\end{aligned} \tag{7.2.10}$$

This is the mean-field approximation to the BCS-model, where b_k (and hence Δ_k) must be determined self-consistently, by minimizing the free energy of the system. We return to that below, but first we must diagonalize the Hamiltonian in eq. (7.2.10). Note that we now have terms like $c^\dagger c$, $\quad c^\dagger c^\dagger$, and cc in $\mathcal{H}$, reminiscent of what we had with boson-operators for the case of quantum antiferromagnets. We will now proceed along a similar route, but with the important difference that we are now considering fermions. Introduce new fermion-operators

$$\eta_k = u_k c_{k\uparrow} + v_k c^\dagger_{-k\downarrow} \tag{7.2.11a}$$

$$\gamma_k = u_k c_{-k\downarrow} - v_k c_{k\uparrow} \tag{7.2.11b}$$

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

These operators are fermionic quasi-particles as linear combinations of spin-up and spin-down particles. Thus spin is not a correct quantum number for the new fermions. Note the minus sign in eq. (7.2.11b). This transformations is required to preserve fermionic commutation relations, for instance

$$\left\{\eta_k, \eta_{k'}^\dagger\right\} = \delta_{kk'}, \tag{7.2.12}$$

η_k, γ_k anticommute,

$$\left\{\eta_k, \gamma_{k'}^\dagger\right\} = 0$$

.

$$u_k u_{k'} \delta_{kk'} + v_k v_{k'} \delta_{kk'} = \delta_{kk'},$$

with the +-sign originating in anti-commutation relations. Thus $\underline{u_k^2 + v_k^2 = 1}$. We reach the same conclusion with $\{\gamma_k, \gamma_{k'}\} = \delta_{kk'}$. This relation is the reason for the minus sign in front of v_k in eq. (7.2.11b)!

$$\begin{pmatrix} \eta_k \\ \gamma_k \end{pmatrix} = \overbrace{\begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix}}^{\equiv M} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{pmatrix} \tag{7.2.13}$$

With these signs, $\det M = u_k^2 + v_k^2 = 1$

$$M = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \qquad M^T = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \qquad M^{-1} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \tag{7.2.14}$$

Thus, M is a unitary transformation with the constraint $u_k^2 + v_k^2 = 1 \implies |u_k|, |v_k| \leq 1$. This is very different from the "squeezing" transformation we used in the quantum AFM-case. Going back to eq. (7.2.11), we have

$$\begin{pmatrix} \eta_k \\ \gamma_k \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{pmatrix} \tag{7.2.15a}$$

$$\begin{pmatrix} \eta_k^\dagger \\ \gamma_k^\dagger \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{-k\downarrow} \end{pmatrix} \tag{7.2.15b}$$

$$\begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} \eta_k \\ \gamma_k \end{pmatrix} \tag{7.2.15c}$$

$$\begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} \eta_k^\dagger \\ \gamma_k^\dagger \end{pmatrix} \tag{7.2.15d}$$

Insert this into the Hamiltonian eq. (7.2.10),

$$\begin{aligned}\mathcal{H} = \sum_k \Big\{ &\Big(\varepsilon_k - \mu\Big) \Big(u_k\eta_k^\dagger - v_k\gamma_k^\dagger\Big) \Big(u_k\eta_k - v_k\gamma_k\Big) \\ &+ \Big(\varepsilon_k - \mu\Big) \Big(v_k\eta_k + u_k\gamma_k\Big) \Big(v_k\gamma_k^\dagger + u_k\gamma_k^\dagger\Big) \\ &- \Delta_k \Big(u_k\eta_k^\dagger - v_k\gamma_k^\dagger\Big) \Big(v_k\eta_k + u_k\gamma_k\Big) \\ &- \Delta_k^\dagger \Big(u_k\eta_k^\dagger + u_k\gamma_k^\dagger\Big) \Big(u_k\eta_k - v_k\gamma_k\Big) + \Delta_k b_k^\dagger \Big\}\end{aligned} \tag{7.2.16}$$

As in the quantum antiferromagnet-case, we now collect terms of different types:

$$\eta_k^\dagger\eta_k : (\varepsilon_k - \mu)\, u_k^2 - u_k v_k \Big(\Delta_k + \Delta_k^\dagger\Big) \tag{7.2.17a}$$

$$\gamma_k^\dagger\gamma_k : (\varepsilon_k - \mu)\, v_k^2 + +u_k v_k \Big(\Delta_k + \Delta_k^\dagger\Big) \tag{7.2.17b}$$

$$\eta_k\eta_k^\dagger : (\varepsilon_k - \mu)\, v_k^2 \tag{7.2.17c}$$

$$\gamma_k\gamma_k^\dagger : (\varepsilon_k - \mu)\, u_k^2 \tag{7.2.17d}$$

$$\gamma_k^\dagger\eta_k : -2\,(\varepsilon_k - \mu)\, u_k v_k + \Delta_k v_k^2 - \Delta_k^\dagger u_k^2 \tag{7.2.17e}$$

$$\eta_k^\dagger\gamma_k : -2\,(\varepsilon_k - \mu)\, u_k v_k - \Delta_k u_k^2 + v_k^2\Delta_k^\dagger \tag{7.2.17f}$$

Using the anticommutation relations in eq. (7.2.12), and the corresponding for γ_k, we may express eqs. (7.2.17a) and (7.2.17b) as

$$\eta_k^\dagger\eta_k : (\varepsilon_k - \mu)\left(u_k^2 - v_k^2\right) - u_k v_k \Big(\Delta_k + \Delta_k^\dagger\Big) \tag{7.2.18a}$$

$$\gamma_k^\dagger\gamma_k : (\varepsilon_k - \mu)\left(v_k^2 - u_k^2\right) + u_k v_k \Big(\Delta_k + \Delta_k^\dagger\Big) \tag{7.2.18b}$$

These are the same, except opposite sign. Adjust u_k, v_k such that the coefficients in front of eqs. (7.2.17e) and (7.2.17f) are zero. Fortunately, these two equations are just complex conjugate of each other, so if one is fulfilled, so is the other. If we set these two to 0, we have

$$-2\,(\varepsilon_k - \mu)\, u_k v_k = u_k^2\Delta_k - v_k^2\Delta_k^\dagger \tag{7.2.19}$$

$$-2\,(\varepsilon_k - \mu)\, u_k v_k = u_k^2\Delta_k^\dagger - v_k^2\Delta_k^\dagger. \tag{7.2.20}$$

By adding these two equations, we get

$$-4\underbrace{(\varepsilon_k - \mu)}_{\equiv\tilde{\varepsilon}_k} u_k v_k = \left(u_k^2 - v_k^2\right)\Big(\Delta_k + \Delta_k^\dagger\Big)$$

$$\Delta_k + \Delta_k^\dagger = 2\,\mathrm{Re}\{\Delta_k\} \equiv 2\tilde{\Delta}_k$$

$$-2\tilde{\varepsilon}_k u_k v_k = \left(u_k^2 - v_k^2\right)\tilde{\Delta}_k$$

Since we have $u_k^2 + v_k^2 = 1$, we may write

$$\begin{aligned}
u_k &= \cos\theta \\
v_k &= \sin\theta \\
-\tilde{\varepsilon}_k \sin 2\theta &= \tilde{\Delta}_k \cos 2\theta
\end{aligned}$$

$$\tan 2\theta = -\frac{\tilde{\Delta}_k}{\tilde{\varepsilon}_k} \tag{7.2.21}$$

This is an equation for θ, and thus u_k, v_k, which gives coefficients of $\gamma_k^\dagger \eta_k, \eta_k^\dagger \gamma_k$ equal to zero. Choose $\tilde{\Delta}_k \geq 0$

$$\begin{aligned}
\tan 2\theta < 0; &\quad \tilde{\varepsilon} > 0 \\
\tan 2\theta > 0; &\quad \tilde{\varepsilon} < 0 \\
\frac{\sin^2(2\theta)}{\cos^2(2\theta)} &= \left(\frac{\tilde{\Delta}_k}{\tilde{\varepsilon}_k}\right)^2 \equiv b^2 \\
\cos^2(2\theta) &= \frac{1}{1+b^2} \\
\cos(2\theta) &= \begin{cases} \frac{-1}{\sqrt{1+b^2}}; & \tilde{\varepsilon} > 0 \\ \frac{1}{\sqrt{1+b^2}}; & \tilde{\varepsilon} < 0 \end{cases}
\end{aligned}$$

Coefficient in front of $\eta_k^\dagger \eta_k$:

$$\begin{aligned}
\tilde{\varepsilon}_k \cos 2\theta - \tilde{\Delta}_k \sin 2\theta &= \cos(2\theta)\left(\tilde{\varepsilon}_k + \left(\frac{\tilde{\Delta}_k}{\tilde{\varepsilon}_k}\right)^2\right) \\
&= -\frac{\mathrm{sign}\tilde{\varepsilon}_k}{\tilde{\varepsilon}_k} \frac{\left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)}{(1+b^2)^{\frac{1}{2}}} \\
&= -\frac{\mathrm{sign}\tilde{\varepsilon}_k}{\frac{\tilde{\varepsilon}_k}{|\tilde{\varepsilon}_k|}} \left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}} \\
&= -\left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}}
\end{aligned}$$

Coefficient in front of $\gamma_k^\dagger \gamma_k$: $\left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}}$. Thus, we have finally diagonalized the Hamiltonian

$$\mathcal{H} = \sum_k \left[2\left(\varepsilon_k - \mu\right) + \Delta_k b_k^\dagger + E_k\left(\gamma_k^\dagger \gamma_k - \eta_k^\dagger \eta_k\right)\right], \tag{7.2.22}$$

where the summation over spins has been made, and with

$$E_k \equiv \left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}}. \tag{7.2.23}$$

b_k and $\tilde{\Delta}_k$ are as yet undetermined. They will have to be determined by minimizing the free energy of this system. The long-lived fermionic excitation are described by $(\eta_k, \eta_k^\dagger)$, $(\gamma_k, \gamma_k^\dagger)$.

Check signs

$$\mathcal{H} = E_0 + \sum_k E_k \left(\gamma_k^\dagger \gamma_k - \eta_k^\dagger \eta_k\right) \tag{7.2.24}$$

$$E_0 = \sum_k \left[2\left(\varepsilon_k - \mu\right) + \Delta_k b_k^\dagger\right] \tag{7.2.25}$$

If we have a fermionic system with a Hamiltonian

$$\mathcal{H} = \sum_k (\varepsilon_k - \mu) c_k^\dagger c_k,$$

the grand canonical partition function is given by

$$\mathcal{Z}_g = \prod_k \left(1 + \mathrm{e}^{-\beta(\varepsilon_k - \mu)}\right). \tag{7.2.26}$$

Is the present case, this gives

$$\mathcal{Z}_g = \mathrm{e}^{-\beta E_0} \prod_k \left(1 + \mathrm{e}^{\beta E_k}\right)\left(1 + \mathrm{e}^{-\beta E_k}\right). \tag{7.2.27}$$

In the limit of large number of particles, all ensembles are equivalent. To expedite th computations, we will consider $\mathcal{Z}_g$ ti be equal to $\mathcal{Z} = \mathrm{e}^{-\beta F}$, where F is the Helmholz free energy for a system.

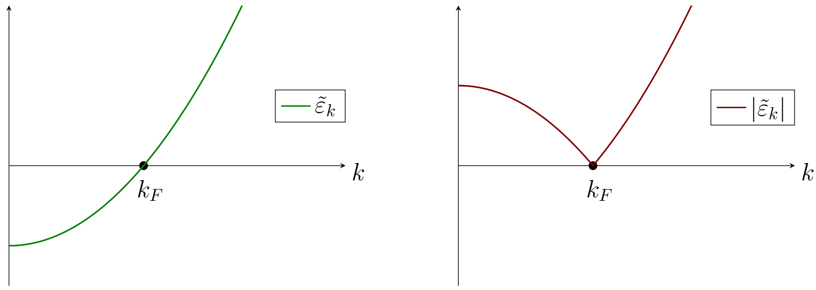
$$F = E_0 - \frac{1}{\beta} \sum_k \left[\ln\left(1 + \mathrm{e}^{-\beta E_k}\right) + \ln\left(1 + \mathrm{e}^{\beta E_k}\right)\right] \tag{7.2.28}$$

We now minimize with respect to Δ_k or $b_k^\dagger$ for a particular value of k. It does not matter which one of these we use. We look for

$$\frac{\partial F}{\partial \Delta_k} = 0, \tag{7.2.29}$$

or

$$b_k^\dagger - \frac{1}{\beta}\left(\frac{1}{1 + \mathrm{e}^{-\beta E_k}}(-\beta)\frac{\partial E_k}{\partial \Delta_k}\mathrm{e}^{-\beta E_k} + \frac{1}{1 + \mathrm{e}^{\beta E_k}}(\beta)\frac{\partial E_k}{\partial \Delta_k}\mathrm{e}^{\beta E_k}\right) = 0$$



(a) $\tilde{\varepsilon}_k$

(b) $|\tilde{\varepsilon}_k|$

Figure 7.3: Typical excitation spectrum at $\Delta_k = 0$.

$$
\begin{aligned}
b_k^\dagger &= \frac{\partial E_k}{\partial \Delta_k}\left(\frac{\mathrm{e}^x}{1+e^x} - \frac{\mathrm{e}^{-x}}{1+e^{-x}}\right) \\
&= \frac{\partial E_k}{\partial \Delta_k} \cdot \tanh\left(\frac{x}{2}\right); \quad x = \beta E_k \\
\frac{\partial E_k}{\partial \Delta_k} &= \frac{\Delta_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}},
\end{aligned}
$$

where we have set Δ_k to be real, such that $\tilde{\Delta}_k = \Delta_k$.

$$
b_k^\dagger = \frac{\Delta_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}} \tanh\left(\frac{\beta E_k}{2}\right) \tag{7.2.30}
$$

We close this to an equation for Δ_k by using the definitions in eq. (7.2.9) to obtain

$$
\Delta_k = -\sum_{k'} V_{kk'} \Delta_{k'} \chi_{k'} \tag{7.2.31}
$$

$$
\chi_k = \frac{1}{(\tilde{\varepsilon}_k^2 + \Delta_k^2)^{\frac{1}{2}}} \tanh\left(\frac{\beta E_k}{2}\right) \tag{7.2.32}
$$

This is the so-called BCS gap-equation. The reason for this name that it is an equation for Δ_k, which represents a gap in the excitation-spectrum. To see this, we first consider the excitation spectrum at $\Delta_k = 0$, depicted in fig. 7.3 Note that on the Fermi-surface ($k = k_F$), there is zero gap in the excitation spectrum $\Delta_k = 0$. From fig. 7.4, we see that Δ_k represents a gap <u>on the Fermi-surface</u> in the excitation spectrum of the Bogoliubov fermions. We will now solve eq. (7.2.31) for the same model for $V_{kk'}$ that we used in the

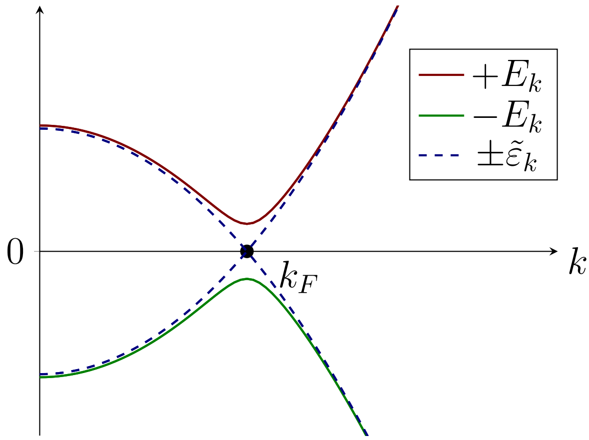


Figure 7.4: $\Delta_k \neq 0$ represents a gap in the excitation spectrum at the Fermi surface, here greatly exaggerated. The difference in the minimum of $+E_k$ and the maximum of $-E_k$ is $2\Delta_k$. This gap always tracks the Fermi surface.

Cooper problem, namely a constant attractive potential in a thin shell around the Fermi-surface. With the understanding that k, k' lie within this thin shell, we have

$$\Delta_k = V \sum_{k'} \Delta_{k'} \chi_{k'} \tag{7.2.33}$$

This means that Δ_k is independent of k, and we can divide by $\Delta = \Delta_k$ and get

$$1 = V \sum_{k'} \frac{1}{(\tilde{\varepsilon}_{k'}^2 + \Delta^2)^{\frac{1}{2}}} \tanh\left(\frac{\beta E_{k'}}{2}\right). \tag{7.2.34}$$

Now use

$$\sum_k g(\tilde{\varepsilon}_k) = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \sum_k \delta(\varepsilon - \tilde{\varepsilon}_k) g(\tilde{\varepsilon}) = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon N(\varepsilon) g(\varepsilon), \tag{7.2.35}$$

$$1 = V \int_{-\omega_0}^{\omega_0} \mathrm{d}\varepsilon \frac{N(\varepsilon)}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh\left(\frac{\beta\sqrt{\varepsilon^2 + \Delta^2}}{2}\right) \tag{7.2.36}$$

Note: ε must lie within a thin energy-shell around the Fermi surface! We have denoted the width of this shell $2\omega_0$

$$-\omega_0 < \varepsilon < \omega_0$$

when energies ε are measured relative μ. Consider now $N(\varepsilon)$ a rather slowly varying function of ε in the thin shell around the Fermi-surface, such that $N(\varepsilon) \simeq N(\varepsilon_F) = N(\mu)$. Introduce $\lambda \equiv VN(\varepsilon_F)$, such that

$$1 = \lambda \int_{-\omega_0}^{\omega_0} \mathrm{d}\varepsilon \frac{1}{\sqrt{\varepsilon^2+\Delta^2}} \tanh\left(\frac{\beta\sqrt{\varepsilon^2+\Delta^2}}{2}\right). \tag{7.2.37}$$

eq. (7.2.37) is difficult to solve, but we will look at two special cases, at $T = 0$ and $T = T_C$.

i) $T = 0$

At $T = 0$, $\tanh\left(\frac{\beta\sqrt{\varepsilon^2+\Delta^2}}{2}\right) = 1$, such that [3]

$$\begin{aligned} 1 &= \lambda \int_0^{\omega_0} \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2+\Delta^2}} \\ &= \lambda \int_0^{\frac{\omega_0}{\Delta}} \frac{\mathrm{d}x}{\sqrt{x^2+1}} \\ &= \lambda \sinh^{-1}\left(\frac{\omega_0}{\Delta}\right) \\ &= \lambda \ln\left(\frac{\omega_0}{\Delta} + \sqrt{\left(\frac{\omega_0}{\Delta}\right)+1}\right) \\ \Longrightarrow \quad \frac{\omega_0}{\Delta} &= \sinh\left(\frac{1}{\lambda}\right) = \frac{1}{2}\left(\mathrm{e}^{\frac{1}{\lambda}} - \mathrm{e}^{\frac{-1}{\lambda}}\right) \end{aligned} \tag{7.2.38}$$

Now consider $\lambda \ll 1 \implies \frac{2\omega_0}{\Delta} \simeq \mathrm{e}^{\frac{1}{\lambda}}$. Reinserting $\hbar$ we obtain

$$\Delta = 2\hbar\omega_0 \mathrm{e}^{\frac{-1}{\lambda}}. \tag{7.2.39}$$

Notice the similar expression in eqs. (7.1.4) and (7.2.39).

ii) The critical temperature

We see from the gap-equation that as T increases, the tanh-factor decreases. Thus, to obtain a solution to the gap-equation requires smaller Δ. As T increases, Δ decreases. Sooner or later, we will reach a temperature whre

[3] The subsequent λ is now redefined by a factor 2, not any more considering per-spin density of states.

$\Delta \to 0^+$. This will be the critical temperature, T_C, which is determined by the equation

$$1 = \lambda \int_0^{\omega_0} \mathrm{d}\varepsilon \, \frac{\tanh\left(\frac{\beta\varepsilon}{2}\right)}{\varepsilon}. \tag{7.2.40}$$

Introducing $x = \frac{\beta\varepsilon}{2}$,

$$\begin{aligned}\frac{1}{\lambda} &= \int_0^{\frac{\beta\omega_0}{2}} \frac{\mathrm{d}x}{x} \tanh(x) \\ &= \ln(x)\tanh(x)\Big|_0^{\frac{\beta\omega_0}{2}} - \int_0^{\frac{\beta\omega_0}{2}} \mathrm{d}x \, \frac{\ln(x)}{\cosh^2(x)}.\end{aligned}$$

Again, we consider $\lambda \ll 1 \implies \frac{\beta\omega_0}{2} \gg 1$. In the last term, we may replace the upper limit by ∞.

$$\frac{1}{\lambda} \simeq \ln\left(\frac{\beta\omega_0}{2}\right) - \underbrace{\int_0^{\infty} \mathrm{d}x \, \frac{\ln(x)}{\cosh^2(x)}}_{=\ln\left(\frac{\pi}{4}\mathrm{e}^{-\gamma}\right) \equiv \ln(C)}, \tag{7.2.41}$$

where $\gamma \simeq 0.5772156649$ is the Euler-Mascheroni constant.

$$\frac{1}{\lambda} = \ln\left(\frac{\beta\omega_0}{2C}\right) \tag{7.2.42}$$

$$\frac{\beta\omega_0}{2C} = \mathrm{e}^{\frac{1}{\lambda}} \tag{7.2.43}$$

$$k_B T_C = \frac{2}{\pi}\mathrm{e}^{\gamma}\omega \mathrm{e}^{\frac{-1}{\lambda}} \tag{7.2.44}$$

Note how extremely sensitive both Δ and $k_B T_C$ is to λ! Note also that the depend on λ in the same way. So if we take their ratios, this dependence cancels, as does the prefactor.

$$\frac{2\Delta(T=0)}{k_B T_C} = \frac{4\omega_0 \mathrm{e}^{\frac{-1}{\lambda}}}{\frac{2}{\pi}\mathrm{e}^{\gamma}\omega_0 \mathrm{e}^{\frac{-1}{\lambda}}} \tag{7.2.45}$$

$$= 2\pi \mathrm{e}^{-\gamma} \simeq 3.53, \tag{7.2.46}$$

which is a universal number! This prediction of the theory turned out to be remarkably accurate for real superconductors where $\lambda \ll 1$. Examples are Hg, Al, Sn. For Pb, the ratio is somewhat larger, and this is attributed to the fact that λ is larger than in Hg, Al, Sn. The opening up of a gap on the Fermi-surface means that the electron many-body state is protected from scattering by this gap. As a result, the resistivity of the electron gas drops abruptly to 0 at $T = T_C$.

> Superconductivity-onset is thus a phase-transition associated with the opening of a gap Δ_k on the Fermi-surface.

Often, this gap Δ_k is referred to as an order-parameter of the system. The original Hamiltonian is invariant under the transformation

$$c_{k\sigma} \to \mathrm{e}^{i\theta} c_{k\sigma}, \tag{7.2.47}$$

where θ is a global phase factor. This is therefore a symmetry of the problem, a global $U(1)$-symmetry as mentioned above. Δ_k is nonzero if and only if b_k is nonzero. The quantity

$$\langle b_k \rangle = \langle c_{-k\downarrow} c_{k\uparrow} \rangle \tag{7.2.48}$$

is, however, not invariant under this global U(1)-transformation. Thus, in the superconducting state, the U(1)-symmetry of $\mathcal{H}$ is spontaneously broken.

7.3 The Meissner Effect

Another truly remarkable property of superconductors is its electromagnetic properties, which are radically different from those of metals. Inside a metal, we have $\mathbf{E} = 0$. However, an externally applied magnetic field $\mathbf{B}$ will essentially penetrate a metal completely

If there is any tendency for the system to resist admitting the external **B**-field, then this is called diamagnetism. In a metal ($T > T_C$) this diamagnetism is very weak, see fig. 7.5a. In a superconductor ($T < T_C$) this is very different. If we take a metal and cool it down and then apply an external field, the magnetic field is excluded, as shown in fig. 7.5b.

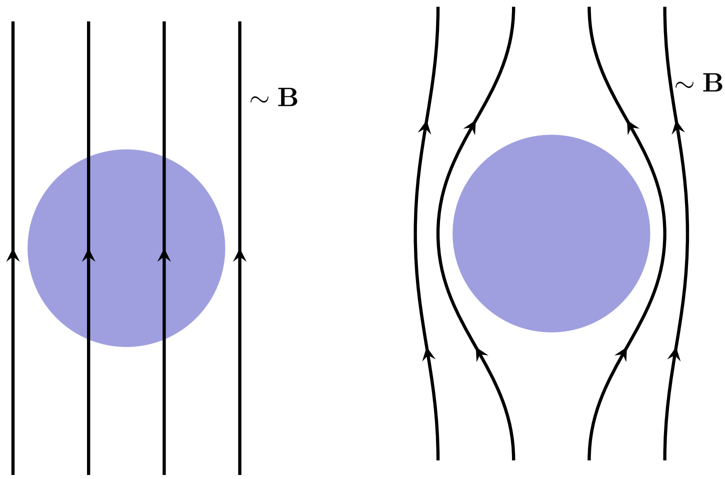
Now, the magnetic field is entirely excluded from the superconductor. This is called the Meissner-effect. We will now relate the Meissner-effect to the onset of a gap Δ_k below T_C.

> The Meissner-effect is the essential phenomenon characterizing a superconductor.

Start with the Maxwell-equations relating magnetic field to a current $\mathbf{J}$.

$$\boldsymbol{\nabla} \cdot \mathbf{B} = 0 \implies \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} \tag{7.3.1}$$

$$\boldsymbol{\nabla} \times \mathbf{B} = \mu_0 \mathbf{J} \tag{7.3.2}$$



(a) $T > T_C$ (metal)

(b) $T < T_C$ (cooled before applied magnetic field)

Figure 7.5: Meissner effect.

Now, as always, we need a constitutive relation for the current $\mathbf{J}$. Obviously, the standard one, $\mathbf{J} = \sigma\mathbf{E}$, where σ is conductivity and $\mathbf{E}$ is electric field, will not work, since it gives Ohmic resistance.

Supercurrent:

$$\mathbf{J}_s = e^* n_s \mathbf{v}_s. \tag{7.3.3}$$

e^*: An effective "quasiparticle" charge

n_s: density of superconducting charge-carriers (Bogoliubov quasiparticles)

$\mathbf{v}_s$: velocity of such quasiparticles

$\mathbf{v} = \frac{\mathbf{p}}{m^*}$, m^*: Mass of quasiparticle.

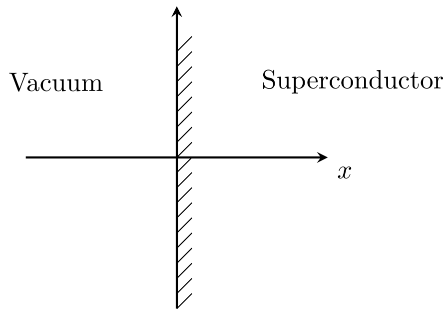


Figure 7.6: Semi-infinite superconductor

In the presence of an electromagnetic field,

$$\mathbf{p} \to \mathbf{p} - e^* \mathbf{A} \tag{7.3.4}$$

$$\mathbf{J}_s = \frac{e^*}{m} n_s \left(-e^* \mathbf{A}\right) = -\frac{\left(e^*\right)^2}{m} \mathbf{A} \tag{7.3.5}$$

$$\boldsymbol{\nabla} \times \left(\boldsymbol{\nabla} \times \mathbf{A}\right) = \mu_0 \mathbf{J}_s = -\frac{\mu_0 \left(e^*\right)^2 n_s}{m} \mathbf{A} \tag{7.3.6}$$

$$\boldsymbol{\nabla} \times \left(\boldsymbol{\nabla} \times \mathbf{A}\right) = \boldsymbol{\nabla} \left(\boldsymbol{\nabla} \cdot \mathbf{A}\right) - \boldsymbol{\nabla}^2 \mathbf{A} \tag{7.3.7}$$

$$\implies -\boldsymbol{\nabla}^2 \mathbf{A} + \frac{\mu_0 \left(e^*\right)^2 n_s}{m} \mathbf{A} = 0, \tag{7.3.8}$$

where we have restricted ourselves to the gauge where $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$ (Coulomb gauge). Define

$$\frac{1}{\lambda^2} \equiv \frac{\mu_0 \left(e^*\right)^2 n_s}{m}. \tag{7.3.9}$$

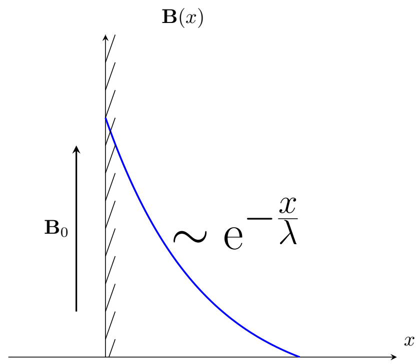
λ : A length (by dimensional analysis of equation for $\mathbf{A}$).

Consider for simplicity a semi-infinite superconductor as in fig. 7.6. Here, $\mathbf{A} = \mathbf{A}(x)$. At $x = 0 : \mathbf{A}(x = 0) = \mathbf{A}_0$.

$$\frac{\mathrm{d}^2 \mathbf{A}}{\mathrm{d}x^2} = \frac{1}{\lambda^2} \mathbf{A} \tag{7.3.10}$$

$$\implies \mathbf{A}(x) = \mathbf{A}_0(x) \mathrm{e}^{-\frac{x}{\lambda}} \tag{7.3.11}$$

$$\mathbf{B}(x) = \boldsymbol{\nabla} \times \mathbf{A} \tag{7.3.12}$$



$B_i = \varepsilon_{ijl}\partial_j A_l$. $j = x(= 1)$ since there is only x-dependence.

$$B_y = \varepsilon_{213}\partial_x A_z = -\partial_x A_z = \frac{1}{\lambda} A_{0z} \mathrm{e}^{\frac{-x}{\lambda}}$$
$$B_z = \varepsilon_{312}\partial_x A_y = +\partial_x A_y = -\frac{1}{\lambda} A_{0y} \mathrm{e}^{\frac{-x}{\lambda}}$$

Thus,

$$\mathbf{B}(x) = \mathbf{B}_0 \mathrm{e}^{\frac{-x}{\lambda}}. \tag{7.3.13}$$

Now we see the physical meaning of λ: It is a characteristic length for how far a magnetic field penetrates a superconductor. It is referred to as the London penetration length. Thus, a magnetic field only exists withing a layer of thickness λ from the surface of the superconductor. There is no magnetic field in the bulk of the superconductor. This is the Meissner-effect.

Meissner-effect : $\lambda^{-1} > 0$.

No Meissner-effect: $\lambda^{-1} = 0$.

The expression for λ is

$$\lambda = \left(\frac{m}{\mu_0 n_s \left(e^*\right)^2} \right)^{\frac{1}{2}}, \tag{7.3.14}$$

a magnetic penetration length. $\lambda^{-1} > 0$ if and only if $n_s > 0$. $\lambda^{-1} = 0$ otherwise. How does n_s relate to $\Delta_k^\dagger$? $\Delta_k^\dagger$ originates with $b_k^\dagger = \langle c_{-k\downarrow} c_{k\uparrow} \rangle^\dagger$ which is the expectation value of the creation operator of a Cooper pair.

Fourier-transformed to real-space it is the wavefunction $\psi(\mathbf{r})$ of a Cooper-pair. $n_s \sim |\psi|^2$, thus $n_s \neq 0$ if and only if $\Delta_k \neq 0$.[4] Thus the onset of Δ_k for $T < T_C$ also means the onset of the Meissner-effect.

The onset of Δ_k at $T < T_C$ explains:

i) loss of resistivity $\rho(T)$

ii) onset of Meissner-effect

7.4 Multi-band superconductors

In many new materials, we may have a situation where several energy-bands can cross the Fermi-level. In such a situation, we will have multiple Fermi-surfaces that can participate in superconductivity. A prominent example of this is superconductivity in the iron-particles, where at least three bands are involved in superconductivity. These materials are potentially important and of great interest because they are high-T_C superconductors, and because they feature interesting new physics precisely because multiple bands are involved in superconductivity. Let us try to set up a theory of such superconductors within the framework we have used up until now. We introduce an index α for an energy band $\varepsilon_{k\alpha}$. A BCS-reduced Hamiltonian is

$$\mathcal{H} = \sum_{k,\alpha,\sigma} (\varepsilon_{k\alpha} - \mu) c^\dagger_{k\alpha\sigma} c_{k\alpha\sigma} + \sum_{\substack{k,k' \\ \alpha,\beta}} V^{\alpha\beta}_{kk'} P^\dagger_{k\alpha} P_{k'\beta} \tag{7.4.1}$$

where

$$P^\dagger_{k\alpha} \equiv c^\dagger_{k\alpha\uparrow} c^\dagger_{-k\alpha\downarrow}. \tag{7.4.2}$$

$V^{\alpha\beta}_{kk'}$ scatters a pair of electrons at $k, -k$ in band α to $(k', -k')$ in band β. We now perform a mean-field approximation exactly as in the one-band case.

$$P^\dagger_{k\alpha} = b^\dagger_{k\alpha} + \delta P^\dagger_{k\alpha}, \tag{7.4.3}$$

[4]Says iff $\Delta_k = 0$ in the notes, which doesn't seem right.s

and ignore $(\delta P^{\dagger}_{k\alpha})^2$-terms. This gives:

$$\begin{aligned}\mathcal{H} &= \sum_{k,\alpha,\sigma} (\varepsilon_{k\alpha} - \mu) c^{\dagger}_{k\alpha\sigma} c_{k\alpha\sigma} \\ &+ \sum_{\substack{k,k'\\ \alpha,\beta}} V^{\alpha\beta}_{kk'} \left[b^{\dagger}_{k\alpha} c^{\dagger}_{-k'\beta\downarrow} c_{k'\beta\uparrow} + b_{k'\beta} c^{\dagger}_{k\alpha\uparrow} c^{\dagger}_{-k\alpha\downarrow} - b^{\dagger}_{k\alpha} b_{k'\beta} \right],\end{aligned} \tag{7.4.4}$$

where

$$b^{\dagger}_{k\alpha} \equiv \langle c^{\dagger}_{k\alpha\uparrow} c^{\dagger}_{-k\alpha\downarrow} \rangle \tag{7.4.5}$$

$$b_{k\beta} \equiv \langle c_{-k\beta\downarrow} c_{k\beta\uparrow} \rangle \,. \tag{7.4.6}$$

Now define

$$\Delta_{k\alpha} = - \sum_{k',\beta} V^{\alpha\beta}_{kk'} b_{k'\beta} \tag{7.4.7}$$

$$\Delta^{\dagger}_{k'\beta} = - \sum_{k,\alpha} V^{\alpha\beta}_{kk'} b^{\dagger}_{k\alpha}. \tag{7.4.8}$$

Then, at mean-field level:

$$\begin{aligned}\mathcal{H} &= \sum_{k,\alpha} \Delta_{k\alpha} b^{\dagger}_{k\alpha} \\ &+ \sum_{k,\alpha,\sigma} (\varepsilon_{k\alpha} - \mu) c^{\dagger}_{k\alpha\sigma} c_{k\alpha\sigma} \\ &- \sum_{k,\alpha} \left[\Delta^{\dagger}_{k\alpha} P_{k\alpha} + \Delta_{k\alpha} P^{\dagger}_{k\alpha} \right]\end{aligned} \tag{7.4.9}$$

Note how $\Delta_{k\alpha}, \Delta^{\dagger}_{k\alpha}$ act as source- and sink-fields for Cooper-pairs in band α. However, $\Delta_{k\alpha}, \Delta^{\dagger}_{k\alpha}$ have contributions from all bands, since $V^{\alpha\beta}_{kk'}$ provides inter-band $(\alpha = \beta)$ as well as inter-band $(\alpha \neq \beta)$ scattering. Note also that $\mathcal{H}$ is now "diagonalized " in band-indices, and we may diagonalize the problem exactly as in the one-band case. To this end, we now introduce operators of the same type that we introduced in the one-band case, now generalized to an arbitrary number of band, one set of operators for each band, as follows

$$\begin{aligned}\eta^{\dagger}_{k\alpha} &= u_{k\alpha} c^{\dagger}_{k\alpha\uparrow} + v_{k\alpha} c_{-k\alpha\downarrow} \\ \gamma^{\dagger}_{k\alpha} &= u_{k\alpha} c_{-k\alpha\downarrow} - v_{k\alpha} c^{\dagger}_{k\alpha\uparrow}\end{aligned} \tag{7.4.10}$$

For each band α, the calculations are now exactly as for the one-band case. Thus, we obtain

$$\begin{aligned}\mathcal{H} = \sum_{k,\alpha}\left[(\varepsilon_{k\alpha} - \mu) + \Delta_{k\alpha} b^{\dagger}_{k\alpha}\right] \\ + \sum_{k,\alpha} E_{k\alpha}\left(\gamma^{\dagger}_{k\alpha}\gamma_{k\alpha} - \eta^{\dagger}_{k\alpha}\eta_{k\alpha}\right).\end{aligned} \tag{7.4.11}$$

From this, we obtain the free energy

$$\begin{aligned}F = \sum_{k,\alpha}\left[(\varepsilon_{k\alpha} - \mu) + \Delta_{k\alpha} b^{\dagger}_{k\alpha}\right] \\ - \sum_{k,\alpha}\left[\ln\left(1 + \mathrm{e}^{-\beta E_{k\alpha}}\right) + \ln\left(1 + \mathrm{e}^{\beta E_{k\alpha}}\right)\right]\end{aligned} \tag{7.4.12}$$

We now consider attracctive intra- and interband-interactions $V^{\alpha\beta}_{kk'} = V_{\alpha\beta}$, which are all taken to be constants in k, k' within thin shells around the Fermi-surfaces. Hence, the functions $\Delta^{\dagger}_{k\alpha}$ will also be k-independent, namely

$$\Delta^{\dagger}_{k\alpha} = -\sum_{k',\beta} V^{\alpha\beta}_{kk'} b^{\dagger}_{k'\beta} = \Delta^{\dagger}_{\alpha}. \tag{7.4.13}$$

Define

$$b^{\dagger}_{\beta} = \sum_{k} b^{\dagger}_{k\beta}, \tag{7.4.14}$$

In a vector-matrix notation, we may write this as follows

$$\Delta^{\dagger}_{\alpha} = -\sum_{\beta} V_{\alpha\beta} b^{\dagger}_{\beta} \tag{7.4.15}$$

$$\boldsymbol{\Delta}^{\dagger} = -V \cdot \boldsymbol{b}^{\dagger} \implies \boldsymbol{b}^{\dagger} = -V^{-1} \cdot \boldsymbol{\Delta}^{\dagger}. \tag{7.4.16}$$

where the latter equality supposes that the inverse matrix V^{-1} exists. hThus, we have

$$\begin{aligned}\sum_{k,\alpha} \Delta_{k\alpha} b^{\dagger}_{k\alpha} &= \boldsymbol{\Delta} \cdot \boldsymbol{b}^{\dagger} \\ &= -\boldsymbol{\Delta} \cdot (V^{-1}) \cdot \boldsymbol{\Delta}^{\dagger} \\ &= -\sum_{\alpha,\beta} \Delta_{\alpha} (V^{-1})_{\alpha\beta} \Delta^{\dagger}_{\beta}.\end{aligned} \tag{7.4.17}$$

$$V_{\alpha\beta} = V_{\beta\alpha} \implies (V^{-1})_{\alpha\beta}) = (V^{-1})_{\beta\alpha}. \tag{7.4.18}$$

$$E_0 = \sum_{k,\alpha}(\varepsilon_{k\alpha} - \mu) - \sum_{\alpha,\beta} \Delta_\alpha (V^{-1})_{\alpha\beta} \Delta^\dagger_\beta. \tag{7.4.19}$$

We now find an equation for Δ_α from $\frac{\partial F}{\partial \Delta_\alpha} = 0$.

$$\boxed{\frac{\partial E_0}{\partial \Delta_\alpha} - \sum_k \frac{\Delta^\dagger_\alpha}{2E_{k\alpha}} \tanh\left(\frac{\beta E_{k\alpha}}{2}\right) = 0.} \tag{7.4.20}$$

$$-\sum_\beta (V^{-1})_{\alpha\beta}\Delta^\dagger_\beta - \underbrace{\Delta^\dagger_\alpha \chi_\alpha}_{\equiv \tilde{\Delta}^\dagger_\alpha} = 0 \tag{7.4.21}$$

$$\chi_\alpha \equiv \sum_k \frac{1}{2E_{k\alpha}} \tanh\left(\frac{\beta E_{k\alpha}}{2}\right) \tag{7.4.22}$$

On matrix-vector form, we have

$$-V^{-1} \cdot \mathbf{\Delta}^\dagger = \tilde{\mathbf{\Delta}}^\dagger \tag{7.4.23}$$

$$\mathbf{\Delta}^\dagger = -V \cdot \tilde{\mathbf{\Delta}}^\dagger, \tag{7.4.24}$$

or equivalently

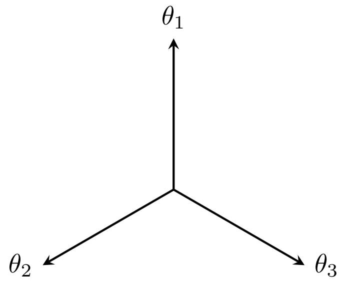
$$\Delta^\dagger_\alpha = -\sum_{k,\beta} V_{\alpha\beta} \frac{\Delta^\dagger_\beta}{2E_{k\beta}} \tanh\left(\frac{\beta E_{k\beta}}{2}\right). \tag{7.4.25}$$

$$\Delta_\alpha = |\Delta_\alpha| \mathrm{e}^{i\theta_\alpha} \tag{7.4.26}$$

Notice how phases θ_α of Δ_α do not necessarily cancel in the multiband-case, unlike the one-band case. This will lead to new physical effects with no counterpart in the one-band case, as follows. Consider again the term in F

$$\begin{aligned} &-\sum_{\alpha,\beta} \Delta_\alpha (V^{-1})_{\alpha\beta} \Delta^\dagger_\beta \\ &= -\sum_\alpha |\Delta_\alpha|^2 (V^{-1})_{\alpha\beta} - 2\sum_{\alpha<\beta} |\Delta_\alpha||\Delta_\beta| (V^{-1})_{\alpha\beta} \cos(\theta_\alpha - \theta_\beta). \end{aligned} \tag{7.4.27}$$

In the second term, $\alpha \neq \beta$. If $(V^{-1})_{\alpha\beta} > 0$, then this term is minimized by $\theta_\alpha - \theta_\beta = 0$ ($\cos(\theta_\alpha - \theta_\beta) = 1$). If some $(V^{-1})_{\alpha\beta} < 0$, the phases $\{\theta_\alpha\}$ of the gaps may be frustrated. Some $\theta_\alpha - \theta_\beta$ would like to be 0, while others would like to be π. In general, for $N \geq 3$, these constraints are not compatible, and the system is forced to choose a compromise. A situation that could arise could be the following ($N = 3$)



Here, we may rotate the triad like a "rigid" body, this is a $U(1)$ symmetry. Swapping $\theta_2 \leftrightarrow \theta_3$; $\theta_1 \to \theta_1$ is like an "Ising"-transformation. In this case, the system may break a $U(1) \times Z_2$-symmetry in separate phase-transitions, leading to novel phase-transitions within the superconducting state.

7.5 Ginzburg-Landau theory of superconductors

We have seen how the appearance of $b^\dagger \neq 0$ leads to superconductivity, i.e. the expectation value of the creation operator of a Copper-pair obtains a nonzero value. Let us formulate this in real space and define a wave-function $\psi(\boldsymbol{r})$ for Cooper-pairs. This wave-function then describes a superconductor. It is a local field where $|\psi|^2$ describes the local density of Copper-pairs. We now set up an energy for the superconductor in terms of this field $\psi(\boldsymbol{r})$. Since this field has charge $e^*(e^* = 2e$, where $e =$ electron charge) this matter field ψ must be minimally coupled to a gauge-field $\boldsymbol{A}$ (where the magnetic field $B_\mu = \varepsilon_{\mu\nu\lambda}\partial_\nu A_\lambda$), and the magnetic field density is given by $B_\mu B_\mu = (\boldsymbol{\nabla}\times\boldsymbol{A})^2$.

$$\begin{aligned}\mathcal{H} &= \frac{\hbar^2}{2m}\left|\left(-i\boldsymbol{\nabla} - e^*\boldsymbol{A}\right)\psi\right|^2 + \alpha|\psi|^2 + \frac{u}{2}|\psi|^4 + \frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{A})^2 \\ \psi &= |\psi|\mathrm{e}^{i\theta}\end{aligned} \tag{7.5.1}$$

This is a phenomenological model of superconductivity written down long before the advent of the BCS-theory, and with very limited knowledge of what $\psi(\boldsymbol{r})$ actually represented! However, after the BCS-theory was formulated, L.P: Gorkov derived the GL-theory from the BCS-theory, and it became clear that

$$\Delta(\boldsymbol{r}) = \mathcal{F}^{-1}(\Delta_k) \iff \psi(\boldsymbol{r}). \tag{7.5.2}$$

$\langle\psi(\boldsymbol{r})\rangle$ then serves as an order-parameter of the superconductor.

- 1. term in equation $\mathcal{H}$: Kinetic enegy
- 2. term in equation $\mathcal{H}$: "Chemical potential"-term for Cooper-pairs
- 3. term in equation $\mathcal{H}$: Contact repulsion term between Cooper-pairs .
- 4. term in equation $\mathcal{H}$: Magnetic field energy.

Note that

$$\begin{aligned} \alpha =& \alpha(T) \\ =& \alpha_0(T - T_C^{MF}), \end{aligned} \tag{7.5.3}$$

where T_C^{MF} is a mean-field critical temperature of a superconductor. $T < T_C^{MF} \implies \alpha < 0$, and thus the "chemical potential"-term makes it energetically advantageous to allow non-zero Cooper-pair density $|\psi|^2$.

Landau theory: Ignore kinetic term

$$\mathcal{H}_L = \alpha|\psi|^2 + \frac{u}{2}|\psi|^4. \tag{7.5.4}$$

Determine $|\psi|$ by minimizing $\mathcal{H}$ with respect to $|\psi|$:

$$\frac{\mathrm{d}\mathcal{H}_L}{\mathrm{d}|\psi|} = 0 \tag{7.5.5}$$

$$\begin{aligned} \frac{\mathrm{d}\mathcal{H}_L}{\mathrm{d}|\psi|} =& 2\alpha|\psi| + 2u|\psi|^3 \\ =& |\psi|(2\alpha + 2u|\psi^2) \\ i)\ |\psi| =& 0 \\ ii)\ |\psi| =& \left(-\frac{\alpha}{u}\right)^{\frac{1}{2}} \end{aligned} \tag{7.5.6}$$

Knowing that $|\psi|$ is real and non-negative, it is clear that

- $\alpha > 0$: Only one real solution, $|\psi| = 0 \implies \mathcal{H}_L = 0$ (minimum)
- $\alpha < 0$: Two real solutions:
  - $|\psi| = 0 \implies \mathcal{H}_L = 0$
  - $|\psi| = \sqrt{\frac{|\alpha|}{u}} \implies \mathcal{H}_L = \alpha\frac{|\alpha|}{u} + \frac{u}{2}\frac{|\alpha|^2}{u^2}$
  - $\mathcal{H}_L^{Min} = -\frac{|\alpha|^2}{2u} < 0$

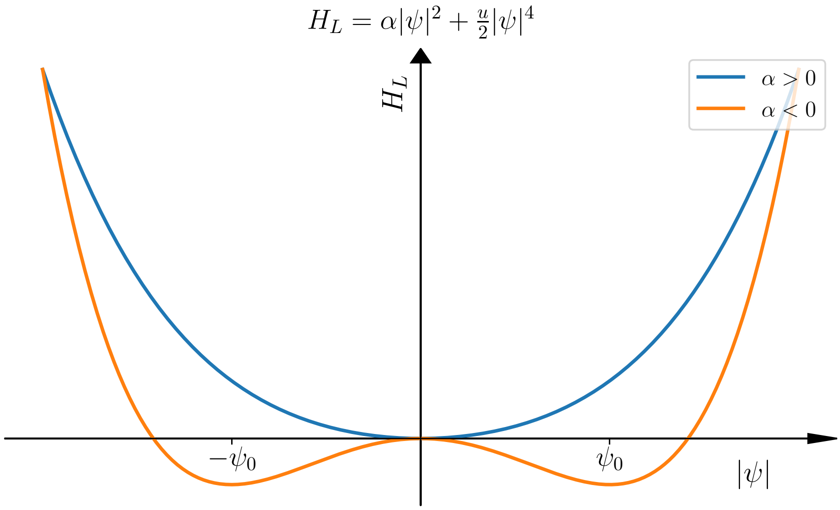


Figure 7.7: The Landau Hamiltonian, $\mathcal{H}_L$, as a function of $|\psi|$. Both signs of α are included, where $\alpha < 0$, results in a minima in $\mathcal{H}_L$ at a nonzero $|\psi|$, denoted ψ_0.

$|\psi| = \sqrt{\frac{|\alpha|}{u}}$ gives a lower energy than $|\psi| = 0$ so $|\psi| = \sqrt{\frac{|\alpha|}{u}}$ is the correct solution for $\alpha < 0$. $\mathcal{H}_L^{min} = -\frac{|\alpha|^2}{2u}$. $\mathcal{H}$ as a function of $|\psi|$ is plotted in the figure below.

For $\alpha < 0$, we define

$$\psi_0 = \sqrt{\frac{\alpha_0}{u}}(T_C^{MF} - T)^{\frac{1}{2}}. \tag{7.5.7}$$

Observe that the critical exponent $\beta = \frac{1}{2}$ and that ψ_0 is a real number for $\alpha < 0$, i.e. at $T < T_C^{MF}$.

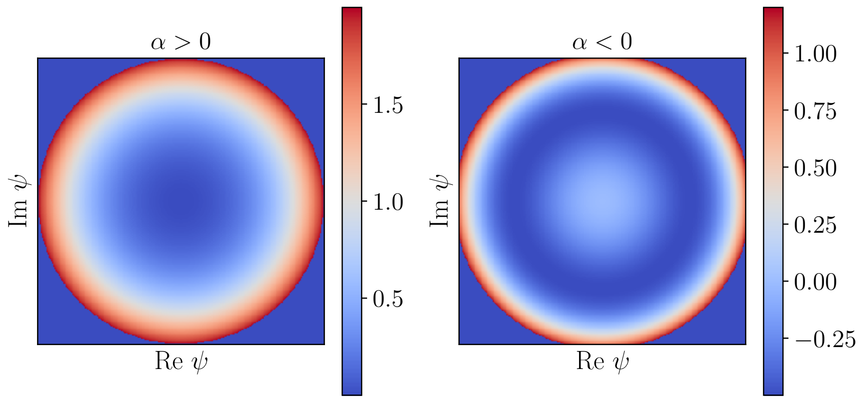


Figure 7.8: The Landau Hamiltonian, $\mathcal{H}_L$, as a function of the complex variable ψ. For $\alpha > 0$ it is a simple paraboloid, monototonically increasing as the modulus of ψ increases. However for $\alpha < 0$, there exists a nonzero value of $|\psi|$ that yields a minima for $\mathcal{H}_L$. It results in a Hamiltonian that bears a resemblence to a "Sombrero hat". Note that the minimum is only unique for the modulus, there is still a massively degenerate $\mathcal{H}_L$-minimum if the phase is included.

Even though $\mathcal{H}_L$ only depends on the modulus of ψ, ψ is still a complex number that can be written on the form $\psi = |\psi|\mathrm{e}^{i\theta}$. So we have the energy landscape in the complex ψ-space as illustrated in the figure above.

Note that from the "Sombrero-hat"-picture, fluctuations in θ cost no energy in Landau-theory. On the other hand we see that fluctuations in $|\psi|$ around ψ_0 do cost energy.

Phase-fluctuations are "massless". Amplitude-fluctuations are "massive".

Consider now also the kinetic energy and allow for phase-fluctuations and amplitude fluctuations. In other words, we allow

$$\begin{aligned} \psi =& (\psi_0 + \psi_1)\mathrm{e}^{i\theta} \\ \psi_0 =& \sqrt{\frac{|\alpha|}{u}}\ ;\ \psi_1 \text{ real.} \end{aligned} \tag{7.5.8}$$

Consider first the Landau terms

$$V(|\psi|) = \alpha|\psi|^2 + \frac{u}{2}|\psi|^4. \tag{7.5.9}$$

Expanding equation eq. (7.5.8) to second order in ψ_1 for $\alpha < 0$ yields

$$
\begin{aligned}
&V(|\psi|)\\
&\quad=\alpha(\psi_0^2+2\psi_0\psi_1+\psi_1^2)\\
&\quad+\frac{u}{2}(\psi_0^4\ 4\psi_0^3\psi_1+6\psi_0^2\psi_1^2+\mathcal{O}(\psi_1^3))\\
&\quad=\alpha_0\psi_0^2+\frac{u}{2}\psi_0^4+3u\psi_0^2\psi_1^2+\alpha\psi_1^2+\psi_1(2\alpha\psi_0+2u\psi_0^3), \text{last term}=0\\
&\quad=-\frac{\alpha^2}{2u}+\psi_1^2(\alpha-3\alpha)\\
&\quad=-\frac{\alpha^2}{2u}+2|\alpha|\psi_1^2\\
&\quad=\mathcal{H}_L^{min}+2\alpha\psi_1^2.
\end{aligned}
\tag{7.5.10}
$$

Consider next the kinetic energy term $\frac{\hbar^2}{2m}\left|\left(\frac{\boldsymbol{\nabla}}{i}-e^*\boldsymbol{A}\right)\psi\right|^2$

$$
\begin{aligned}
&\left(-i\boldsymbol{\nabla}-e^*\boldsymbol{A}\right)(\psi_0+\psi_1)\mathrm{e}^{i\theta}\\
=&-i\boldsymbol{\nabla}\psi_1\mathrm{e}^{i\theta}-e^*\boldsymbol{A}\psi_1\mathrm{e}^{i\theta}\\
+&(\boldsymbol{\nabla}\theta-e^*\boldsymbol{A})(\psi_0+\psi_1)\mathrm{e}^{i\theta}\\
\simeq&\left(-i\boldsymbol{\nabla}\psi_1+(\boldsymbol{\nabla}\theta-e^*\boldsymbol{A})\psi_0\right)\mathrm{e}^{i\theta}.
\end{aligned}
\tag{7.5.11}
$$

Here we have kept only terms that are linear in the fluctuations fields $\psi_1, \theta, \boldsymbol{A}$, since we will square the above expression to get the kinetic energy.

$$
\begin{aligned}
&\frac{\hbar^2}{2m}\left|\left(-i\boldsymbol{\nabla}-e^*\boldsymbol{A}\right)\psi\right|^2\\
=&\frac{\hbar^2}{2m}\left[(\boldsymbol{\nabla}\theta-e^*\boldsymbol{A})^2\psi_0^2+(\boldsymbol{\nabla}\psi_1)^2\right].\\
\mathcal{H}=&\mathcal{H}_L^{min}+\frac{\hbar^2\psi_0^2}{2m}(\boldsymbol{\nabla}\theta-e^*\boldsymbol{A})^2\\
+&\frac{\hbar^2}{2m}(\boldsymbol{\nabla}\psi_1)^2+2|\alpha|\psi_1^2++\frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{A})^2.
\end{aligned}
\tag{7.5.12}
$$

When $\alpha < 0$, we see that amplitude-fluctuations ψ_1 are always massive, even if we make $\boldsymbol{\nabla}\psi_1$ arbitrarily small. Fluctuations in the phase θ, on the other hand are massless, which means they are much easier to excite, and can be made to have arbitrarily low energy by making $\boldsymbol{\nabla}\theta$ arbitrarily small. The same is true for the $(\boldsymbol{\nabla}\times\boldsymbol{A})^2$-term. We therefore focus on the fluctuations in θ and $\boldsymbol{A}$, and discard the ψ_1-part. Also discarding $\mathcal{H}_L^{min}$ and introducing

$$
\rho_s \equiv \frac{\hbar^2\psi_0^2}{m},
\tag{7.5.13}
$$

we have

$$\mathcal{H} = \frac{\rho_s}{2}(\boldsymbol{\nabla}\theta - e^*\boldsymbol{A})^2 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A})^2. \tag{7.5.14}$$

This is the theory descrbing the relevant fluctuations around the Landau mean-field theory.

By introducing the current

$$\begin{aligned} \boldsymbol{j} =& -\frac{\partial \mathcal{H}}{\partial(e^*\boldsymbol{A})} \\ =& \rho_s(\boldsymbol{\nabla}\theta - e^*\boldsymbol{A}), \end{aligned} \tag{7.5.15}$$

we can describe the current in the superconducting state with phase-ordering as

$$\boldsymbol{j} = -e^*\rho_s\boldsymbol{A}. \tag{7.5.16}$$

Equation eq. (7.5.16) is exactly the consitutive relation for $\boldsymbol{j}$ that we used in combination with Maxwell's equations to give the Meissner-effect.

Note that the theory has a local $U(1)$ gauge-invariance, $e^*\boldsymbol{A'} = e^*\boldsymbol{A} - \boldsymbol{\nabla}\theta$. This transformation leaves $\mathcal{H}$ in equation eq. (7.5.14) invariant

$$\mathcal{H} = \frac{\rho_s}{2}{e^*}^2\boldsymbol{A'}^2 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A}')^2. \tag{7.5.17}$$

Note that it now appears that the gauge-field (photon) has acquired a mass

$$m_A^2 \equiv {e^*}^2\rho_s. \tag{7.5.18}$$

Also note that we <u>used</u> the $U(1)$ gauge-invariance to arrive at this conclusion. We thus have

$$\boxed{\rho_s \neq 0 \iff \psi_0 \neq 0 \iff \mathrm{Cooper-pairs.}}$$

ψ_0 plays the role of a Higgs-field, and the presence of a Higgs condensate (in this case, a superconductor) gives the photon a <u>mass m_A</u>. This leads to the Meissner-effect.

The Ginzburg-Landau theory for a superconductor is identical in form to the Higgs-sector of the Standard model.

> The Bogoliubov quasiparticles described by η_k and γ_k in the BCS-theory are fermionic analogs of the so-called Higgs-particle.

7.6 The interacting Bose gas

It is well known that an ideal (non-interacting) Bose gas can undergo a phase-transition into a condensed state where the ground state is macroscopically occupied. If the dimensionality of the system is $\underline{d}$, and the single-particle excitation energy is

$$\varepsilon_k = \alpha k^\nu, \tag{7.6.1}$$

then Bose-Einstein condensation (BEC) can take place if $d/\nu > 1$. Here, k is a wavenumber. If the total number of particles in the system is N, the number of particles in the condensate is N_0, and the number of excited states is $N_{>0}$, then

$$N = N_0 + N_{>0}, \tag{7.6.2}$$

or equivalently

$$\frac{N_0}{N} = 1 - \frac{N_{>0}}{N}. \tag{7.6.3}$$

The Hamiltonian of such a non-interacting system is

$$\mathcal{H} = \sum_k \varepsilon_k a_k^\dagger a_k, \tag{7.6.4}$$

where the $a^\dagger$'s create bosons with quantum number k, while the a's correspondingly destroy the same. We take ε_k to be minimum at $k = 0$ (e.g $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$, where m is the mass of the particles). The ground state energy is

$$E_0 = \varepsilon_0 \langle a_0^\dagger a_0 \rangle = \varepsilon_0 \langle \hat{N}_0 \rangle \tag{7.6.5}$$

$$\hat{N}_0 = a_0^\dagger a_0 \tag{7.6.6}$$

Eigenvalue of $\hat{N}_0$: $N_0 = \#$ particles in condensate

$$N_0 = \langle a_0^\dagger a_0 \rangle . \tag{7.6.7}$$

Now, we set $\langle a_0^\dagger \rangle = \langle a_0 \rangle = \sqrt{N_0}$ which expresses the fact that particles condense in the ground state.

$$\hat{N} = \hat{N}_0 + \sum_{k \neq 0} a_k^\dagger a_k \tag{7.6.8}$$

$$\begin{aligned} N &= N_0 + \sum_{k \neq 0} \langle a_k^\dagger a_k \rangle \\ &= N_0 + \sum_{k \neq 0} \frac{1}{e^{\beta \varepsilon_k} - 1} \end{aligned} \tag{7.6.9}$$

which is an equation for N_0 as a function of T. How does all of this change when interactions among bosons are introduced? We now write the Hamiltonian

$$\mathcal{H} = \sum_k \varepsilon_k a_k^\dagger a_k + \sum_{k_1,\ldots,k_4} U_{k_1,\ldots,k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta_{k_1+k_2,k_3+k_4}. \tag{7.6.10}$$

Let us consider weakly interacting Bose gases of alkali atoms $\mathrm{Li}, \mathrm{Na}, \mathrm{Rb}\ldots$. The interactions are typically van der Waals forces $V(r) \sim \frac{1}{r^6}$. We will model these interactions as contact interactions, i.e.

$$U_{k_1,\ldots,k_4} = \frac{U}{2V} = \text{constant}. \tag{7.6.11}$$

(i.e. $\mathcal{H}$ is the analog of a Bose-Hubbard model). $V =$ volume.

$$\mathcal{H} = \sum_k \varepsilon_k a_k^\dagger a_k + \frac{U}{2V} \sum_{k_1,\ldots,k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta_{k_1+k_2,k_3+k_4}. \tag{7.6.12}$$

We now consider a condensed state, where we specifically assume

$$N = N_0 + N_{>0} \tag{7.6.13}$$
$$N_0 \gg N_{>0} \tag{7.6.14}$$
$$N_0 \gg 1. \tag{7.6.15}$$

Thus (for later use), we have

$$N^2 = (N_0 + N_{>0})^2 \simeq N_0^2 + 2N_0 N_{>0}. \tag{7.6.16}$$

We now set $a_0 = \langle a_0 \rangle = \sqrt{N_0}$ etc, and expand $\mathcal{H}$ to quadratic order in a_k, with $k \neq 0$, neglecting cubic and quartic terms. Furthermore, we set $\varepsilon_0 = 0$.
<u>Kinetic term:</u>

$$\sum_k \varepsilon_k a_k^\dagger a_k = \sum_{k\neq 0} \varepsilon_k a_k^\dagger a_k. \tag{7.6.17}$$

<u>Interaction term:</u>

$$\begin{aligned} &\frac{U}{2V} \sum_{k_1,\ldots,k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta_{k_1+k_2,k_3+k_4} \\ &= \frac{U}{2V} N_0^2 + \text{terms where } \underline{\text{at least one}}\ k_i \neq 0. \end{aligned} \tag{7.6.18}$$

- Consider now first the case where one $k_i \neq 0$, i.e. three $k_i = 0$. We then see that $\delta_{k_1+k_2,k_3+k_4} = 0$. Thus, there are <u>no</u> terms <u>linear</u> in a_k or $a_k^\dagger$, with $k \neq 0$.

- Consider next the case where two k_i's $\neq 0$, i.e. two k_i's $= 0$. There are 6 possibilities: $\binom{4}{2} = 6$. We need to pick 2 k_i's out of the 4 k_1, k_2, k_3, k_4.

$$\begin{array}{lll}
(k_1, k_2) = 0, & (k_3, k_4) \neq 0 & \Longrightarrow a_{k_3} a_{-k_3} \\
(k_1, k_3) = 0, & (k_2, k_4) \neq 0 & \Longrightarrow a^\dagger_{k_2} a_{k_2} \\
(k_1, k_4) = 0, & (k_3, k_2) \neq 0 & \Longrightarrow a^\dagger_{k_2} a_{k_2} \\
(k_2, k_3) = 0, & (k_1, k_4) \neq 0 & \Longrightarrow a^\dagger_{k_1} a_{k_1} \\
(k_2, k_4) = 0, & (k_1, k_3) \neq 0 & \Longrightarrow a^\dagger_{k_1} a_{k_1} \\
(k_3, k_4) = 0, & (k_1, k_2) \neq 0 & \Longrightarrow a^\dagger_{k_1} a^\dagger_{-k_1}
\end{array}$$

To quadratic order in $a_k, a_k^\dagger$, the interaction term then becomes

$$\frac{U}{2V} N_0 4 \sum_{k\neq 0} a_k^\dagger a_k + \frac{U}{2V} N_0 \sum_{k \neq 0} \left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right). \tag{7.6.19}$$

Hence, we obtain for $\mathcal{H}(\varepsilon_0 = 0)$

$$\begin{aligned}
\mathcal{H} = & \frac{U}{2V} N_0^2 + \sum_{k\neq 0} \left(\varepsilon_k + \frac{2U}{V} \right) a_k^\dagger a_k \\
& + \frac{U}{2V} N_0 \sum_{k\neq 0} \left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right)
\end{aligned} \tag{7.6.20}$$

An important point to note now, is that at this stage, $\mathcal{H}$ is expressed in terms of $\hat{N}_0$, not $\hat{N}$. This is a bit inconvenient, since N_0 is an unknown quantity, while it is N that we prescribe, and which is therefore known. It therefore behooves us to re-express $\mathcal{H}$ in terms of N rather than N_0. We proceed as follows:

$$\begin{aligned}
\mathcal{H} = & \frac{U}{2V} N_0^2 + \frac{U}{2V} 2N_0 \sum_{k \neq 0} a_k^\dagger a_k \\
& + \sum_{k\neq 0} \left(\varepsilon_k + \frac{U}{V} N_0 \right) a_k^\dagger a_k \\
& + \frac{U}{2V} N_0 \sum_{k\neq 0} \left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right)
\end{aligned}$$

In the first line: (use eq. (7.6.16))

$$\frac{U}{2V} (N_0^2 + 2N_0 N_{>0}) \simeq \frac{U}{2V} N^2. \tag{7.6.21}$$

In all other terms, we replace N_0 with N, to the approximation we are computing:

$$\begin{aligned} N_0 N_{>0} &= (N - N_{>0}) N_{>0} \\ &= N N_{>0} - N_{>0}^2 \\ &\simeq N N_{>0}. \end{aligned} \tag{7.6.22}$$

Furthermore, using $\varepsilon_k = \varepsilon_{-k}$, we symmetrize the term

$$\sum_{k \neq 0} \left(\varepsilon_k + \frac{U}{V} N \right) a_k^\dagger a_k = \frac{1}{2} \sum_{k \neq 0} \left(\varepsilon_k + \frac{U}{V} N \right) \left(a_k^\dagger a_k + a_{-k}^\dagger a_{-k} \right) \tag{7.6.23}$$

Finally, we therefore have the following form for the Hamiltonian

$$\begin{aligned} \mathcal{H} = \frac{U}{2V} N^2 &+ \frac{1}{2} \sum_{k \neq 0} \left(\varepsilon_k + \frac{U}{V} N \right) \left(a_k^\dagger a_k + a_{-k}^\dagger a_{-k} \right) \\ &+ \frac{U}{2V} N \sum_{k \neq 0} \left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right) \end{aligned} \tag{7.6.24}$$

We will now diagonalize this Hamiltonian proceeding more or less along the same lines as we did for the antiferromagnet, or the anisotropic ferromagnet. We introduce new boson operators as follows

$$\begin{aligned} a_k &= u_k A_k - v_k A_{-k}^\dagger \\ a_k^\dagger &= u_k A_k^\dagger - v_k A_{-k} \end{aligned} \tag{7.6.25}$$

$$\mathcal{H} = \frac{U}{2V} N^2 + \frac{1}{2} \sum_{k \neq 0} \varepsilon_1 \left(a_k^\dagger a_k + a_{-k}^\dagger a_{-k} \right) + \frac{1}{2} \sum_{k \neq 0} \varepsilon_2 \left((a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right) \tag{7.6.26}$$

$$\left. \begin{aligned} \varepsilon_1 &\equiv \varepsilon_k + U n \\ \varepsilon_2 &\equiv U n \end{aligned} \right\} n = \frac{N}{V} \tag{7.6.27}$$

Note the constant shift of the energy ε_k, which is a mean-field way of accounting for interactions in the problem. Consider the k-dependent terms k by k:

$$\begin{aligned} a_k^\dagger a_k &= \left(u_k A_k^\dagger - v_k A_{-k} \right) \left(u_k A_k - v_k A_{-k}^\dagger \right) \\ &= u_k^2 A_k^\dagger A_k + v_k^2 A_{-k} A_{-k}^\dagger \\ &- v_k u_k \left(A_k A_{-k} + A_k^\dagger A_{-k}^\dagger \right) \end{aligned} \tag{7.6.28}$$

Thus, we have

$$
\begin{aligned}
a_k^\dagger a_k + a_{-k}^\dagger a_{-k} = u_k^2 &\left(A_k^\dagger A_k + A_{-k}^\dagger A_{-k}\right) \\
&+ v_k^2 \left(A_{-k} A_{-k}^\dagger + A_k A_k^\dagger\right) \\
&- 2 v_k u_k \left(A_k^\dagger A_{-k}^\dagger + A_k A_{-k}\right).
\end{aligned}
\tag{7.6.29}
$$

$$
\begin{aligned}
a_k^\dagger a_{-k}^\dagger &= \left(u_k A_k^\dagger - v_k A_{-k}\right)\left(u_k A_{-k} - v_k A_k^\dagger\right) \\
&= u_k^2 A_k^\dagger A_{-k}^\dagger + v_k^2 A_k A_{-k} \\
&- v_k u_k \left(A_k^\dagger A_k + A_{-k} A_{-k}^\dagger\right)
\end{aligned}
\tag{7.6.30}
$$

$$
\begin{aligned}
a_k a_{-k} = v_k^2 A_{-k}^\dagger A_k^\dagger + u_k^2 A_{-k} A_k \\
- v_k u_k \left(A_k^\dagger A_k + A_{-k} A_{-k}^\dagger\right)
\end{aligned}
\tag{7.6.31}
$$

$$
\begin{aligned}
a_k^\dagger a_{-k}^\dagger + a_k a_{-k} = u_k^2 &\left(A_k^\dagger A_{-k}^\dagger + A_{-k} A_k\right) \\
&+ v_k^2 \left(A_k A_{-k} + A_{-k}^\dagger A_k^\dagger\right) \\
&- 2 u_k v_k \left(A_k^\dagger A_k + A_{-k} A_{-k}^\dagger\right).
\end{aligned}
\tag{7.6.32}
$$

Insert all of these terms into eq. (7.6.26)

$$
\begin{aligned}
&\varepsilon_1 \left(a_k^\dagger a_k + a_{-k}^\dagger a_{-k}\right) + \varepsilon_2 \left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k}\right) \\
&= \varepsilon_1 \Big[u_k^2 \left(A_k^\dagger A_k + A_{-k}^\dagger A_{-k}\right) + v_k^2 \left(A_{-k}^\dagger A_{-k} + A_k^\dagger A_k\right) + 2 v_k^2 \\
&\quad -2 v_k u_k \left(A_k^\dagger A_{-k}^\dagger + A_k A_{-k}\right)\Big] \\
&\quad + \varepsilon_2 \Big[u_k^2 \left(A_k^\dagger A_{-k}^\dagger + A_{-k} A_k\right) + v_k^2 \left(A_k A_{-k} + A_{-k}^\dagger A_k^\dagger\right) \\
&\quad\quad -2 u_k v_k \left(A_k^\dagger A_k + A_{-k}^\dagger A_{-k}\right) - 2 u_k v_k\Big]
\end{aligned}
\tag{7.6.33}
$$

From this, we now identify the coefficients of the normal and anomalous terms involving A-operators, as follows

$$
\begin{aligned}
A_k^\dagger A_k :&\quad \varepsilon_1 (u_k^2 + v_k^2) - 2 \varepsilon_2 u_k v_k \\
A_{-k}^\dagger A_{-k} :&\quad \varepsilon_1 (u_k^2 + v_k^2) - 2 \varepsilon_2 u_k v_k \\
A_k^\dagger A_{-k}^\dagger :&\quad \varepsilon_2 (u_k^2 + v_k^2) - 2 \varepsilon_1 u_k v_k \\
A_k A_{-k} :&\quad \varepsilon_2 (u_k^2 + v_k^2) - 2 \varepsilon_1 u_k v_k
\end{aligned}
\tag{7.6.34}
$$

There will be constant A-independent terms appearing when commuting $A_k A_k^\dagger = 1 + A_k^\dagger A_k$, and these will contribute to the ground state energy:

$$-2\varepsilon_2 u_k v_k + 2v_k^2 \varepsilon_1 \tag{7.6.35}$$

We now parametrize, as in the case of antorferromagnets of isotrpoic ferromagnets, the coherence factors u_k and v_k in terms of hyperbolic squeezing factors

$$\begin{aligned} u_k^2 - v_k^2 = 1 \rightarrow &\begin{cases} u_k = \cosh(\theta) \\ v_k = \sinh(\theta) \end{cases} \\ u_k^2 + v_k^2 &= \cosh(2\theta) \\ 2u_k v_k &= \sinh(2\theta) \end{aligned}$$

We now adjust the squeezing-parameter θ such that all anomalous terms $A_k A_{-k}^\dagger$ and $A_k A_{-k}$ vanish.

$$\begin{aligned} \varepsilon_2(u_k^2 + v_k^2) &= \varepsilon_1 u_k v_k \\ u_k^2 &= \frac{1}{2}\left(1 + \frac{\varepsilon_1}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}}\right) \\ v_k^2 &= \frac{1}{2}\left(-1 + \frac{\varepsilon_1}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}}\right) \\ 4u_k^2 v_k^2 &= \frac{\varepsilon_2^2}{\varepsilon_1^2 - \varepsilon_2^2} \\ 2u_k v_k &= \frac{\varepsilon_2}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}} \\ u_k^2 + v_k^2 &= \frac{\varepsilon_1}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}}. \end{aligned}$$

The coefficients of $A_k^\dagger A_k$ and $A_{-k}^\dagger A_{-k}$ are then found to be

$$\frac{1}{2}\left[\varepsilon_1(u_k^2 + v_k^2) - \varepsilon_2 2u_k v_k\right] = \frac{1}{2}\left(\frac{\varepsilon_1^2 - \varepsilon_2^2}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}}\right) = \frac{1}{2}\sqrt{\varepsilon_1^2 - \varepsilon_2^2}. \tag{7.6.36}$$

Thus,

$$\begin{aligned} \mathcal{H} = &\frac{U}{2V}N^2 + \frac{1}{2}\sum_{k\neq 0}\left(2v_k^2\varepsilon_1 - 2\varepsilon_2 u_k v_k\right) \\ &+ \frac{1}{2}\sum_{k\neq 0} E_k\left(A_k^\dagger A_k + A_{-k}^\dagger A_{-k}\right) \end{aligned} \tag{7.6.37}$$

with

$$\begin{aligned} E_k &= \sqrt{\varepsilon_1^2 - \varepsilon_2^2} = \sqrt{(\varepsilon_k + nU)^2 - (nU)^2} \\ &= [\varepsilon_k(\varepsilon_k + 2nU)]^{\frac{1}{2}} \end{aligned} \tag{7.6.38}$$

Note the delicate cancellation of the $(nU)^2$-terms.

When $U = 0$, $E_k = \varepsilon_k$. When $U \neq 0$, the spectrum changes drastically as $k \to 0$. While $\varepsilon_k \sim k^2$,

$$E_k = \left(\frac{\hbar^2}{2m} 2Un\right)^{\frac{1}{2}} k \equiv \hbar c k; \qquad k \to 0,\, U \neq 0. \tag{7.6.39}$$

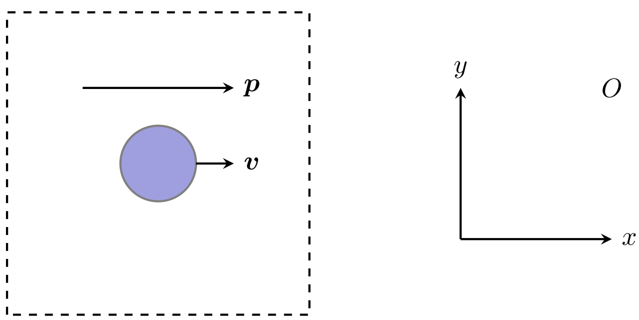
$$c = \left(\frac{Un}{m}\right)^{\frac{1}{2}} \tag{7.6.40}$$

may be interpreted as the velocity of a density-wave. Later, we shall see that c corresponds to the maximum velocity associated with superfluid flow in the condensate. This is called the critical superfluid velocity, which is seen to vanish when $U \to 0$. Thus, an ideal Bose-Einstein condensate is not a superfluid. Superfluidity and the presence of colective excitations require interactions to be present in the problem.

7.6.1 Landau criterion for superfluidity

Subsection or section?

Let us consider a fluid in motion with total momentum $\boldsymbol{p}$ with respect to some fixed reference frame. Imagine that we insert a small object and drag it through the fluid with some velocity $\boldsymbol{v}$ with respect to the same fixed frame.



Energy of fluid in frame O:

$$E = \frac{p^2}{2M}, \tag{7.6.41}$$

where $M = Nn$, N is the number of particles in fluid element we consider. The same energy in the fram of the moving object is

$$\begin{aligned} E(\boldsymbol{v}) &= \frac{1}{2M}\left(\boldsymbol{p} - M\boldsymbol{v}\right)^2 . \\ &= E - \boldsymbol{p}\cdot\boldsymbol{v} + \frac{1}{2}Mv^2 \end{aligned} \tag{7.6.42}$$

The ground state energy of the fluid in frame O:

$$E_0 = 0. \tag{7.6.43}$$

The ground state energy of the fluid in the frame of the moving object

$$E_{\mathrm{GS}}(\boldsymbol{v}) = E_0 + \frac{1}{2}Mv^2. \tag{7.6.44}$$

Imagine now that out of the ground state, we create a single excitation of momentum $\boldsymbol{p}$, with energy $\underline{\varepsilon_p}$. In frame O:

$$E_{\mathrm{ex}} = E_0 + \varepsilon_p. \tag{7.6.45}$$

But that means that in the frame moving with the obstacle, we have

$$E_{\mathrm{ex}}(\boldsymbol{v}) = E_0 + \varepsilon_p - \boldsymbol{p}\cdot\boldsymbol{v} + \frac{1}{2}Mv^2 \tag{7.6.46}$$

$$\Delta E = E_{\mathrm{ex}}(\boldsymbol{v}) - E_{\mathrm{GS}}(\boldsymbol{v}) = \varepsilon_p - \boldsymbol{p}\cdot\boldsymbol{v}. \tag{7.6.47}$$

In other words, dragging an object through the fluid changes the energy required to make an excitation. If $\varepsilon_p - \boldsymbol{v}\cdot\boldsymbol{p} < 0$, the the system gains energy by creating excitations, i.e. energy is lowered byu this. This happens at a velocity

$$v = \frac{\varepsilon_p}{p}. \tag{7.6.48}$$

The minimum velocity required, is called the critical velocity, and is given by

$$v_C = \min \frac{\varepsilon_p}{p}. \tag{7.6.49}$$

This is the lowest velocity one can drag an obstacle thourgh the fluid and create single-particle excitations, i.e. scattering. Below this velocity, no scattering takes place and the fluid is superfluid. For the non-interacting Bose-gas, we have $\varepsilon = \frac{p^2}{2m}$, for which

$$v_C = \min \frac{p}{2m} = 0. \tag{7.6.50}$$

An ideal Bose gas is not a superfluid. With interactions, we found

$$E_p = \sqrt{\varepsilon_p(\varepsilon_p + Un)} = \sqrt{\frac{Un}{m}}p + \cdots \tag{7.6.51}$$

$$v_C = \min \sqrt{\frac{Un}{m}} = \sqrt{\frac{Un}{m}}. \tag{7.6.52}$$

The interacting Bose gas can flow with a velocity up to $v_C = \sqrt{\frac{Un}{m}}$ without scattering and therefore exhibits superfluidity. Repulsive interactions are required to stabilize superfluidity.

7.6.2 Condensate fraction

We have the following relation between the total # particles in the system, N, and the number of particles in the condensate, N_0:

$$N = N_0 + \sum_{k\neq 0} \langle a_k^\dagger a_k \rangle \tag{7.6.53}$$

Introducing the Bogoliubov operators, we then have

$$\begin{aligned} N &= N_0 + \sum_{k\neq 0} \left[u_k^2 \langle A_k^\dagger A_k \rangle + v_k^2 \langle A_{-k} A_{-k}^\dagger \rangle \right] \\ &= N_0 + \sum_{k\neq 0} v_k^2 + \sum_{k\neq 0} (u_k^2 + v_k^2) \langle A_k^\dagger A_k \rangle \\ &= N_0 + \sum_{k\neq 0} v_k^2 + \sum_{k\neq 0} \frac{u_k^2 + v_k^2}{\mathrm{e}^{\beta E_k} - 1}. \end{aligned} \tag{7.6.54}$$

At $T = 0$, the last term gives no contribution, such that we have

$$N = N_0 + \sum_{k\neq 0} v_k^2. \tag{7.6.55}$$

The condensate fraction may then be expressed as

$\frac{N_0}{N} = 1 - \frac{1}{N}\sum_k v_k^2$?

$$\frac{N_0}{N} = 1 - \sum_{k \neq 0} v_k^2 \tag{7.6.56}$$

$$v_k^2 = \frac{1}{2}\left(-1 + \frac{\varepsilon_1}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}}\right) \tag{7.6.57}$$

$$\varepsilon_1 = \varepsilon_k + Un; \quad \varepsilon_2 = Un$$

$$U \to 0 \implies v_k^2 = 0 \implies$$

$$\frac{N_0}{N} = 1. \tag{7.6.58}$$

With finite interactions, we get a depletion of the condensate fraction even at $T = 0$. Consider now the case $d = 3$.

$$D(\varepsilon) = K\sqrt{\varepsilon} \tag{7.6.59}$$

$$\frac{N_0}{N} = 1 - \frac{K}{2}\int_0^\infty \mathrm{d}\varepsilon \sqrt{\varepsilon}\left(-1 + \frac{\varepsilon_1}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}}\right) \tag{7.6.60}$$

$$\varepsilon = \varepsilon_1 - Un$$

$$\varepsilon_1^2 - \varepsilon_2^2 = (\varepsilon_1 - \varepsilon_2)(\varepsilon_1 + \varepsilon_2) \tag{7.6.61}$$

$$\frac{N_0}{N} = 1 - \frac{K}{2}\int_{Un}^\infty \mathrm{d}x \sqrt{x - Un}\left(-1 + \frac{x}{\sqrt{x^2 - (Un)^2}}\right) \tag{7.6.62}$$

$$= 1 - \frac{K}{2}(I_1 - I_2) \tag{7.6.63}$$

$$I_1 = \int_{Un}^\infty \mathrm{d}x \frac{x}{\sqrt{x + Un}} \tag{7.6.64}$$

$$I_2 = \int_{Un}^\infty \mathrm{d}x \sqrt{x - Un}. \tag{7.6.65}$$

These integrals will be performed with upper limit A, and then let $A \to \infty$.

$$I_2 = \frac{2}{3}(A - Un)^{\frac{2}{3}}, \tag{7.6.66}$$

$$\begin{aligned} I_1 &= \left[\left(\frac{1}{3}(x + Un) - Un\right) 2\sqrt{x + Un}\right]_{Un}^{A} \\ &= \left(\frac{2}{3}(A + Un) - 2Un\right)\sqrt{A + Un} - \frac{2}{3}Un \cdot 2\sqrt{2Un}, \end{aligned} \tag{7.6.67}$$

$$\lim_{A\to\infty}(I_1 - I_2) = \frac{4}{3}Un\sqrt{2Un} = \frac{2}{3}(2Un)^{\frac{2}{3}}\,. \tag{7.6.68}$$

The filling fraction is

$$\boxed{\frac{N_0}{N} = 1 - \frac{K}{3}(2Un)^{\frac{3}{2}}\,.} \tag{7.6.69}$$

Problems

Problem 7.1. The creation and destruction operator of a Cooper-pair is given by

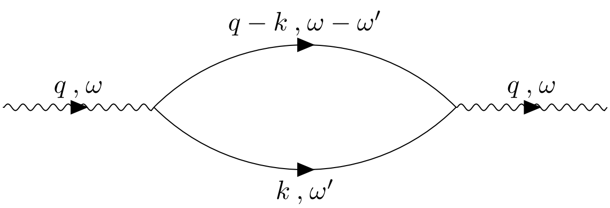
$$
\begin{aligned}
b_{\mathbf{k}} &= c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \\
b_{\mathbf{k}}^{\dagger} &= c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k},\downarrow}^{\dagger}
\end{aligned}
$$

a) Compute the commutators $\left[b_{\mathbf{k}}, b_{\mathbf{k}'}^{\dagger}\right]$ and $[b_{\mathbf{k}}, b_{\mathbf{k}'}]$, and the anti-commutator $\{b_{\mathbf{k}}, b_{\mathbf{k}'}\}$. Compare your results with what you find if the operators had been boson-operators.

b) Imagine that you had two different condensed matter systems, one with a relatively strong attraction between electrons, and one with a relatively weak attraction between electrons. Which one of these two system would you think a description of Cooper-pairs as bosons would be the best approximation?

Problem 7.2. In Problem 1 we considered creation an destruction operators for a Cooper-pair. Consider now a bosonic *pair-fluctuation field* $\varphi(\mathbf{q}, \omega)$ which can split into two electrons, and two electrons can recombine into the field $\varphi(\mathbf{q}, \omega)$.

A Feynman-diagram for such a process is given in the Figure below.



$$= \chi_0(\mathbf{q}, \omega)\ K(\mathbf{q}, \omega)\ \chi_0(\mathbf{q}, \omega)$$

The wavy line is the Green's function for the free field $\varphi(\mathbf{q}, \omega)$, denoted $\chi_0(\mathbf{q}, \omega)$. Denote the bubble-diagram by $K(\mathbf{q}, \omega)$. Consider now a Dyson-equation for the Green's function $\chi(\mathbf{q}, \omega)$ for the pairing field

$$\chi(\mathbf{q},\omega)^{-1} = \chi_0(\mathbf{q},\omega)^{-1} - K(\mathbf{q},\omega)$$
$$\chi_0(\mathbf{q},\omega)^{-1} = V$$

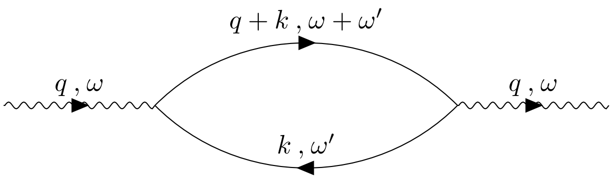
Here, $V =$ is a constant attractive interaction that works in a thin shell around the Fermi-surface.

a) Use the Feynman-rules to compute the integral over ω' in the bubble-diagram, taking care to express your answer in terms of $T = 0$ Fermi-distribution $\theta(\varepsilon_F - \varepsilon_{\mathbf{k}})$ and its complementary distribution $\theta(\varepsilon_{\mathbf{k}} - \varepsilon_F)$, and corresponding quantities with $\mathbf{k} \to \mathbf{k} + \mathbf{q}$.

b) Generalize this to finite temperatures $T > 0$ by replacing the θ-functions by finite-temperature Fermi-distributions and simplify the expression by letting $\mathbf{q} \to 0$.

c)$\chi(\mathbf{q},\omega)$ may be given a physical interpretation as a *pair-susceptibility*, i.e. the ability an electron system has to form pairs of electrons, Cooper-pairs. The divergence of this susceptibility indicates an instability of the Fermi-sea of electrons. Find the temperature at which this instability takes place by explicitly computing the remaining $\mathbf{k}$-sum. (Hint: Consider the case $\mathbf{q} = 0$ and convert the sum over $\mathbf{k}$ to an energy integral and approximate the single-particle density of states by its value on the Fermi-surface.)

Note how very differently the particle-particle bubble $K(\mathbf{q},\omega)$ behaves from the particle-hole bubble $\Pi(\mathbf{q},\omega)$ we considered in class.



$= D_0(\mathbf{q},\omega)\ \Pi(\mathbf{q},\omega)\ D_0(\mathbf{q},\omega)$

There, we found that $\lim_{\mathbf{q}\to 0} \Pi(\mathbf{q},\omega = 0) = -2N(\varepsilon_F)$. This is essentially T-independent.

Problem 7.3. In class, we have introduced new operators $\eta_{\mathbf{k}}, \gamma_{\mathbf{k}}$ to diagonalize the mean-field BCS-Hamiltonian using transformation coefficients $(u_{\mathbf{k}}, v_{\mathbf{k}})$ that are real. Let us generalize this to the case where $(u_{\mathbf{k}}, v_{\mathbf{k}})$ can be complex. As in class, we choose $V_{\mathbf{k},\mathbf{k}'}$ to be a constant within a thin shell around the Fermi surface. We will use the following transformation

$$\begin{pmatrix} \eta_{\mathbf{k}} \\ \gamma_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ -v^*_{\mathbf{k}} & u^*_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^\dagger_{-\mathbf{k},\downarrow} \end{pmatrix}$$

a) Show that preservation of anti-commutation relations gives the constraint

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$$

b) We next want to diagonalize the problem such that only terms of the form $\gamma^\dagger_{\mathbf{k}}\gamma_{\mathbf{k}}$ and $\eta^\dagger_{\mathbf{k}}\eta_{\mathbf{k}}$ appear in the Hamiltonian. Show that the condition for this is given by

$$\begin{aligned} -2(\varepsilon_{\mathbf{k}} - \mu)u_{\mathbf{k}}v_{\mathbf{k}} &= u^2_{\mathbf{k}}\Delta - v^2_{\mathbf{k}}\Delta^* \\ -2(\varepsilon_{\mathbf{k}} - \mu)u^*_{\mathbf{k}}v^*_{\mathbf{k}} &= (u^*_{\mathbf{k}})^2\Delta^* - (v^*_{\mathbf{k}})^2\Delta \end{aligned}$$

c) Show that the coefficient of $\gamma^\dagger_{\mathbf{k}}\gamma_{\mathbf{k}}$ is given by

$$E_{\mathbf{k}} = (\varepsilon_{\mathbf{k}} - \mu)\left(|v_{\mathbf{k}}|^2 - |u_{\mathbf{k}}|^2\right) + \Delta v^*_{\mathbf{k}}u_{\mathbf{k}} + \Delta^* v_{\mathbf{k}}u^*_{\mathbf{k}}$$

and that the corresponding coefficient of $\eta^\dagger_{\mathbf{k}}\gamma_{\mathbf{k}}$ is given by $-E_{\mathbf{k}}$.

d) We next parametrize $u = \cos\chi\ e^{i\varphi_u}$, $v = \sin\chi\ e^{i\varphi_v}$, $\Delta = |\Delta|e^{i\varphi}$. Use the constraint in **b** to find constraints on the phases $\varphi_u, \varphi_v, \varphi$. Conclude from this that $E_{\mathbf{k}}$ is real.

e) Use the definition of Δ as given in class to show that in this case, the phase of the gap may be cancelled out of the self-consistent equation for Δ. Hence, in this case, we can consider Δ to be real and positive without loss of generality.

Problem 7.4. In this problem, we will consider a generalization of the BCS-theory to a situation where electrons originating with two energy-bands can participate in superconductivity. Such a situation arises in transition metal elements, where scattering of electrons in s- and d-orbitals constributes to the resistivity in the normal state. The generalization of the BCS-reduced Hamiltonian to this case is straightforward. We denote the single-particle excitation energies of the electrons on the s- and d-bands as $\varepsilon_{\mathbf{k}s}$ and $\varepsilon_{\mathbf{k}d}$, respectively.

The BCS-reduced Hamiltonian for this case is given by

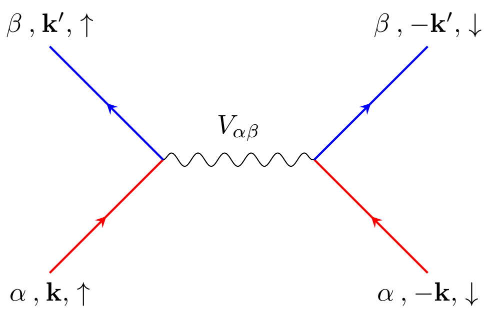
$$\begin{aligned}\mathcal{H} &= \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}s} - \mu)\ c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}d} - \mu)\ d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \\ &- V_{ss} \sum_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}',\uparrow} c^\dagger_{-\mathbf{k}',\downarrow} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} - V_{dd} \sum_{\mathbf{k},\mathbf{k}'} d^\dagger_{\mathbf{k}',\uparrow} d^\dagger_{-\mathbf{k}',\downarrow} d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} \\ &- V_{sd} \sum_{\mathbf{k},\mathbf{k}'} \left[d^\dagger_{\mathbf{k}',\uparrow} d^\dagger_{-\mathbf{k}',\downarrow} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} + c^\dagger_{\mathbf{k}',\uparrow} c^\dagger_{-\mathbf{k}',\downarrow} d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} \right]\end{aligned}$$

Here, $(V_{ss}, V_{dd}, V_{sd}) > 0$ are attractive interactions operative provided both $\mathbf{k}, \mathbf{k}'$ both are located within a thin shell around the Fermi-surface of the s- and d-bands. The c- and d-operators are fermionic creation- and destruction operators of the s and d-bands, respectively. Note that the Hamiltonian decouples into two independent single-band problems if $V_{sd} = 0$.

The V_{ss}- and V_{dd}-terms are intra-band scattering processes on the s- and d-bands, respectively. The V_{sd}-term is an inter-band scattering between the s- and the d-band.

The summations of $\mathbf{k}, \mathbf{k}'$ are close to the Fermi-surface both for the s- and the d-band, so the regions in $\mathbf{k}$-space will be quite different in the two cases. Furthermore, we will denote the single-particle densities of states on the Fermi-surface in the s- and d-bands as N_s and N_d, respectively.

The Feynman-diagram illustrating the various scattering processes is given below.



a) We next perform a mean-field approximation along the same lines that we did in class for the single-band case. Introduce mean-field expectation values

$$
\begin{aligned}
b_{\mathbf{k},s} &= \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle \\
b_{\mathbf{k},d} &= \langle d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} \rangle
\end{aligned}
$$

and write

$$
\begin{aligned}
c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} &= b_{\mathbf{k},s} + \delta b_{\mathbf{k},s} \\
d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} &= b_{\mathbf{k},d} + \delta b_{\mathbf{k},d}
\end{aligned}
$$

and discard terms $\mathcal{O}(\delta b_{\mathbf{k},s})^2$ and $\mathcal{O}(\delta b_{\mathbf{k},s})^2$. Show that the mean-field Hamiltonian may be written on form

$$
\begin{aligned}
\mathcal{H} = & \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}s} - \mu) \; c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}d} - \mu) \; d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \\
& - V_{ss} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',s} \; c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} + h.c. \right] - V_{dd} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',d} \; d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} + h.c. \right] \\
& - V_{sd} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',d} \; c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} + h.c. + b^\dagger_{\mathbf{k}',s} \; d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} + h.c. \right] \\
& + V_{ss} \sum_{\mathbf{k},\mathbf{k}'} b^\dagger_{\mathbf{k}',s} \; b_{\mathbf{k},s} + V_{dd} \sum_{\mathbf{k},\mathbf{k}'} b^\dagger_{\mathbf{k}',d} \; b_{\mathbf{k},d} + V_{sd} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',d} \; b_{\mathbf{k},s} + b^\dagger_{\mathbf{k}',s} \; b_{\mathbf{k},d} \right]
\end{aligned}
$$

b) Introduce the two quantities Δ_1 and Δ_2 (to be dermined selfconsistently)

$$
\begin{aligned}
\Delta_1 &\equiv V_{ss} \sum_{\mathbf{k}} b_{\mathbf{k},s} + V_{sd} \sum_{\mathbf{k}} b_{\mathbf{k},d} \\
\Delta_2 &\equiv V_{sd} \sum_{\mathbf{k}} b_{\mathbf{k},s} + V_{dd} \sum_{\mathbf{k}} b_{\mathbf{k},d}
\end{aligned}
$$

Express the mean-field Hamiltonian in terms of Δ_1 and Δ_2 instead of $b_{\mathbf{k},s}$ and $b_{\mathbf{k},d}$. Try to give a physical interpretation of Δ_1 and Δ_2. (Hint: Try to infer what Δ_1 and Δ_2 mean based on how they appear in the Hamiltonian).

c) To diagonalize the mean-field problem, we will introduce new fermionic operators $e_{\mathbf{k},\sigma}$ and $f_{\mathbf{k},\sigma}$ as follows

$$
\begin{aligned}
c_{\mathbf{k},\uparrow} &= \cos(\theta_{\mathbf{k}})e_{\mathbf{k},\uparrow} + \sin(\theta_{\mathbf{k}})e^{\dagger}_{-\mathbf{k},\downarrow} \\
c_{\mathbf{k},\downarrow} &= \cos(\theta_{\mathbf{k}})e_{\mathbf{k},\downarrow} - \sin(\theta_{\mathbf{k}})e^{\dagger}_{-\mathbf{k},\uparrow} \\
d_{\mathbf{k},\uparrow} &= \cos(\varphi_{\mathbf{k}})f_{\mathbf{k},\uparrow} + \sin(\varphi_{\mathbf{k}})f^{\dagger}_{-\mathbf{k},\downarrow} \\
d_{\mathbf{k},\downarrow} &= \cos(\varphi_{\mathbf{k}})f_{\mathbf{k},\downarrow} - \sin(\varphi_{\mathbf{k}})f^{\dagger}_{-\mathbf{k},\uparrow}
\end{aligned}
$$

The parameters $\theta_{\mathbf{k}}$ and $\varphi_{\mathbf{k}}$ are determined by substituting these expressions into $\mathcal{H}$ and equating the coefficients of terms $e^{\dagger}e^{\dagger}$ and ee to zero, and likewise for the f-operators. Show that this procedure yields the following equations determining $\theta_{\mathbf{k}}$ and $\varphi_{\mathbf{k}}$

$$
\begin{aligned}
\varepsilon_{\mathbf{k}s}\sin(2\theta_{\mathbf{k}}) + D_s\cos(2\theta_{\mathbf{k}}) &= 0 \\
\varepsilon_{\mathbf{k}d}\sin(2\varphi_{\mathbf{k}}) + D_d\cos(2\varphi_{\mathbf{k}}) &= 0
\end{aligned}
$$

and give expressions for D_s and D_d.
Find the excitation energies of the Bogoliubov quasiparticles (e, f) defined above.

d) Find an expression for the free energy of the system.

e) Minimize the free energy w.r.t the quantities Δ_1 and Δ_2 and show that the coupled equations for these two quantities may be written

$$
\begin{aligned}
\Delta_\alpha &= \sum_{\beta=1}^{2} V_{\alpha\beta}\Delta_\beta\ \chi_\beta; \alpha = (1,2) \\
\chi_\beta &\equiv \sum_{\mathbf{k}} \frac{1}{2E_{\beta\mathbf{k}}}\tanh\left(\frac{\beta E_{\beta\mathbf{k}}}{2}\right)
\end{aligned}
$$

f) With the real transformation coefficients we have used so far, Δ_α will be real. Imagine that we had used complex transformation coefficients instead, like in Problem 1. We would then get the same equations for Δ_α as above, but with the possibility of complex gaps, $\Delta_\alpha = |\Delta_\alpha|e^{i\varphi_\alpha}$. We may thus cancel out an overall phase from the gap-equations, and be left with *one and only one* relative phase $\varphi_{12} = \varphi_1 - \varphi_2$. Show, using the gap-equations, that $\varphi_{12} = (0, \pi)$ mod (2π). Therefore, the gaps again may both be taken to be real, but they may have opposite signs. What is the criterion for Δ_1 and Δ_2 having equal or opposite signs?

Note: This sort of simplification in general is not possible when one has more than two bands involved in the superconductivity. This leads to qualitatively new effects. Important examples of N-band superconductors with $N \geq 3$ are the iron-pnictide high-T_c superconductors currently of considerable interest.

g) Find an expression for the critical temperature of the system using the same technique that we used in class for the single-band case.