Contents

1 Introduction

The types of systems we will look at are mainly defined by

- electrons interacting with each other,
- electrons interacting with crystal vibrations and lattice imperfections (but not perfect lattices),
- lattice ions interacting with each other.

In principle the problem we are facing is therefore defined by the Schrödinger equation:

$$\mathcal{H}|\psi\rangle = i\hbar \frac{\partial |\psi\rangle}{\partial t}.$$

<u>Exercise:</u> find the eigenstates and the excitation spectrum.

Hamilton operators:

$$\mathcal{H} = \mathcal{H}_{\text{e-e}} + \mathcal{H}_{\text{e-ion}} + \mathcal{H}_{\text{ion-ion}}.$$

(Plus possible external perturbations, such as an external electromagnetic field.)

$$\mathcal{H}_{\text{e-e}} = \sum_i \frac{p_i^2}{2m} + \sum_{i,j} V_{\text{Coul}}^{\text{e-e}}(\boldsymbol{r}_i - \boldsymbol{r}_j),$$

$$\mathcal{H}_{\text{ion-ion}} = \sum_i \frac{P_i^2}{2M} + \sum_{i,j} V_{\text{Coul}}^{\text{ion-ion}}(\boldsymbol{R}_i - \boldsymbol{R}_j),$$

$$\mathcal{H}_{\text{e-ion}} = \sum_{i,j} V_{\text{Coul}}^{\text{e-ion}}(\boldsymbol{R}_i - \boldsymbol{r}_j).$$

$|\psi\rangle$: many-particle state that "describes" the system.

1.1 Statistical mechanics

We need one extra parameter to describe the "macroscopic" physics: T. This is introduced as follows ($\mathcal{H}$ doesn't include T):

Suppose we know the excitation spectrum of the system as well as the eigenstate

$$\mathcal{H}|\psi_{N_i}\rangle = E_{N_i}|\psi_{N_i}\rangle,$$

where i is the index for the i-th eigenstate $|\psi_{N_i}\rangle$. There may exist many such $|\psi_{N_i}\rangle$ with the same energy E_{N_i} (degeneracy). We can then find the partition function

$$\mathcal{Z} = \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \sum_n \langle n|e^{-\beta\mathcal{H}}|n\rangle, \qquad \beta = \frac{1}{k_B T},$$

where $\{|n\rangle\}$ is a complete basis that satisfies the identity $\sum_n |n\rangle\langle n|$. Which basis shall we choose? It doesn't matter:

$$\begin{aligned}\mathcal{Z} &= \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \mathrm{Tr}(SS^{-1}e^{-\beta\mathcal{H}}) = \mathrm{Tr}(S^{-1}e^{-\beta\mathcal{H}}S) \\ &= \sum_n \langle n|S^{-1}e^{-\beta\mathcal{H}}S|n\rangle = \sum_{n'} \langle n'|e^{-\beta\mathcal{H}}|n'\rangle\,,\end{aligned}$$

where $|n'\rangle = S|n\rangle$ and $S^{-1} = S^\dagger$ is a unitary "similarity transformation". Choose $\{|n\rangle\} = \{|N\rangle\}$ such that

$$\mathcal{H}|N\rangle = E_N|N\rangle \qquad \Rightarrow \qquad \mathcal{Z} = \sum_i e^{-\beta E_{N_i}},$$

where E_{N_i} is the i-th excitation energy for an N-particle system and $|N_i\rangle$ is the corresponding eigenstate.

All information about interesting many-particle effects are encoded in $\mathcal{Z}$, but in general it is difficult to get explicit information from it. Suppose we have an operator that is described by an observable $\hat{\mathcal{O}}$ with the statistical mean

$$\boxed{\langle\hat{\mathcal{O}}\rangle = \frac{1}{\mathcal{Z}}\,\mathrm{Tr}\Big(\hat{\mathcal{O}}e^{-\beta\mathcal{H}}\Big)}$$

$$\begin{aligned}\underbrace{\langle\hat{\mathcal{O}}\rangle}_{\substack{\text{statistical mean,}\\ \text{usually what's}\\ \text{measured in}\\ \text{a lab}}} &= \frac{1}{\mathcal{Z}}\sum_i \langle N_i|\hat{\mathcal{O}}e^{-\beta\mathcal{H}}|N_i\rangle = \frac{1}{\mathcal{Z}}\sum_{i,j}\langle N_i|\hat{\mathcal{O}}|N_j\rangle\, e^{-\beta E_{N_i}}\delta_{ij} \\ &= \frac{1}{\mathcal{Z}}\sum_i \underbrace{\langle N_i|\hat{\mathcal{O}}|N_i\rangle}_{\substack{\text{mean value in}\\ \text{e.g. state}|N_i\rangle}}\, e^{-\beta E_{N_i}},\end{aligned}$$

where we used that

$$\sum_i |N_i\rangle\langle N_i| = 1, \qquad \text{(completeness)}$$

$$\langle N_i|N_j\rangle = \delta_{ij}. \qquad \text{(orthonormality)}$$

Hence this is a coupling between quantum mechanics and thermodynamics. In the ground state $T \to 0$ and $\beta \to \infty$. The lowest state has energy $E_{N_1} = E_{N_0} + \Delta E$, if $e^{-\beta\Delta E} \ll 1$, then

$$\mathcal{Z} \approx e^{-\beta E_{N_0}} = e^{-e\beta F},$$

where $F = U - TS = E_{N_0}$ (the entropy term disappears as $T \to 0$) is the Helmholtz free energy. We can now write

$$\langle\hat{\mathcal{O}}\rangle = \frac{1}{e^{-\beta E_{N_0}}}\,\langle N_0|\hat{\mathcal{O}}|N_0\rangle\, e^{-\beta E_{N_0}} = \underbrace{\langle N_0|\hat{\mathcal{O}}|N_0\rangle}_{\substack{\text{expectation value}\\ \text{in the ground state}}}.$$

For systems where the lowest excited state is separated from the ground state with an energy gap, it is often enough to look at the ground state's expectation values.

Example: electronic insulator or semiconductor with a gap between $\sim 0.1 - 1\text{eV}$.

Counterexample: in good metals, such as for example Cu, Ag, Au etc, there is no gap in the excitation spectrum.

1.2 Many-particle state vector for fermions

We build such state vectors from single-particle states: think of a set quantum number λ describing a single-particle state. The corresponding single-particle state vector is given by $|n_\lambda\rangle$ (Dirac ket) and the adjoint state by $\langle n_\lambda|$ (Dirac bra). $|n_\lambda\rangle$ can be created from a vacuum via a creation operator $c_\lambda^\dagger$:

$$|n_\lambda\rangle = c_\lambda^\dagger |0\rangle ,$$

where λ isn't yet specified. The set will be chosen as appropriate, "good" quantum numbers, and will depend on the problem we are looking at. λ will consist of quantum numbers that describe single-particle states.

Example: translation-invariant systems of fermions with spin

$$\lambda = (\boldsymbol{k}, \sigma)$$

$\boldsymbol{k}$: wave number, a conserved ("good") quantum number

σ : spin $\uparrow$ or $\downarrow$ for spin-1/2 fermions

$c_{\boldsymbol{k},\sigma}^\dagger$ creates a fermion with wave number $\boldsymbol{k}$ and spin σ:

$$|n_{\boldsymbol{k},\sigma}\rangle = c_{\boldsymbol{k},\sigma}^\dagger |0\rangle , \qquad \varphi_{\boldsymbol{k},\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{\nu}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \qquad |0\rangle = c\,|\boldsymbol{k},\sigma\rangle .$$

Example: semiconductor heterostructure in a strong external magnetic field (homogeneous)

$$\lambda = \boldsymbol{k}, \qquad \varphi_{\boldsymbol{k},\sigma} = \underbrace{u_{\boldsymbol{k},\sigma}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}_{\text{Bloch function}} .$$

2D Electron gas completely spin-polarised $\Rightarrow$ spin degrees of freedom "frozen out" $\Rightarrow$ "spinless fermions" (QHE).

Example: Lattice fermion model where the electrons mainly "live" at one lattice point, and then tunnel from one lattice point to another

$$\lambda = (i,\sigma), \qquad |n_{i,\sigma}\rangle = c^\dagger_{i,\sigma}|0\rangle, \qquad \varphi_{i,\sigma} = \phi^i_w(\boldsymbol{r}_i),$$

where i is a lattice point.

1.3 Many-particle states

An N-particle state is given by

$$|N\rangle = |n_{\lambda_1}, n_{\lambda_2}, \cdots, n_{\lambda_N}\rangle = c^\dagger_{\lambda_1}\cdots c^\dagger_{\lambda_N}|0\rangle,$$

where

$$|0\rangle = |0_{\lambda_1}, \cdots, 0_{\lambda_N}\rangle \qquad \text{and} \qquad |N\rangle = \prod_{i=1}^{N} c^\dagger_{\lambda_i}|0\rangle = \prod_{i=1}^{N}|n_{\lambda_i}\rangle .$$

This is often called a Fock state.

In the case of fermions we can have maximum one fermion in each single-particle state.

1.4 The formulation of many-particle theory as a quantum field theory

The fermions are considered as quantized excitations of a matter field in the same way as photons are considered as quantized excitations of an electromagnetic field. The general field operator for a fermion is given by

$$\psi^\dagger(\boldsymbol{r},t) = \sum_\lambda c^\dagger_\lambda(t)\varphi^*_\lambda(\boldsymbol{r}).$$

$\psi^\dagger(\boldsymbol{r},t)$: Operator that requires a fermion at the point $(\boldsymbol{r},t)$ with any quantum number.

$c^\dagger_\lambda(t)$: Operator that requires a fermion with a certain quantum number λ at time t.

$\varphi^*_\lambda(\boldsymbol{r})$: Function that describes the spatial part (and in some cases the spin part) of the state that is required.

Heisenberg picture:

$$\hat{\mathcal{O}}(t) = e^{i\mathcal{H}t/\hbar}\,\hat{\mathcal{O}}\,e^{-i\mathcal{H}t/\hbar},$$

where $\hat{\mathcal{O}}$ is an operator in the Schrödinger picture.

In the case of fermions the field is quantized with the help of the anticommutator relation

$$\underbrace{\left[\psi^\dagger(\boldsymbol{r},t), \psi(\boldsymbol{r}',t)\right]_+}_{\text{same } t} = \delta(\boldsymbol{r}-\boldsymbol{r}').$$

We assume that the basis functions $\{\varphi_\lambda\}$ form a complete set and that the set is orthonormalized.

<u>Orthonormalization</u>

$$\boxed{\sum_{\boldsymbol{r}} \varphi^*_{\lambda'}(\boldsymbol{r})\varphi_\lambda(\boldsymbol{r}) = \delta_{\lambda,\lambda'}.} \tag{1}$$

Completeness:

$$f(\boldsymbol{r}) = \sum_\lambda b_\lambda \varphi_\lambda(\boldsymbol{r}),$$

where f is an arbitrary function, and b_λ is given by

$$b_\lambda = \sum_{\boldsymbol{r}'} \varphi^*_\lambda(\boldsymbol{r}')f(\boldsymbol{r}').$$

Therefore:

$$f(\boldsymbol{r}) = \sum_{\boldsymbol{r}'} \underbrace{\sum_\lambda \varphi^*_\lambda(\boldsymbol{r}')\varphi_\lambda(\boldsymbol{r})}_{\delta(\boldsymbol{r}-\boldsymbol{r}')}\, f(\boldsymbol{r}').$$

Completeness relation:

$$\boxed{\sum_\lambda \varphi^\star_\lambda(\boldsymbol{r}')\varphi_\lambda(\boldsymbol{r}) = \delta(\boldsymbol{r}-\boldsymbol{r}').}$$

What commutation relations should be satisfied? In the case of fermions this is the anticommutator relation

$$\left[\psi^\dagger(\boldsymbol{r},t), \psi(\boldsymbol{r}',t)\right]_+ = \delta(\boldsymbol{r}-\boldsymbol{r}') = \sum_{\lambda_1,\lambda_2} \varphi^*_{\lambda_1}(\boldsymbol{r})\varphi_{\lambda_2}(\boldsymbol{r}')\left[c^\dagger_{\lambda_1}, c^\dagger_{\lambda_2}\right]_+.$$

In case that

$$\left[c^\dagger_{\lambda_1}, c_{\lambda_2}\right]_+ = \delta_{\lambda_1,\lambda_2},$$

we get, from completeness:

$$\sum_{\lambda_1} \varphi^*_{\lambda_1}(\boldsymbol{r})\varphi_{\lambda_2}(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'),$$

$$\left[c^\dagger_{\lambda'}(t), c_\lambda(t)\right]_+ = \delta_{\lambda,\lambda'}.$$

In addition it is trivially shown that

$$\left[\psi(\boldsymbol{r}, t), \psi(\boldsymbol{r}', t)\right]_+ = 0 \Rightarrow \left[c_\lambda, c_{\lambda'}\right]_+ = 0,$$

$$\left[\psi^\dagger(\boldsymbol{r}, t), \psi^\dagger(\boldsymbol{r}', t)\right]_+ = 0 \Rightarrow \left[c^\dagger_\lambda, c^\dagger_{\lambda'}\right]_+ = 0,$$

thus fully specifying the characteristics of the field operators ψ and c.

<u>**Interpretation of the anticommutation relations**</u>

The fact that there cannot be two fermions in the same state (the Pauli principle) is expressed as follows:

$$c^\dagger_\lambda c^\dagger_\lambda \left|0\right\rangle = 0 \qquad \Rightarrow \qquad \left[c^\dagger_\lambda, c^\dagger_\lambda\right]_+ = 0,$$

whereas the annihilation of the vacuum leads to

$$c_\lambda c_\lambda \left|0\right\rangle = 0 \qquad \Rightarrow \qquad \left[c_\lambda, c_\lambda\right]_+ = 0.$$

For $\lambda_1 \neq \lambda_2$ we get

$$\left[c^\dagger_{\lambda_1}, c_{\lambda_2}\right]_+ = 0 \qquad \Rightarrow \qquad \left|n_{\lambda_1}, n_{\lambda_2}\right\rangle = -\left|n_{\lambda_2}, n_{\lambda_1}\right\rangle,$$

antisymmetry under exchange of two single-particle states.

The next step is to express the <u>operators</u> that represent observables via field operators. This is the appropriate formulation (as we will see). The introduction of creation and annihilation operators (with anticommutation relations for fermions) is called <u>second quantization</u>.

1.5 Single-particle operators

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

where $\hat{U}_i$ only works on element number i in $\left|N\right\rangle$.

Example: Kinetic energy:

$$\hat{T}\left|N\right\rangle = \sum_i \frac{p_i^2}{2m}\left|N\right\rangle .$$

Example: Crystal potential that every single electron feels when they move around in a lattice

$$V\left|N\right\rangle = \sum_i \hat{V}\left|N\right\rangle , \qquad \hat{V}_i = \sum_{\boldsymbol{R}_j} V(\boldsymbol{r}_i - \boldsymbol{R}_j),$$

where:

$$\boldsymbol{r}_i : \text{electron coordinate,}$$

$$\boldsymbol{R}_j : \text{ion coordinate.}$$

Placing the matrix element of a single-particle operator between two many-particle states $|N\rangle$ and $|N'\rangle$:

$$\langle N'|\hat{U}|N\rangle = \sum_i \langle N'|\hat{U}_i|N\rangle .$$

Writing out $|N\rangle$ and $|N'\rangle$ we get

$$|N\rangle = |n_1\rangle \cdots |n_N\rangle , \qquad |N'\rangle = |n_1'\rangle \cdots |n_N'\rangle ,$$

$$\langle n_1'| \cdots \langle n_N'| \left(\sum_i \hat{U}_i\right) |n_1\rangle \cdots |n_N\rangle = \sum_i \langle n_i'|\hat{U}_i|n_i\rangle \prod_{k\neq i} \langle n_k'|n_k\rangle .$$

Normalization:

$$\frac{\langle N'|\hat{U}|N\rangle}{\langle N'|N\rangle} = \frac{\sum_i \langle n_i'|U_i|n_i\rangle \prod_{k\neq i}\langle n_k'|n_k\rangle}{\prod_k \langle n_k'|n_k\rangle} = \sum_i \frac{\langle n_i'|\hat{U}_i|n_i\rangle}{\langle n_i'|n_i\rangle} \frac{\prod_{k\neq i}\langle n_k'|n_k\rangle}{\prod_{k\neq i}\langle n_k'|n_k\rangle} = \sum_i \frac{\langle n_i'|\hat{U}_i|n_i\rangle}{\langle n_i'|n_i\rangle}.$$

Single-particle operators are defined by matrix elements in single-particle Hilbert space.

1.6 Two-particle operators

$$\hat{V}\,|n_1\rangle \cdots |n_N\rangle = \frac{1}{2}\sum_{i,j} \hat{V}_{i,j}\,|n_1\rangle \cdots |n_N\rangle .$$

The operator $\hat{V}_{i,j}$ works on the elements i and j. The factor 1/2 is there because the summation is over distinct pairs.

Example: Coulomb interaction between electrons.

The matrix element is given by

$$\frac{\langle N'|\hat{V}|N\rangle}{\langle N'|N\rangle} = \frac{1}{2}\sum_{i,j} \frac{\langle n_i', n_j'|\hat{V}_{i,j}|n_j, n_j\rangle}{\langle n_i', n_j'|n_i, n_j\rangle}.$$

Two-particle operators are defined by their matrix elements in the Hilbert space of two-particle states.

$$\hat{V}_{i,j} = \hat{V}_{j,i} \quad \text{for} \quad i \neq j, \qquad \hat{V}_{i=j} = 0,$$

the latter because a two-particle operator is working on a single-particle state.

2 Electrons with interaction

The Hamilton operators consist of a sum of single-particle and two-particle operators:

$$\mathcal{H} = \underbrace{\sum_i \left(\frac{p_i^2}{2m} + U(\boldsymbol{r}_i) \right)}_{\text{Single-particle operator.}} + \underbrace{\sum_{i<j} V_{\text{Coul}}(\boldsymbol{r}_i - \boldsymbol{r}_j)}_{\substack{\text{Two-particle operator.} \\ \text{It is this part that} \\ \text{makes the problem} \\ \text{difficult to solve.}}} .$$

$$= \sum_i \mathcal{H}_1(i) + \frac{1}{2} \sum_{i,j} \mathcal{H}_2(\boldsymbol{r}_i, \boldsymbol{r}_j).$$

We first find the second-quantized form of the two parts in $\mathcal{H}_i$.

2.1 Second quantization of single-particle operators

If we know $\mathcal{H}$ expressed in a classical way, how can we express it using annihilation and creation operator? We will start by finding the second-quantized form of $\mathcal{H}_1$. Define φ_λ and ε_λ such that

$$\mathcal{H}_1(\boldsymbol{r})\varphi_\lambda(\boldsymbol{r}) = \varepsilon_\lambda \varphi_\lambda(\boldsymbol{r}).$$

We thus assume that we are able to find the eigenfunctions and eigenvalues of the non-interacting system

$$\mathcal{H}_1 = -\frac{\hbar^2}{2m} \nabla^2 + U(\boldsymbol{r}), \qquad \nabla = \frac{\partial}{\partial \boldsymbol{r}}. \tag{2}$$

What we intend to show is that we can find a second-quantized form of $\mathcal{H}_1$ that has the <u>same</u> matrix elements as equation (2).

We proceed as follows:

$$\langle \lambda_1 | \mathcal{H}_1 | \lambda_2 \rangle = \int d\boldsymbol{r} d\boldsymbol{r}' \underbrace{\langle \lambda_1 | \boldsymbol{r} \rangle}_{\varphi^*_{\lambda_1}(\boldsymbol{r})} \langle \boldsymbol{r} | \mathcal{H}_1 | \boldsymbol{r}' \rangle \underbrace{\langle \boldsymbol{r}' | \lambda_2 \rangle}_{\varphi_{\lambda_2}(\boldsymbol{r}')} . \tag{3}$$

We now need the matrix element

$$\langle \boldsymbol{r} | \mathcal{H}_1 | \boldsymbol{r}' \rangle = \langle \boldsymbol{r} | \sum_i \mathcal{H}_1(\boldsymbol{r}_i) | \boldsymbol{r}' \rangle ,$$

where

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

$|\boldsymbol{r}\rangle$: Eigenfunction of the position operator.

The latter satisfies the following relations:

$$\hat{\boldsymbol{r}}\,|\boldsymbol{r}\rangle = \boldsymbol{r}\,|\boldsymbol{r}\rangle\,,$$

$$\langle\boldsymbol{r}|\hat{\boldsymbol{r}}|\boldsymbol{r}'\rangle = \boldsymbol{r}'\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$

$$\langle\boldsymbol{r}|U(\boldsymbol{r})|\boldsymbol{r}'\rangle = \sum_n c_n\,\langle\boldsymbol{r}|\hat{\boldsymbol{r}}^n|\boldsymbol{r}'\rangle = \sum_n c_n \boldsymbol{r}'^n\delta(\boldsymbol{r}-\boldsymbol{r}') = U(\boldsymbol{r}')\delta(\boldsymbol{r}-\boldsymbol{r}').$$

<u>But:</u> We also need

$$\langle\boldsymbol{r}|\boldsymbol{p}_i^2|\boldsymbol{r}'\rangle = \sum_{\boldsymbol{r}_i}\langle\boldsymbol{r}|\hat{\boldsymbol{p}}_i|\boldsymbol{r}_i\rangle\,\langle\boldsymbol{r}_i|\hat{\boldsymbol{p}}_i|\boldsymbol{r}'\rangle\,.$$

Let's have a look at $\langle\boldsymbol{r}|\hat{\boldsymbol{p}}|\boldsymbol{r}'\rangle$. For simplicity, we will look at a single spatial dimension, the result will be trivial to generalize. We got $[\hat{x},\hat{p}]_- = i\hbar$:

$$\langle x|\,[\hat{x},\hat{p}]_-\,|x'\rangle = \langle x|\hat{x}\hat{p}|x'\rangle - \langle x|\hat{p}\hat{x}|x'\rangle = (x-x')\,\langle x|\hat{p}|x'\rangle = i\hbar\delta(x-x').$$

The δ distribution is defined as

$$\int_{-\infty}^{\infty} dx\,\delta(x)f(x) = f(0),$$

now look at the distribution $x\,\delta'(x)$:

$$\int_{-\infty}^{\infty} dx\,x\delta'(x)f(x) = -\int_{-\infty}^{\infty} dx\,\delta(x)\,[x\,f(x)]' = -f(0).$$

From this we conclude that

$$\boxed{x\,\delta'(x) = -\delta(x),}$$

and thus

$$(x-x')\,\langle x|\hat{p}|x'\rangle = i\hbar\,\delta(x-x') \qquad \Rightarrow \qquad \langle x|\hat{p}|x'\rangle = -\frac{\hbar}{i}\,\frac{\delta(x-x')}{x-x'} = \frac{\hbar}{i}\,\frac{d}{dx}\delta(x-x').$$

Similarly,

$$\langle x|\hat{p}^2|x'\rangle = \sum_{x_1}\langle x|\hat{p}|x_1\rangle\,\langle x_1|\hat{p}|x'\rangle = -\hbar^2\sum_{x_1}\underbrace{\frac{d}{dx}\delta(x-x_1)}_{g(x-x_1)}\cdot\underbrace{\frac{d}{dx_1}\delta(x_1-x')}_{f'(x_1-x')}$$

$$= -\hbar^2\int_{-\infty}^{\infty} dx_1\,g(x-x_1)f'(x_1-x') = +\hbar^2\int_{-\infty}^{\infty} dx_1\,f(x_1-x')g'(x-x_1)$$

$$= \hbar^2\int_{-\infty}^{\infty} dx_1\,\delta(x_1-x')\frac{d}{dx_1}\frac{d}{dx}\delta(x-x_1) = \hbar^2\frac{d}{dx'}\frac{d}{dx}\delta(x-x')$$

$$= -\hbar^2\frac{d^2}{dx^2}\delta(x-x').$$

Generalizing this result gives

$$\langle x|F(\hat{p})|x'\rangle = F\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\delta(x-x').$$

This is immediately generalized to multiple dimensions:

$$\langle \boldsymbol{r}|\frac{\hat{\boldsymbol{p}}^2}{2m}|\boldsymbol{r}'\rangle = -\frac{\hbar^2}{2m}\nabla^2\delta_{\boldsymbol{r},\boldsymbol{r}'},$$

with which we get

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

Substituting this back into equation (3) we find

$$\begin{aligned}
\langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle &= \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, \varphi^*_{\lambda_1}\left(-\frac{\hbar^2}{2m}\nabla_1^2 + U(\boldsymbol{r}_1)\right)\delta_{\boldsymbol{r},\boldsymbol{r}'}\varphi_{\lambda_2}(\boldsymbol{r}_2)\\
&= \int d\boldsymbol{r}\, \varphi^*_{\lambda_1}(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right)\varphi_{\lambda_2}(\boldsymbol{r})\\
&= \varepsilon_{\lambda_2}\int d\boldsymbol{r}\, \varphi^*_{\lambda_1}(\boldsymbol{r})\varphi_{\lambda_2}(\boldsymbol{r})\\
&= \varepsilon_{\lambda_2}\delta_{\lambda_1,\lambda_2},
\end{aligned}$$

where we used equation (1) in the last step. Emphasizing that this is a matrix element, we can write

$$\left(\hat{\mathcal{H}}_1\right)_{\lambda_1,\lambda_2} = \varepsilon_{\lambda_2}\delta_{\lambda_1,\lambda_2}. \tag{4}$$

Can we find a form of $\mathcal{H}_1$ expressed in terms of c_λ and $c^\dagger_\lambda$ that gives the same matrix elements?

$$\underline{\text{Ansatz:}} \qquad \mathcal{H}_1 = \sum_\lambda \epsilon_\lambda c^\dagger_\lambda c_\lambda.$$

$$\langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle \;:\; \left(\psi(\boldsymbol{r}) = \sum_\lambda c_\lambda\varphi_\lambda(\boldsymbol{r})\right)$$

$$|\lambda_2\rangle = c^\dagger_{\lambda_2}|0\rangle$$

$$\langle\lambda_1| = |0\rangle\, c_{\lambda_1} = \left(c^\dagger_{\lambda_1}|0\rangle\right)^\dagger \neq 0$$

$$\langle 0|c_{\lambda_1}\left(\sum_\lambda \varepsilon_\lambda c^\dagger_\lambda c_\lambda\right)c^\dagger_{\lambda_2}|0\rangle = \sum_\lambda \varepsilon_\lambda\,\langle 0|c_{\lambda_1}c^\dagger_\lambda\underbrace{c_\lambda c^\dagger_{\lambda_2}}_{\delta_{\lambda_2,\lambda}-c^\dagger_{\lambda_2}c_\lambda}|0\rangle = \sum_\lambda \varepsilon_\lambda\delta_{\lambda_2\lambda}\,\langle 0|\underbrace{c_{\lambda_1}c^\dagger_\lambda}_{\delta_{\lambda_1,\lambda}-c^\dagger_\lambda c_{\lambda_1}}|0\rangle$$

$$= \sum_\lambda \varepsilon\delta_{\lambda_2,\lambda}\delta_{\lambda_1,\lambda} = \varepsilon_{\lambda_1}\delta_{\lambda_2,\lambda_1}.$$

This is ok because it is the same matrix element as in equation (4). We conclude that the second-quantized form of $\mathcal{H}$ for non-interacting fermion system is given by

$$\boxed{\mathcal{H}_1 = \sum_\lambda \varepsilon_\lambda c_\lambda^\dagger c_\lambda.} \tag{5}$$

Since the set of quantum numbers λ isn't specified at all, this is a very general form.

$$\boxed{c_\lambda^\dagger c_\lambda \ : \ \text{number operator.}}$$

The number operator measures the number of fermions in a single-particle state specified by λ, and energy ε_λ. The total energy $\mathcal{H}_1$ is therefore the energy of each single-particle state multiplied by the number of fermions i that state, summed over single-particle states. We could have found a corresponding form <u>without</u> assuming that we have found a basis set $\{\varphi_\lambda\}$ of eigenfunctions of $\mathcal{H}_1$.

$$\langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle = \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, \varphi^*_{\lambda_1}(\boldsymbol{r}_1)\left(\sum_i \mathcal{H}_1(\boldsymbol{r}_i)\right)\varphi_{\lambda_2}(\boldsymbol{r}_2) = \int d\boldsymbol{r}\, \varphi^*_{\lambda_1}\mathcal{H}_1(\boldsymbol{r})\varphi_{\lambda_2}(\boldsymbol{r}).$$

$$\text{Ansatz:} \qquad \mathcal{H}_1 = \sum_{\lambda_1,\lambda_2} \epsilon_{\lambda_2,\lambda_1} c^\dagger_{\lambda_1} c_{\lambda_2}.$$

$$\langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle = \sum_{\lambda,\lambda'} \langle 0|c_{\lambda_1}\varepsilon_{\lambda,\lambda'}c^\dagger_{\lambda'}c_\lambda c^\dagger_{\lambda_2}|0\rangle = \sum_{\lambda,\lambda'} \varepsilon_{\lambda',\lambda}\,\langle 0|\underbrace{c_{\lambda_1}c^\dagger_{\lambda'}}_{\delta_{\lambda',\lambda_1}-c^\dagger_{\lambda'}c_{\lambda_1}}\underbrace{c_\lambda c^\dagger_{\lambda_2}}_{\delta_{\lambda,\lambda_2}-c^\dagger_{\lambda_2}c_\lambda}|0\rangle$$

$$= \sum_{\lambda,\lambda'} \varepsilon_{\lambda',\lambda}\delta_{\lambda',\lambda_1}\delta_{\lambda,\lambda_2} = \varepsilon_{\lambda_1,\lambda_2}$$

$$\Rightarrow \qquad \boxed{\mathcal{H}_1 = \sum_{\lambda_1,\lambda_2} \langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle\, c^\dagger_{\lambda_1}c_{\lambda_2}.} \tag{6}$$

Here the matrix element $\langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle$ is known when the "classical" expression for $\mathcal{H}_1$ is known, and the basis $\{\varphi_\lambda\}$ is chosen:

$$\langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle = \int d\boldsymbol{r}\varphi^*_{\lambda_1}(\boldsymbol{r})\mathcal{H}_1\varphi_{\lambda_2}(\boldsymbol{r}).$$

$\mathcal{H}_1$ is now written in the so-called second-quantized form. Since we found this result without using that $\{\varphi_\lambda\}$ must be eigenfunctions of

$$\mathcal{H}_1 = -\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}),$$

we can write down an expression for an arbitrary single-particle operator

$$T = \sum_i T(i),$$

when the "classical" expression for (the single-particle operator) $T(i)$ is known:

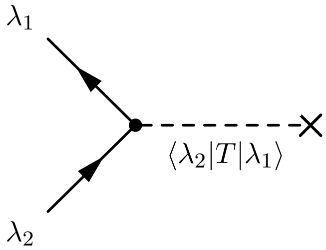
$$T(i) = T(\{\boldsymbol{r}_i, \boldsymbol{p}_i\}) = \sum_i T_i\left(\boldsymbol{r}_i, \frac{\hbar}{i}\nabla_i\right) = T\left(\boldsymbol{r}_i, \frac{\hbar}{i}\nabla_i\right), \qquad \nabla_i = \frac{\partial}{\partial \boldsymbol{r}_i}.$$

$$\langle\lambda_1|T(i)|\lambda_2\rangle = \int d\boldsymbol{r}_i\, \varphi^*_{\lambda_1}(\boldsymbol{r}_i)\, T\left(\boldsymbol{r}_i, \frac{\hbar}{i}\nabla_i\right) \varphi_{\lambda_2}(\boldsymbol{r}_i).$$

The operator T is then given by

$$\boxed{T = \sum_{\lambda_1,\lambda_2} \underbrace{\langle\lambda_1|T|\lambda_2\rangle}_{\text{number}}\, c^\dagger_{\lambda_1} c_{\lambda_2}.}$$

Diagrammatically:



2.2 Second quantization of two-particle operators

The Hamilton function for an interacting electron system also has a two-particle contribution

$$\frac{1}{2}\sum_{i,j} \mathcal{H}_2(\boldsymbol{r}_i, \boldsymbol{r}_j) = \frac{1}{2}\sum_{i,j} V_{\text{Coul}}(\boldsymbol{r}_i - \boldsymbol{r}_j).$$

Assume that the classical form of a general two-particle operator is known.

$$V_2 = \frac{1}{2}\sum_{i,j} V_2(\boldsymbol{r}_i - \boldsymbol{r}_j).$$

Ansatz for the second-quantized form:

$$V_2 = \frac{1}{2}\sum_{\lambda_1,\cdots,\lambda_2} \langle\lambda_1, \lambda_2|V_2|\lambda_3, \lambda_4\rangle\, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}\ \langle\lambda_1, \lambda_2|V_2|\lambda_3, \lambda_4\rangle$$

$$= \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3\, d\boldsymbol{r}_4\, \varphi^*_{\lambda_1}(\boldsymbol{r}_1)\varphi^*_{\lambda_2}(\boldsymbol{r}_2) V_2(\boldsymbol{r}_3, \boldsymbol{r}_4)\varphi_{\lambda_3}(\boldsymbol{r}_3)\varphi_{\lambda_4}(\boldsymbol{r}_4)$$

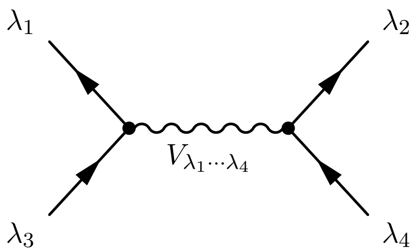
$$\times\delta_{\boldsymbol{r}_1,\boldsymbol{r}_4}\delta_{\boldsymbol{r}_2,\boldsymbol{r}_3}\ \langle\boldsymbol{r}_1\boldsymbol{r}_2|V_2(\boldsymbol{r}_3, \boldsymbol{r}_4)|\boldsymbol{r}_3, \boldsymbol{r}_4\rangle = V_2(\boldsymbol{r}_3, \boldsymbol{r}_4)\delta_{\boldsymbol{r}_1,\boldsymbol{r}_4}\delta_{\boldsymbol{r}_2,\boldsymbol{r}_3}$$

$$= \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2 \varphi^*_{\lambda_1}(\boldsymbol{r}_1)\varphi^*_{\lambda_2}(\boldsymbol{r}_2) V(\boldsymbol{r}_3, \boldsymbol{r}_1)\varphi_{\lambda_3}(\boldsymbol{r}_2)\varphi_{\lambda_4}(\boldsymbol{r}_1).$$

General second-quantized form of $\mathcal{H}$ for a fermion system

$$\mathcal{H} = \sum_{\lambda_1,\lambda_2} \langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle\, c^\dagger_{\lambda_1} c_{\lambda_2} + \sum_{\lambda_1,\cdots,\lambda_4} \langle\lambda_1,\lambda_2|V_2|\lambda_3,\lambda_4\rangle\, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}. \quad (7)$$

Diagrammatic illustration of the two-particle contribution:



Please note: the same number of annihilation and creation operators on each side! "Spreading process" between two electrons because of interaction between them. The expression for $\mathcal{H}$ is completely independent of the choice of the basis set $\{\varphi_\lambda\}$, which is equivalent with the choice of a quantum number.

A few examples of the choice of basis set and quantum numbers.

Example: Basis set and quantum number for nearly free electrons

$$\lambda = (\boldsymbol{k}, \sigma), \qquad \varphi_\lambda(\boldsymbol{r}) = \varphi_{\boldsymbol{k},\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, \chi_\sigma.$$

The spatial part is given by the plane waves $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$. The spin part is given by the spin function χ_σ.

Example: Basis set for nearly free electrons in a periodic crystal potential

$$\lambda = (\boldsymbol{k}, \sigma), \qquad \varphi_{\boldsymbol{k},\sigma}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r})\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, \chi_\sigma.$$

The spatial part is given by the Bloch function

$$u_{\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{R}) = u_{\boldsymbol{k}}(\boldsymbol{r}),$$

with the lattice's periodicity.

<u>Example:</u> Almost localized fermions on a lattice

$$\lambda = (i, \alpha, \sigma), \qquad \varphi_{i,\sigma}(\boldsymbol{r}) = \phi^{w}_{\alpha,\sigma}(\boldsymbol{r}, \boldsymbol{R}_i),$$

i: Lattice point

α: Atom orbital

σ: Spin index

$\boldsymbol{r}$: Electron coordinate

$\boldsymbol{R}_i$: Ion coordinate

ϕ^w: Wannier orbital function that describes the state the electron "lives" in at lattice point i.

Such choices represent explicit realizations of the general expression for $\mathcal{H}$ in equation (7). For example, in good metals such as Al it will be natural to choose a plane wave basis. In a semiconductor where the crystal potential is important for creating a gap in the band structure, a Bloch function will be a natural basis. In strongly interacting electron systems where the kinetic energy is dominated by the potential energy, the Wannier basis will be "good".

2.3 The interacting electron gas

We will now look at a few concrete realizations of $\mathcal{H}$ in second quantization. The system we will look at is the interacting electron gas.

The plane wave basis is used to describe nearly free (free = non-interacting) fermions in periodic lattices. Considering the electrons to almost not interact at all means that the kinetic energy of the electrons dominates the interaction energy between them. We will later come back to why the Coulomb energy often can be ignored i <u>good metals</u> (but not in "bad" metals, insulators and semiconductors). Metals that are good conductors, and therefore suited for a plane wave basis, are for example Al, Sn, Fe, Cu, Ag etc.

The Hamiltonian for the interacting electron gas is in the classical form given by

$$\mathcal{H} = \underbrace{\sum_i \frac{p_i^2}{2m} + \sum_i U(\boldsymbol{r}_i)}_{\mathcal{H}_1} + \underbrace{\frac{1}{2}\sum_{i,j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}}_{\mathcal{H}_2}.$$

In the second-quantized form this becomes

$$\mathcal{H} = \sum_{\lambda_1,\lambda_2} \langle \lambda_1 | \mathcal{H}_1 | \lambda_2 \rangle \, c^\dagger_{\lambda_1} c_{\lambda_2} + \frac{1}{2} \sum_{\lambda_1,\cdots,\lambda_4} \langle \lambda_1, \lambda_2 | \mathcal{H}_2 | \lambda_3, \lambda_4 \rangle \, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}.$$

The basis is given by

$$\varphi_\lambda(\boldsymbol{r}, s) = \varphi_{\boldsymbol{k},\sigma}(\boldsymbol{r}, s) = \frac{1}{\sqrt{V}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, \chi_\sigma(s), \qquad \lambda = (\boldsymbol{k}, \sigma)$$

$$\boldsymbol{r} : \text{Spatial coordinate}$$

$$s : \text{Spin coordinate}$$

The spin part of the wave function is represented by a two-component spinor (in the case of $S = 1/2$ fermions, for a general spin s the spinor will in the non-relativistic case be a $(2S+1)$-component spinor, but we'll restrict ourselves to $S = 1/2$ fermions).

$S = 1/2$: quantize the spin along the z-axis, and use the z-component of the spin as the spin quantum number σ, $\sigma =\uparrow$ or $\sigma =\downarrow$ ($S_z = +1/2, -1/2$):

$$\chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{matrix} \leftarrow s = 1 \\ \leftarrow s = 2 \end{matrix}, \qquad \chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{matrix} \leftarrow s = 1 \\ \leftarrow s = 2 \end{matrix}.$$

The spin coordinate s indicates the components in the spinors $\chi_\sigma(s)$:

$$\chi_\uparrow(1) = 1, \qquad \chi_\uparrow(2) = 0, \qquad \chi_\downarrow(1) = 0, \qquad \chi_\downarrow(2) = 1.$$

Orthonormality:

$$\sum_x \varphi^*_\lambda(x)\varphi_{\lambda'}(x) = \delta_{\lambda,\lambda'},$$

where $\sum_x$ is the summation over the coordinates in the basis function:

$$\sum_x = \sum_s \sum_{\boldsymbol{r}}, \qquad \delta_{\lambda,\lambda'} = \underbrace{\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\sigma,\sigma'}}_{\delta \text{ function of \underline{all} quantum numbers}}.$$

Completeness:

$$\sum_\lambda \varphi^*_\lambda(x)\varphi_\lambda(x') = \delta(x - x'),$$

where

$$\delta(x - x') = \underbrace{\delta_{s,s'}\delta(\boldsymbol{r} - \boldsymbol{r}')}_{\delta \text{ function over \underline{all} coordinates}}.$$

The field operators are now given by

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

$$\left[c_{\boldsymbol{k},\sigma}(t), c^\dagger_{\boldsymbol{k}',\sigma'}(t) \right]_+ = \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\sigma,\sigma'},$$

$$\left[c_{\boldsymbol{k},\sigma}(t), c_{\boldsymbol{k}',\sigma'}(t) \right]_+ = \left[c^\dagger_{\boldsymbol{k},\sigma}(t), c^\dagger_{\boldsymbol{k}',\sigma'}(t) \right]_+ = 0,$$

where $c^\dagger_{\boldsymbol{k},\sigma}(t)$ needs a fermion with quantum number $\boldsymbol{k}$ and spin σ at time t.

Orthonormality of the spatial part:

$$\frac{1}{V}\int d\boldsymbol{r}\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \delta_{\boldsymbol{k},\boldsymbol{k}'}.$$

Orthonormality of the spin part:

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

(This can also be verified directly by using the spinor components we have introduced.)

Completeness of the spatial part:

$$\frac{1}{V}\sum_{\boldsymbol{k}} e^{-\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta(\boldsymbol{r}-\boldsymbol{r}').$$

Completeness of the spin part:

$$\sum_\sigma \chi^*_\sigma(s_1)\chi_\sigma(s_2) = \delta_{s_1,s_2}.$$

The plane waves are eigenfunctions of

$$\sum_i \frac{p_i^2}{2m} = \sum_i\left(-\frac{\hbar^2\nabla_i^2}{2m}\right).$$

By using the result in equation (5) we immediately find the second quantized form for this contribution to $\mathcal{H}_1$:

$$\sum_i \frac{p_i^2}{2m} \quad\Rightarrow\quad \sum_{\boldsymbol{k},\sigma}\varepsilon_{\boldsymbol{k},\sigma}c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},\sigma}, \qquad \varepsilon_{\boldsymbol{k},\sigma} = \frac{\hbar^2\boldsymbol{k}^2}{2m}.$$

The next contribution to $\mathcal{H}_1$ is the external (crystal) potential $\sum_i U(\boldsymbol{r}_i)$. We will use the general result in equation (6):

$$\sum_i U(\boldsymbol{r}_i) = \sum_{\lambda_1,\lambda_2}\langle\lambda_1|U|\lambda_2\rangle\, c^\dagger_{\lambda_1}c_{\lambda_2} = \sum_{\substack{\boldsymbol{k}_1,\boldsymbol{k}_2\\ \sigma_1,\sigma_2}}\langle\boldsymbol{k}_1,\sigma_1|U|\boldsymbol{k}_2,\sigma_2\rangle\, c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2}.$$

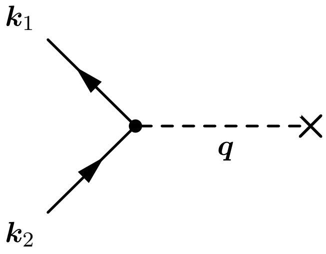
$$\begin{aligned}\langle\lambda_1|U|\lambda_2\rangle &= \sum_x \varphi^*_{\lambda_1}(x)\; U(x)\; \varphi_{\lambda_2}(x)\\ &= \sum_s\int d\boldsymbol{r}\,\chi^*_{\sigma_1}(s)\,\frac{1}{\sqrt{V}}\,e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}\,\underbrace{U(\boldsymbol{r})}_{\text{spin-independent potential}}\,\chi_{\sigma_2}(s)\,\frac{1}{\sqrt{V}}\,e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}\\ &= \underbrace{\sum_s\chi^*_{\sigma_1}(s)\chi_{\sigma_2}(s)}_{\delta_{\sigma_1,\sigma_2}}\;\underbrace{\frac{1}{V}\int d\boldsymbol{r}\,U(\boldsymbol{r})\,e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}}}_{\equiv\tilde{U}(\boldsymbol{k}_1-\boldsymbol{k}_2)},\end{aligned}$$

where $\tilde{U}(\boldsymbol{q})$ is the Fourier transform of the crystal potential:

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

$$\boxed{\tilde{U}(\boldsymbol{q}) = \frac{1}{V}\int d\boldsymbol{r}\, U(\boldsymbol{r})\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}},}$$

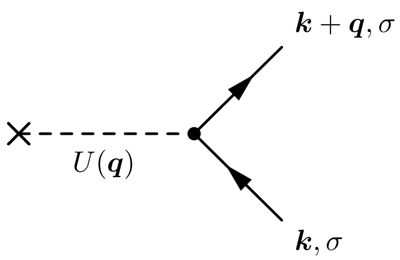
and $\boldsymbol{k}_1 - \boldsymbol{k}_2$ is the transferred momentum $\boldsymbol{q}$:



The plane waves are scattered by the crystal potential (plane waves are eigenfunctions in free space):

$$\mathcal{H}_1 = \sum_i \left(\frac{p_i^2}{2m} + U(\boldsymbol{r}_i)\right) \qquad \Rightarrow \qquad \mathcal{H}_1 = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \tilde{U}(\boldsymbol{q}) c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma},$$

in plane wave basis, where the second term represents the scattering of the electrons in plane wave states by the crystal potential.



It remains to second quantize the Coulomb parts in the plane wave basis. (Note that, in second quantized form, the information about what basis is used, is encoded in the interpretation of the creation/annihilation operators.)

2.4 Electron-electron interaction

$$\frac{1}{2}\sum_{\lambda_1,\cdots,\lambda_4} \langle \lambda_1, \lambda_2 | \mathcal{H}_2 | \lambda_3, \lambda_4 \rangle\, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}:$$

$$\langle \lambda_1, \lambda_2 | \mathcal{H}_2 | \lambda_3, \lambda_4 \rangle = \sum_{x_1, x_2} \varphi^*_{\lambda_1}(x_1) \varphi^*_{\lambda_2}(x_2) \underbrace{\mathcal{H}_2(x_1, x_2)}_{= \frac{e^2}{4\pi\varepsilon_0} \Rightarrow \substack{\text{doesn't work on the spin} \\ \text{part of the basis function}}} \varphi_{\lambda_3}(x_2) \varphi_{\lambda_4}(x_1)$$

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

$$\times \frac{1}{V^2} \int d\boldsymbol{r}_1 \, d\boldsymbol{r}_2 \, e^{-i\boldsymbol{k}_1 \cdot \boldsymbol{r}_1 - i\boldsymbol{k}_2 \cdot \boldsymbol{r}_2} \left(\frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \right) \frac{1}{4\pi\varepsilon_0} \, e^{i\boldsymbol{k}_3 \cdot \boldsymbol{r}_2 + i\boldsymbol{k}_4 \cdot \boldsymbol{r}_1}$$

$$= \delta_{\sigma_1, \sigma_4} \delta_{\sigma_2, \sigma_3} \cdot \text{Integral.} \tag{8}$$

The potential only depends on $\boldsymbol{r}_1 - \boldsymbol{r}_2$. We therefore try to make such a combination in the plane waves as well, to bring up another Fourier transformation.

$$\text{Integral} = \frac{1}{V^2} \int d\boldsymbol{r}_1 \, d\boldsymbol{r}_2 \, V(\boldsymbol{r}_1 - \boldsymbol{r}_2) \underbrace{e^{-i(\boldsymbol{k}_1 - \boldsymbol{k}_4) \cdot \boldsymbol{r}_1} \, e^{-(\boldsymbol{k}_2 - \boldsymbol{k}_3) \cdot \boldsymbol{r}_2}}_{e^{-i(\boldsymbol{k}_1 - \boldsymbol{k}_4) \cdot (\boldsymbol{r}_1 - \boldsymbol{r}_2)} \, e^{-i\boldsymbol{r}_2 \cdot (\boldsymbol{k}_1 - \boldsymbol{k}_4 + \boldsymbol{k}_2 - \boldsymbol{k}_3)}}$$

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$$

$$d\boldsymbol{r} = d\boldsymbol{r}_1 \qquad \text{(Integrate over } \boldsymbol{r}_1\text{, but treat } \boldsymbol{r}_2 \text{ as constant.)}$$

The integral is factorized:

$$\text{Integral} = \frac{1}{V^2} \int d\boldsymbol{r} \, V(\boldsymbol{r}) \, e^{-i(\boldsymbol{k}_1 - \boldsymbol{k}_4) \cdot \boldsymbol{r}} \times \underbrace{\int d\boldsymbol{r}_2 \, e^{-i(\boldsymbol{k}_1 - \boldsymbol{k}_4 + \boldsymbol{k}_2 - \boldsymbol{k}_3) \cdot \boldsymbol{r}_2}}_{\boxed{\substack{\boldsymbol{k}_1 - \boldsymbol{k}_4 = \boldsymbol{k}_3 - \boldsymbol{k}_2 \\ \boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_3 + \boldsymbol{k}_4}} \quad \substack{V\delta_{\boldsymbol{k}_1 - \boldsymbol{k}_4, \boldsymbol{k}_3 - \boldsymbol{k}_2} \\ = V\delta_{\boldsymbol{k}_1 + \boldsymbol{k}_2, \boldsymbol{k}_3 + \boldsymbol{k}_4}}}$$

$$= \underbrace{\delta_{\boldsymbol{k}_1 + \boldsymbol{k}_2, \boldsymbol{k}_3 + \boldsymbol{k}_4}}_{\substack{\text{momentum conservation} \\ \text{in scattering caused by} \\ \text{Coulomb interaction} \\ \text{between electrons}}} \quad \tilde{V}(\boldsymbol{k}_1 - \boldsymbol{k}_4),$$

where $\tilde{V}$ is the Fourier transform of the Coulomb potential:

$$\tilde{V}(\boldsymbol{q}) = \frac{1}{V} \int d\boldsymbol{r} \, e^{-i\boldsymbol{q} \cdot \boldsymbol{r}} \, V(\boldsymbol{r}).$$

Simplification:

$$\boldsymbol{q} = \boldsymbol{k}_1 - \boldsymbol{k}_4 \quad \text{(Momentum transfer in collision between electrons.)}$$

$$\boldsymbol{k} = \boldsymbol{k}_1 - \boldsymbol{q}$$

Must eliminate $\boldsymbol{k}_3$ as well:

$$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_3 + \boldsymbol{k}_4 = \boldsymbol{k}_3 + \boldsymbol{k}_1 - \boldsymbol{q}$$

$$\Rightarrow \boldsymbol{k}_2 = \boldsymbol{k}_3 - \boldsymbol{q}, \qquad \boldsymbol{k}_3 = \boldsymbol{k_2} + \boldsymbol{q}.$$

After the above, equation (8) contains

- 4 sums over spin and momentum $\boldsymbol{k}$,
- 2 δ functions of spin $\Rightarrow$ 2 spin sums remain,
- 1 δ function of $\boldsymbol{k}$ $\Rightarrow$ 3 $\boldsymbol{k}$ sums remain.

These sums can for example be over σ_1, σ_2 and $\boldsymbol{k}_1$, $\boldsymbol{k}_2$ and $\boldsymbol{q}$:

$$\frac{1}{2} \sum_{\substack{\boldsymbol{k}_1,\cdots,\boldsymbol{k}_4 \\ \sigma_1,\cdots,\sigma_4}} \delta_{\sigma_1,\sigma_4} \delta_{\sigma_2,\sigma_3} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4} \tilde{V}(\boldsymbol{k}_1 - \boldsymbol{k}_4) c^\dagger_{\boldsymbol{k}_1,\sigma_1} c^\dagger_{\boldsymbol{k}_2,\sigma_2} c_{\boldsymbol{k}_3,\sigma_3} c_{\boldsymbol{k}_4,\sigma_4}$$
$$= \frac{1}{2} \sum_{\substack{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{q} \\ \sigma_1,\sigma_2}} \tilde{V}(\boldsymbol{q}) c^\dagger_{\boldsymbol{k}_1,\sigma_1} c^\dagger_{\boldsymbol{k}_2,\sigma_2} c_{\boldsymbol{k}_2+\boldsymbol{q},\sigma_2} c_{\boldsymbol{k}_1-\boldsymbol{q},\sigma_1}.$$

This 2-particle scattering is shown in the following diagram. Here the momentum is conserved, as well as the spin in each fermion line, as the Coulomb interaction is spin independent.

The complete Hamiltonian

In total the Hamiltonian looks as follows when using the plane wave basis:

$$\boxed{\begin{aligned}\mathcal{H} = &\sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \tilde{U}(\boldsymbol{q}) c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma} \\ &+ \frac{1}{2} \sum_{\substack{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q} \\ \sigma,\sigma'}} \tilde{V}(\boldsymbol{q}) c^\dagger_{\boldsymbol{k},\sigma} c^\dagger_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k}'+\boldsymbol{q},\sigma'} c_{\boldsymbol{k}-\boldsymbol{q},\sigma}.\end{aligned}}$$

i) For a static, regular crystal lattice, it is the Coulomb term that makes the problem difficult to solve. $\tilde{U}$ then represents a relatively trivial complication. The Coulomb interaction is difficult in a many-particle problem.

ii) If the crystal lattice itself has dynamics that are coupled to the electron gas (which is realistic), the second term in $\mathcal{H}$ will describe, as we will later see, a coupling between the fermion gas and lattice vibrations (which is a phonon gas). They will also give the second term a many-particle effect!

2.5 The atom orbital basis (the lattice fermion model)

We think about a system where the fermions are mostly strongly bound to ions. They will sometimes tunnel to and from one lattice point to another. So this is almost the "opposite" situation of what we had before.

$$\varphi_\lambda(x) = \phi_{i,n}(\boldsymbol{r})\chi_\sigma(s)$$

n : A quantum number that tells what atom orbital the electron at lattice point i "lives" at (e.g. 1s, 2s, 2p, 3d etc).

We write the external potential as

$$U = \sum_i U(\boldsymbol{r}_i), \qquad U(\boldsymbol{r}_i) = \sum_j U_a(\boldsymbol{r}_i, \boldsymbol{R}_j),$$

$\boldsymbol{r}_i$: Electron coordinate,

$\boldsymbol{R}_j$: Ion coordinate.

The crystal potential that the electron feels, is established by the entire lattice. We write U the following way:

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

The point with splitting the potential like this is that, as the electrons are assumed to spend most of their time at a single ion lattice point, the basis functions are chosen as eigenfunctions of electrons around isolated atoms.

$$\left[\frac{\boldsymbol{p}_i^2}{2m} + U_a(\boldsymbol{r}_i, \boldsymbol{R}_i)\right] \varphi_{n,i,\sigma}(\boldsymbol{r_i}) = \varepsilon_n \varphi_{n,i,\sigma}(\boldsymbol{r}_i),$$

$$\varphi_\lambda(x) = \phi_{n,i}(\boldsymbol{r})\chi_\sigma(s),$$

$$x = \boldsymbol{r}, s, \qquad \lambda = (n, i, \sigma).$$

If we now bring in the rest of the crystal potential, these basis functions will no longer be eigenfunctions; we get "scattering". This "scattering" term leads to tunneling from one ion to another. <u>The tunneling represents the electron's kinetic energy.</u> The kinetic energy in the lattice fermion model therefore has its origin in electrostatic interactions! The details are as follows.

Field operators

$$\psi_j^\dagger(\boldsymbol{r}, s, t) = \sum_{n,\sigma} c^\dagger_{n,\sigma,j}(t)\phi^*_{n,j}(\boldsymbol{r})\chi^*_\sigma(s),$$

$$\left[c_{n,\sigma,j}, c^\dagger_{n',\sigma',j'}\right]_+ = \delta_{n,n'}\delta_{\sigma,\sigma'}\delta_{j,j'},$$

$$\left[c_{n,\sigma,j}, c_{n',\sigma',j'}\right]_+ = \left[c^\dagger_{n,\sigma,j}, c^\dagger_{n',\sigma',j'}\right]_+ = 0.$$

Orthogonality

$$\sum_s \int d\boldsymbol{r}\, \varphi^*_{n,\sigma,j}(\boldsymbol{r}, s)\varphi_{n',\sigma',j'}(\boldsymbol{r}, s) = \delta_{n,n'}\delta_{\sigma,\sigma'}\delta_{j,j'}.$$

Completeness

$$\sum_{n,\sigma,j} \varphi^*_{n,\sigma,j}(\boldsymbol{r}, s)\varphi_{n,\sigma,j}(\boldsymbol{r}', s') = \delta_{s,s'}\delta(\boldsymbol{r} - \boldsymbol{r}').$$

Single-particle part of $\mathcal{H}$:

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

Our basis functions are assumed to be eigenfunctions of the first contribution in $\mathcal{H}_1$. We again use the result in equation (5) to write the second quantized form down directly:

$$\sum_i \left[\frac{\boldsymbol{p}_i^2}{2m} + U_a(\boldsymbol{r}_i, \boldsymbol{R}_i)\right] \quad \Rightarrow \quad \sum_{n,\sigma,i} \varepsilon_{n,\sigma,i} c^\dagger_{n,\sigma,i} c_{n,\sigma,i},$$

where $\varepsilon_{n,\sigma,i}$ is the energy of the electron in the <u>isolated</u> atom orbital n at lattice point i. If this energy is assumed to be independent of i, the system is assumed to be translationally invariant (with discrete translation symmetry). We can easily generalize this, by stating that $\varphi_{n,\sigma,i}(\boldsymbol{r})$ satisfies the eigenvalue problem

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

We then get:

$$\sum_i \left[\frac{\boldsymbol{p}_i^2}{2m} + U_a(\boldsymbol{r}_i, \boldsymbol{R}_i)\right] \quad \Rightarrow \quad \sum_{n,\sigma,i} \varepsilon_{n,i} c^\dagger_{n,\sigma,i} c_{n,\sigma,i}.$$

The system is now no longer translation invariant, if we let $\varepsilon_{n,i}$ vary from one lattice point to another. We can look at such variation as a simple model for <u>irregularity</u> in the system if for example the variation in $\varepsilon_{n,i}$ is random from lattice point to lattice point. $\varepsilon_{n,i}$ can also vary in a <u>regular</u> way between lattice points. For example, every other lattice point can have energy $E_0 + \Delta$, with the rest having energy $E_0 - \Delta$. This is then a fermion system with two types of atom orbitals in the lattice, such that we need two types of creation operators. Thus: a two-component fermion system.

We now look at the term

$$\sum_i \sum_{j \neq i} U_a(\boldsymbol{r}_i, \boldsymbol{R}_j) \quad \Rightarrow \quad \sum_{\lambda_1, \lambda_2} \langle \lambda_1 | \mathcal{H}_1 | \lambda_2 \rangle \, c^\dagger_{\lambda_1} c_{\lambda_2},$$

by using the result in equation (6):

$$= \sum_{\substack{n_1,\sigma_1,i_1\\ n_2,\sigma_2,i_2}} \underbrace{\langle n_1,\sigma_1,i_1| \sum_{j\neq i} U_a |n_2,\sigma_2,i_2\rangle}_{\text{No summation over } i \text{ here!}} c^\dagger_{n_1,\sigma_1,i_1} c_{n_2,\sigma_2,i_2}$$

$$\times\ \langle n_1,\sigma_1,i_1| \underbrace{\sum_{j\neq i}}_{\text{Note: } \sum_i \boldsymbol{r}_i \to \int d\boldsymbol{r}} U_a(\boldsymbol{r}_i,\boldsymbol{R}_j)|n_2,\sigma_2,i_2\rangle$$

$$= \sum_s \int d\boldsymbol{r}\, \varphi^*_{N_1,\sigma_1,i_1}(\boldsymbol{r},s) \left(\sum_{j\neq i} U_a(\boldsymbol{r},\boldsymbol{R}_j)\right) \varphi_{n_2,\sigma_2,i_2}(\boldsymbol{r},s)$$

$$= \underbrace{\sum_s \chi^*_{\sigma_1}(s)\chi_{\sigma_2}(s)}_{\delta_{\sigma_1,\sigma_2}} \underbrace{\int d\boldsymbol{r}_i \phi_{n_1,i_1}(\boldsymbol{r}) \left(\sum_{j\neq i} U_a(\boldsymbol{r},\boldsymbol{R}_j)\right) \phi_{n_2,i_2}(\boldsymbol{r}),}_{\equiv t^{n_1,n_2}_{i_1,i_2}\text{, a matrix element}}$$

which gives us

$$\sum_i \sum_{j\neq i} U_a(\boldsymbol{r}_i,\boldsymbol{R}_j) = \sum_{\substack{i_1,i_2\\ n_1,n_2\\ \sigma}} t^{n_1,n_2}_{i_1,i_2}\, c^\dagger_{n_1,\sigma,i_1} c_{n_2,\sigma,i_2}.$$

This is a "hopping" process <u>from</u> lattice point i_2 <u>to</u> lattice point i_1.

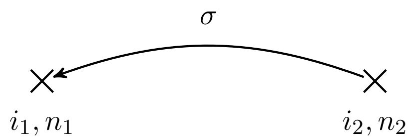


Figure 1: From orbital n_2 at i_2 to orbital n_1 at i_1.

The spin doesn't "flip" during the hopping process. This is because the hopping (the tunneling) has its origin in

$$\sum_i \sum_{j\neq i} U(\boldsymbol{r}_i,\boldsymbol{R}_j),$$

which is assumed to be a simple <u>electrostatic</u>, <u>spin-independent</u> single-particle potential.

$$t^{n_1,n_2}_{i_1,i_2} = \int d\boldsymbol{r}_i \phi^*_{n_1,i_1}(\boldsymbol{r}_i) \left(\sum_{j\neq i} U_a(\boldsymbol{r}_i,\boldsymbol{R}_j)\right) \phi_{n_2,i_2}(\boldsymbol{r}_i).$$

So far we therefore have, in the translation-invariant case:

$$\mathcal{H}_1 = \sum_{n,\sigma,i} \varepsilon_n c^\dagger_{n,\sigma,i} c_{n,\sigma,i} + \underbrace{\sum_{\substack{n_1,i_1 \\ n_2,i_2 \\ \sigma}} t^{n_1,n_2}_{i_1,i_2} c^\dagger_{n_1,\sigma_1,i_1} c_{n_2,\sigma_2,i_2}}_{\text{Contains both intra and interatomic ``hopping'' processes.}} .$$

Before we second quantize the Coulomb term, we will make the following simplifications:

i) Assume that

$$t^{n,n'}_{i,j} = t_{i,j}\delta_{n,n'} + \text{``small terms''}.$$

This means that the tunnelling between lattice points mainly occurs from an orbital at one lattice point to the same orbital at an other one.

ii) Consider only a single orbital per lattice point as applicable. For $S = 1/2$ fermions it can then at most be suitable to consider two fermions per lattice point (the other orbitals either are so low in energy that they are filled and inactive, or have such a high energy that they are never occupied).

$$t^{n_1,n_2}_{i_1,i_2} \to t_{i_1,i_2}.$$

iii) For translation-invariant systems we can set $\varepsilon_n = 0$, such that it only defines the baseline for the energy.

We end up with the following model:

$$\mathcal{H}_1 = \sum_{i_1,j_1,\sigma} t_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma}.$$

Here the atom orbital number n has been dropped because we only consider one kind of orbitals. In general: next and second-next neighbour hopping is enough.

2.6 Coulomb interaction

$$\begin{aligned}
\frac{1}{2}\sum_{i,j} V(\boldsymbol{r}_i - \boldsymbol{r}_j) \Rightarrow \frac{1}{2} \sum_{\lambda_1,\cdots,\lambda_4} \langle \lambda_1, \lambda_2 | V | \lambda_3, \lambda_4 \rangle \, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4} \\
= \frac{1}{2} \sum_{\substack{i_1,\cdots,i_4 \\ \sigma_1,\cdots,\sigma_4}} \langle \sigma_1, i_i; \sigma_2, i_2 | V | \sigma_3, i_3; \sigma_4, i_4 \rangle \, c^\dagger_{\sigma_1,i_1} c^\dagger_{\sigma_2,i_2} c_{\sigma_3,i_3} c_{\sigma_4,i_4}
\end{aligned}$$

$$
\begin{aligned}
\langle \sigma_1, i_i; \sigma_2, i_2 | V | \sigma_3, i_3; \sigma_4; i_4 \rangle &= \sum_{x_1, x_2} \varphi^*_{\lambda_1}(x_1) \varphi^*_{\lambda_2}(x_2) \underbrace{V(x_1, x_2)}_{\text{spin independent}} \varphi_{\lambda_3}(x_2) \varphi_{\lambda_4}(x_1) \\
&= \sum_{s_1, s_2} \chi^*_{\sigma_1}(s_1) \chi_{\sigma_4}(s_1) \chi^*_{\sigma_2}(s_2) \chi_{\sigma_3}(s_2) \\
&\quad \times \int d\boldsymbol{r}_1 \, d\boldsymbol{r}_2 \, \phi^*_{i_1}(\boldsymbol{r}_1) \phi_{i_2}(\boldsymbol{r}_2) V(\boldsymbol{r}_1 - \boldsymbol{r}_2) \phi_{i_3}(\boldsymbol{r}_2) \phi_{i_4}(\boldsymbol{r}_1) \\
&= \delta_{\sigma_1, \sigma_4} \, \delta_{\sigma_2, \sigma_3} \, V_{i_1, i_2, i_3, i_4},
\end{aligned}
$$

where

$$
V_{i_1, \cdots, i_4} = \int d\boldsymbol{r}_1 \, d\boldsymbol{r}_2 \, \phi^*_{i_1}(\boldsymbol{r}_1) \phi^*_{i_2}(\boldsymbol{r}_2) V(\boldsymbol{r}_1 - \boldsymbol{r}_2) \phi_{i_3}(\boldsymbol{r}_2) \phi_{i_4}(\boldsymbol{r}_1).
$$

The integrations over the two coordinates $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ go over all space. The wave function $\phi_i(\boldsymbol{r})$ is centred around lattice point i. We expect the largest contribution to $V_{i_1, \cdots, i_4}$ when $i_1 = i_2 = i_3 = i_4$:

$$
V_{i_1, i_1, i_1, i_1} = \int d\boldsymbol{r}_1 \, d\boldsymbol{r}_2 \, |\phi(\boldsymbol{r}_1)|^2 V(\boldsymbol{r}_1 - \boldsymbol{r}_2) |\phi(\boldsymbol{r}_2)|^2 = U.
$$

If we neglect <u>other</u> contributions to the Coulomb integral, we get

$$
\frac{1}{2} \sum_{i, \sigma_1, \sigma_2} U \, c^\dagger_{i, \sigma_1} c^\dagger_{i, \sigma_2} c_{i, \sigma_2} c_{i, \sigma_1}.
$$

<u>But:</u> This means that $\sigma_2 = -\sigma_1$ because we can have at most two fermions at each lattice point. Because of the Pauli principle these must have opposite spin.

We therefore get:

$$
\frac{1}{2} \sum_{i, \sigma} U \, c^\dagger_{i, \sigma} c^\dagger_{i, -\sigma} c_{i, -\sigma} c_{i, \sigma} = \frac{1}{2} \sum_{i, \sigma} U \, c^\dagger_{i, \sigma} c_{i, \sigma} c^\dagger_{i, -\sigma} c_{i, \sigma} = \frac{1}{2} \sum_{i, \sigma} U \, n_{i, \sigma} n_{i, -\sigma},
$$

where $n_{i, \sigma} = c^\dagger_{i, \sigma} c_{i, \sigma}$ is the number operator. In this approximation we then get, in total:

$$
\mathcal{H} = \sum_{i, j, \sigma} t_{i, j} \, c^\dagger_{i, \sigma} c_{j, \sigma} + \frac{U}{2} \sum_{i, \sigma} n_{i, \sigma} n_{i, -\sigma}.
$$

In this model we have neglected the Coulomb interaction between electrons except for the case where two electrons are located at the same lattice point. It thus is a model where the Coulomb potential is extremely simplified, it seems. A very non-trivial complication with the interaction term in this model, is the interesting "spin structure". This suggests an <u>antiferromagnetic</u> correlation between electrons.

The model is rather famous in condensed matter physics, and is of great interest nowadays. It was introduced in the 60's and solved exactly in one dimension in

1968 [**lieb1968**]. Originally it was introduced to describe metallic magnetism (magnetism in good conductors, such as ferromagnetism) in two and three dimensions. This is a completely unsolved problem; there doesn't really exist a theory for magnetism in iron! The model is called the Hubbard model and despite its apparent simplicity, its properties are generally not known in 2D and 3D. One exception is when $U \gg t_{ij}$, and we have only one electron per lattice point. We will look at this system later on. The model will be an antiferromagnetic insulator! But the electron band is half filled, and normal single-electron physics dictates that the model should be a good metal. This is an example of when band theory collapses.

The model is now studied intensively in two dimensions. The reason is that it is thought that the model exhibits interesting and new physics that distinguishes itself qualitatively from the physics in "normal" good metals, where the picture with a free electron gas works well. Such single-particle physics has collapsed entirely in the Hubbard model in one dimensions, as is seen with the exact solution [**anderson1987**]. Something similar can have happened in 2D.

It is easy to write down the generalisation. Look for example at

$$V_{i_1,\cdots,i_4}, \quad \text{with} \quad \begin{cases} i_1 = i_4 \\ i_2 = i_3 \end{cases}, \quad \text{where } i_1 \text{ and } i_2 \text{ are nearest neighbours.}$$

$$V_{i_1,i_2,i_2,i_1} = V, \quad i_1 \text{ and } i_2 \text{ n.n.}$$

The potential becomes

$$\frac{V}{2}\sum_{\langle i,j\rangle} n_i n_j, \qquad n_i = \sum_{\sigma} n_{i,\sigma},$$

where $\langle i,j\rangle$ is the summation over i, where j are the nearest neighbours of i. We then get:

$$\mathcal{H} = \sum_{i,j} t_{i,j}\, c^{\dagger}_{i,\sigma} c_{i,\sigma} + \frac{U}{2}\sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma} + \frac{V}{2}\sum_{\langle i,j\rangle} n_i n_j.$$

Last term: nearest neighbour electrostatic interaction.

An other type of generalisation: Two different kinds of lattice points, but still only one important orbital and thus a maximum of two fermions at each.

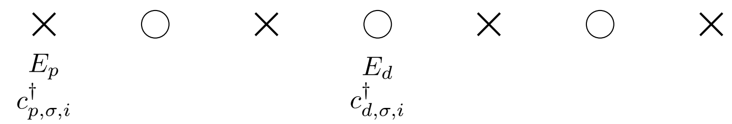


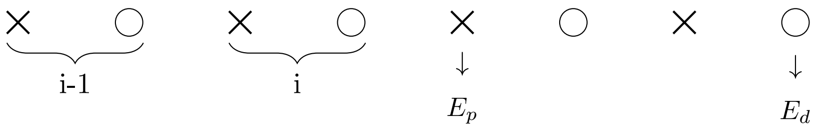
Figure 2: Lattice with two types of lattice points, where $E_p \neq E_d$ and p and d are the orbital indices [].

$$
\begin{aligned}
\mathcal{H} = \sum_{i,\sigma} E_p c^\dagger_{p,\sigma,i} c_{p,\sigma,i} + \sum_{i,\sigma} E_d c^\dagger_{d,\sigma,i} c_{d,\sigma,i} \\
+ \underbrace{U_p \sum_{i,\sigma} n_{p,i,\sigma} n_{p,i,-\sigma}}_{\text{Hubbard type}} + \underbrace{U_d \sum_{i,\sigma} n_{d,i,\sigma} n_{d,i,-\sigma}}_{\text{Hubbard type}} + \text{hopping terms.}
\end{aligned}
$$

The hopping terms can be written in the form

$$
t \sum_{i,\sigma} \left(c^\dagger_{d,i,\sigma} c_{p,i,\sigma} + c^\dagger_{d,i-1,\sigma} c_{p,i,\sigma} + \text{h.c.} \right),
$$

where i is the unit cell index.



Such models are also studied intensively nowadays, and it is now known that they have new and interesting phase transitions, even in one dimension! They contain much "more physics" than the Hubbard model [**sudbo1993**, **sandvik1996**].

3 Second quantization for bosons

We define many-particle states and creation/annihilation operators analogous to what we have done in the fermion case, with corresponding commutation relations. These relations will reflect fundamental boson properties.

Fundamental boson properties

i) Symmetric under exchange of two single-particle states.

ii) No limit on the occupation number in single-particle states.

$$|N\rangle = \prod_{\lambda} |n_\lambda\rangle\,, \qquad a^\dagger_\lambda |0\rangle = |\lambda\rangle\,, \qquad a\,|0\rangle = 0.$$

The operator $a^\dagger_\lambda$ requires a boson with the set of quantum numbers λ. Unlike the fermion case, we can now continue to operate with $a^\dagger_\lambda$ on a single-particle state, without annihilating states, as the Pauli exclusion principle doesn't apply to bosons.

$$(a^\dagger_\lambda)^n |0\rangle \propto |n_\lambda\rangle\,.$$

Normalizing the above:

$$c_n |n_2+1\rangle = a^\dagger_\lambda |n\rangle\,,$$

introducing c_n as a normalization constant. The number operator is given by

$$a^\dagger_\lambda a_\lambda |n_\lambda\rangle = n_\lambda |n_\lambda\rangle\,,$$

and the following commutation relations apply:

$$\left[a_\lambda, a^\dagger_{\lambda'}\right]_- = \delta_{\lambda,\lambda'}, \qquad \left[a_\lambda, a_{\lambda'}\right]_- = \left[a^\dagger_\lambda, a^\dagger_{\lambda'}\right]_- = 0, \qquad [A,B]_- = AB - BA.$$

Calculating the normalization constant:

$$|c_n|^2 \underbrace{\langle n_\lambda+1|n_\lambda+1\rangle}_{=1} = \langle n_\lambda|a_\lambda a^\dagger_\lambda|n_\lambda\rangle = \langle n_\lambda|1+a^\dagger_\lambda a_\lambda|n_\lambda\rangle = 1+n_\lambda,$$

which means that

$$c_n = \sqrt{1+n_\lambda} \qquad \Rightarrow \qquad \begin{cases} |n_\lambda+1\rangle = \dfrac{a^\dagger_\lambda}{\sqrt{1+n_\lambda}}\,|n_\lambda\rangle\,, \\[2ex] |n_\lambda\rangle = \dfrac{(a^\dagger_\lambda)^{n_\lambda}}{\sqrt{n_\lambda!}}\,|0\rangle\,. \end{cases},$$

and

$$|N\rangle = \prod_\lambda \frac{(a^\dagger_\lambda)^{n_\lambda}}{\sqrt{n_\lambda!}}\,|0\rangle\,.$$

Field operators

$$A^\dagger(x,t) = \sum_\lambda a_\lambda^\dagger(t)\varphi_\lambda^*(x),$$

$$\left[A(x,t), A^\dagger(x',t)\right]_- = \delta_{x,x'},$$

$$\left[A(x,t), A(x',t)\right]_- = \left[A^\dagger(x,t), A^\dagger(x',t)\right]_- = 0.$$

We will now second quantize a Hamiltonian for an interacting, material, boson system exactly as we did for fermions.

$$\mathcal{H} = \sum_{\lambda_1,\lambda_2} \langle\lambda_1|\mathcal{H}_1|\lambda_2\rangle\, a_{\lambda_1}^\dagger a_{\lambda_2} + \frac{1}{2}\sum_{\lambda_1,\cdots,\lambda_4} \langle\lambda_1,\lambda_2|V|\lambda_3,\lambda_4\rangle\, a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger a_{\lambda_3} a_{\lambda_4}.$$

Free phonon gas:

$$\mathcal{H} = \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda.$$

Note: For phonons that interact this will be a little bit different, because phonons aren't material particles. We will look at this later.

4 Lattice fermions and spin models

We return to the fermion system and look at special cases where the physics is simpler. Under such simplifying circumstances we will be able to calculate low-temperature properties of the system explicitly. In general:

$$\mathcal{H} = \sum_{\lambda_1,\lambda_2} \langle \lambda_1 | \mathcal{H}_1 | \lambda_2 \rangle \, c^\dagger_{\lambda_1} c_{\lambda_2} + \frac{1}{2} \sum_{\lambda_1,\cdots,\lambda_4} \langle \lambda_1, \lambda_2 | \mathcal{H}_2 | \lambda_3, \lambda_4 \rangle \, c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4}.$$

Lattice fermions

i) One type of fermions.

ii) Translation invariance.

iii) One orbital and at most two fermions per lattice point.

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

First look at the Hubbard model, with $i_1 = i_2 = i_3 = i_4$.

$$\mathcal{H} = \sum_{i,j,\sigma} t_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma}.$$

We will study this model now for a special, but important case:

i) $U \gg t_{i,j}$.

ii) One fermion per lattice point. Since each lattice point has a maximum of two fermions, the system is half-filled.

iii) Equally many "spin up" as "spin down".

iv) $t_{i,j} = \begin{cases} t & i,j = \text{nearest neighbours} \\ 0 & \text{otherwise} \end{cases}$

Since $U/t \gg 1$ we will look at the hopping term as a perturbation. What is the unperturbed ground state? The answer is obvious: one spin (electron) per lattice point. It doesn't matter how "up" and "down" are distributed, since different lattice points don't communicate <u>at all</u> when $t = 0$.

$$|\psi_0\rangle = \underbrace{\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\ \cdots}_{\text{random distribution of spins}}.$$

$|\psi_0\rangle$ is massively 2^N-fold spin degenerate, where N is the number of lattice points.

$$\frac{U}{2}\sum_{i,\sigma} n_{i,\sigma}n_{i,-\sigma}|\psi_0\rangle = E_0|\psi_0\rangle,$$

where $E_0 = 0$ as no lattice point is doubly occupied in $|\psi_0\rangle$. The unperturbed Hamiltonian is given by

$$\mathcal{H}_0 = \frac{U}{2}\sum_{i,\sigma} n_{i,\sigma}n_{i,-\sigma}.$$

We will now introduce the hopping term as perturbation. Note! $|\psi_0\rangle$ is degenerate, such that any combination of the 2^N degenerate eigenstates of $\mathcal{H}_0$ are eigenstates. But: From degenerate perturbation theory we know that not all linear combinations evolve similarly (see for example P.C. Hemmer's "Kvantemekanikk" [**hemmer2000**]).

Assume that we have found such linear combinations, that we from now on will call $|\psi_0\rangle$. The perturbation is given by

$$\mathcal{H}_{\text{hop}} = \sum_{\langle i,j\rangle} t c^\dagger_{i,\sigma}c_{j,\sigma}.$$

First order correction to E_0

$$\Delta E^{(1)} = \langle\psi_0|\mathcal{H}_{\text{hop}}|\psi_0\rangle = \sum_{\langle i,j\rangle,\sigma} t\langle\psi_0|c^\dagger_{i,\sigma}c_{j,\sigma}|\psi_0\rangle,$$

$$c^\dagger_{i,\sigma}c_{j,\sigma}|\psi_0\rangle \;:\; |\uparrow\uparrow\underbrace{\downarrow}_{i}\cdots\underbrace{\uparrow}_{j}\cdots\downarrow\rangle \quad\Rightarrow\quad |\uparrow\uparrow\underbrace{\downarrow\uparrow}_{i}\cdots\underbrace{}_{j}\cdots\downarrow\rangle.$$

The final state is orthogonal to $|\psi_0\rangle$:

$$\langle\psi_0|c^\dagger_{i,\sigma}c_{j,\sigma}|\psi_0\rangle = 0.$$

Second order correction to E_0

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

where

$|n\rangle$: unperturbed excited states,

E_n : excited energies of $\mathcal{H}_0$.

Those $|n\rangle$ that contribute to the sum, must then of course be chosen such that

$$\sum_{i,j,\sigma} t \langle \psi_0 | c^\dagger_{i,\sigma} c_{j,\sigma} | n \rangle \neq 0,$$

where $|n\rangle$ is a linear combination of states where the lattice point j is doubly occupied, and i is unoccupied. In that case we have $E_n = E_0 + U$:

$$\begin{aligned}\Delta E^{(2)} &= -\frac{1}{U} \sum_n \langle \psi_0 | \mathcal{H}_{\text{hop}} | n \rangle \langle n | \mathcal{H}_{\text{hop}} | \psi_0 \rangle = -\frac{1}{U} \langle \psi_0 | \mathcal{H}^2_{\text{hop}} | \psi_0 \rangle \\ &= \langle \psi_0 | \mathcal{H}_{\text{eff}} | \psi_0 \rangle ,\end{aligned}$$

which can be written as a first-order contribution from an effective Hamiltonian $\mathcal{H}_{\text{eff}} = -\mathcal{H}^2_{\text{hop}}/U$, which unlike $\mathcal{H}_{\text{hop}}$ (which is a single-particle operator) is a two-particle operator. The effective Hamiltonian is given by

$$\begin{aligned}\mathcal{H}_{\text{eff}} &= -\frac{1}{U} \sum_{i,j,\sigma} t_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma} \sum_{k,l,\sigma} t_{k,l} c^\dagger_{k,\sigma'} c_{l,\sigma'} \\ &= -\frac{1}{U} \sum_{\substack{i,j,k,l \\ \sigma,\sigma'}} t_{i,j} t_{k,l} c^\dagger_{i,\sigma} c_{j,\sigma} c^\dagger_{k,\sigma'} c_{l,\sigma'} .\end{aligned}$$

If $\mathcal{H}_{\text{eff}}$ is to give a correction to the ground state energy, we must have

$$\langle \psi_0 | \underbrace{c^\dagger_{i,\sigma} c_{j,\sigma} c^\dagger_{k,\sigma'} c_{l,\sigma'}}_{\hat{\mathcal{O}}} | \psi_0 \rangle \neq 0.$$

If we start with $|\psi_0\rangle$, the general result of $\hat{\mathcal{O}}$ will be that we end up with <u>two</u> doubly occupied, and two unoccupied states. This is orthogonal to $|\psi_0\rangle$, such that

$$\langle \psi_0 | \hat{\mathcal{O}} | \psi_0 \rangle = 0,$$

with the exception of

$$\boxed{i = l; \ j = k.}$$

This is an exchange process, without any real charge transport. In that case we will avoid any doubly-occupied final states, such that

$$\langle \psi_0 | \hat{\mathcal{O}} | \psi_0 \rangle \neq 0.$$

In that case we get:

$$\mathcal{H}_{\text{eff}} = -\frac{1}{U}\sum_{i,j,\sigma,\sigma'} t^2 c^\dagger_{i,\sigma} c_{j,\sigma} c^\dagger_{j,\sigma'} c_{i,\sigma'} = -\frac{t^2}{U}\sum_{i,j,\sigma,\sigma'} c^\dagger_{i,\sigma} c_{i,\sigma'} \underbrace{c_{j,\sigma} c^\dagger_{j,\sigma'}}_{=-c^\dagger_{j,\sigma'}c_{j,\sigma}+\delta_{\sigma,\sigma'}}$$

$$= \frac{t^2}{U}\sum_{i,j,\sigma,\sigma'} c^\dagger_{i,\sigma} c_{i,\sigma'} c^\dagger_{j,\sigma'} c_{j,\sigma} - \frac{t^2}{U}\sum_{i,j,\sigma} \underbrace{c^\dagger_{i,\sigma} c_{i,\sigma}}_{\substack{\text{Number operator. Not}\\ \text{kinetic energy because}\\ \underline{\text{same}}\text{ lattice index}\\ \text{in } c^\dagger \text{ and } c!}}.$$

This term has the same form as

$$\sum_{i,\sigma} \varepsilon c^\dagger_{i,\sigma} c_{i,\sigma},$$

which we have already disregarded, as $\varepsilon \;\to\; \varepsilon' = \varepsilon - t^2/U$, this term can be set to zero. Thus the most important term is

$$\mathcal{H}_{\text{eff}} = \frac{t^2}{u}\sum_{\langle i,j\rangle\,\sigma\sigma'} c^\dagger_{i,\sigma} c_{i,\sigma'} c^\dagger_{j,\sigma'} c_{j,\sigma}.$$

<u>Note!</u> This term is of the same form as a two particle operator as advertised, but is not of the form $n_i n_j$. This follows from the expression $c^\dagger_{i,\sigma} c_{i,\sigma'}$ where σ is not necessarily equal to σ' and thus leads to a peculiar spin flipping process. What is the physical interpretation of this two-particle operator? To explore this question we consider the effect of the operators in $\mathcal{H}_{\text{eff}}$ on spin states.
First try:

$$\begin{aligned}&\sum_{\sigma\sigma'} c^\dagger_{i,\sigma} c_{i,\sigma'} c^\dagger_{j,\sigma'} c_{j,\sigma}\\ &= \quad\uparrow\ \ \uparrow\ \ \uparrow\ \ \uparrow\\ &\quad +\downarrow\ \ \uparrow\ \ \uparrow\ \ \downarrow\\ &\quad +\uparrow\ \ \downarrow\ \ \downarrow\ \ \uparrow\\ &\quad +\downarrow\ \ \downarrow\ \ \downarrow\ \ \downarrow\end{aligned}$$

Then we choose a basis and representation

$$|\!\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad |\!\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix},$$

which is an *irreducible basis*, and thus the representations for $c^\dagger_\uparrow c_\uparrow$ etc. becomes irreducible.

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

$$\left.\begin{aligned} \begin{pmatrix}1&0\\0&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} &= \begin{pmatrix}1\\0\end{pmatrix} \\ \begin{pmatrix}1&0\\0&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} &= \mathbf{0} \end{aligned}\right\} \quad \Rightarrow \quad c_\uparrow^\dagger c_\uparrow = \begin{pmatrix}1&0\\0&0\end{pmatrix}$$

$$\left.\begin{aligned} \begin{pmatrix}0&0\\0&1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} &= \mathbf{0} \\ \begin{pmatrix}0&0\\0&1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} &= \begin{pmatrix}0\\1\end{pmatrix} \end{aligned}\right\} \quad \Rightarrow \quad c_\downarrow^\dagger c_\downarrow = \begin{pmatrix}0&0\\0&1\end{pmatrix}$$

$$\left.\begin{aligned} c_\uparrow^\dagger c_\downarrow \begin{pmatrix}1\\0\end{pmatrix} &= \mathbf{0} \\ c_\uparrow^\dagger c_\downarrow \begin{pmatrix}0\\1\end{pmatrix} &= \begin{pmatrix}1\\0\end{pmatrix} \end{aligned}\right\} \quad \Rightarrow \quad c_\uparrow^\dagger c_\downarrow = \begin{pmatrix}0&1\\0&0\end{pmatrix}$$

$$\left.\begin{aligned} c_\downarrow^\dagger c_\uparrow \begin{pmatrix}1\\0\end{pmatrix} &= \begin{pmatrix}0\\1\end{pmatrix} \\ c_\downarrow^\dagger c_\uparrow \begin{pmatrix}0\\1\end{pmatrix} &= \mathbf{0} \end{aligned}\right\} \quad \Rightarrow \quad c_\downarrow^\dagger c_\uparrow = \begin{pmatrix}0&0\\1&0\end{pmatrix}.$$

This yields a 2×2-matrix representation for all the factors in $\mathcal{H}_{\text{eff}}$. <u>Note!</u>: Since $|\boldsymbol{S}| = 1/2$ can be represented by the Pauli-matrices, this indicates that we might try to express $\mathcal{H}_{\text{eff}}$ with $|\boldsymbol{S}| = 1/2$ spin-operators. Pauli matrices:

$$\underbrace{\sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix},\ \sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix},\ \sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix}}_{\text{Irreducible representations for Pauli matrices}}$$

This choice is of course not unique but determined by the choice of representation for $|\uparrow\rangle$ and $|\downarrow\rangle$. The basis is irreducible. The set of Pauli matrices is an irreducible representation for $SU(2)$.

$$\left.\begin{aligned} c_\uparrow^\dagger c_\uparrow &= \frac{1}{2}(1+\sigma_z) \\ c_\downarrow^\dagger c_\downarrow &= \frac{1}{2}(1-\sigma_z) \\ c_\uparrow^\dagger c_\downarrow &= \frac{1}{2}(\sigma_x + i\sigma_y) = \frac{1}{2}\sigma^+ \\ c_\downarrow^\dagger c_\uparrow &= \frac{1}{2}(\sigma_x - i\sigma_y) = \frac{1}{2}\sigma^- \end{aligned}\right\}$$

<u>Note!</u> This connection is independent of the representation of the Pauli spin operators (Pauli matrices).

Inserting this we get

$$\boxed{\sum_{\sigma\sigma'} c_{i,\sigma}^\dagger c_{i,\sigma'} c_{j,\sigma'}^\dagger c_{j,\sigma} = \frac{1}{2}\left(1 + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right).}$$

This can now be regarded as an operator, independent of what representation is used.

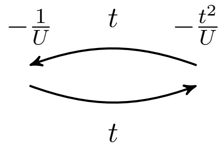
$$\boldsymbol{\sigma} = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}.$$

The first term ($\boldsymbol{T}$) is an uninteresting constant.

Thus we get in the end:

$$\mathcal{H} = \frac{2t^2}{U} \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j = -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j,$$

where we have defined $\boldsymbol{S} = 1/2\boldsymbol{\sigma}$ and $J = -2t^2/u$, i.e. an antiferromagnetic coupling. Exchange:



Thus: With one electron pr. lattice site and $U/t \gg 1$, the Hubbard model described an anti-ferromagnetic insulator! It is an insulator because the spins are "stuck" on the lattice sites and there are no free fermions in the model that can facilitate transport of charge and thus give metallic properties.

We now give a simple qualitative argument for why we get antiferromagnetism in this model when the band is half-filled.

The hopping term introduces kinetic energy in the problem. What the kinetic energy operator tries to do is to de-localize the electron as much as possible, i.e. it smooths out the wave function as much as possible. (Remember $K = -\hbar^2 \nabla^2 \psi/(2m)$, hence kinetic energy wins by reducing the curvature of ψ). What $\mathcal{H}_{\text{hop}}$ does, is it reduces the system's total energy by accessing kinetic energy by delocalize the electron such that we get virtually excited double-occupied states.

$$\begin{aligned}
\text{Start}: &\quad |\uparrow, \downarrow, \uparrow, \downarrow, \downarrow, \quad \uparrow, \ldots\rangle \\
\mathcal{H}_{\text{hop}}: &\quad |\uparrow, \downarrow, \uparrow, \downarrow, \cdot, \;\; \downarrow\uparrow, \ldots\rangle \\
\mathcal{H}_{\text{hop}}: &\quad |\uparrow, \downarrow, \uparrow, \downarrow, \downarrow, \quad \uparrow, \ldots\rangle = \text{End} = \text{Start}
\end{aligned}$$

The energy won by this virtual process is then

$$\boxed{\delta E = -\frac{t^2}{U}}$$

Note!: The spins on the exchange sites must have opposite spins to access the virtual double-occupied state and thus win energy. It is of course beneficial if all the spins in the system can contribute with $\delta E = -t^2/U$, but then the nearest neighbour spins has to be opposite $\Rightarrow$

> Antiferromagnetic correction!

We will now return to the more general fermion model and see how it behaves when the band is half-filled. We then consider the matrix-element $\langle i_1\, i_2 |\, V\, | i_3 i_4\rangle$, but now with the is <u>pairwise</u> equal. Do such terms lead to spin models? There are three possibilities

$$\left.\begin{array}{lll} i) & i_1 = i_2\ ; & i_3 = i_4 \\ ii) & i_1 = i_4\ ; & i_2 = i_3 \\ iii) & i_1 = i_3\ ; & i_2 = i_4 \end{array}\right\} \text{Two-center integral with pairwise equal lattice indexes.}$$

Remember: Hubbard $\Rightarrow$ antiferromagnetic model. Can we get a ferromagnetic model with pairwise equal indexes?

i) $i_1 = i_2\ ;\quad i_3 = i_4 \quad i_1 \neq i_3$

$$\sum_{\substack{i_1 i_3\\ \sigma_1\sigma_2}} \langle i_1\, i_1 |\, V\, | i_3\, i_3\rangle \underbrace{c^\dagger_{i_1\sigma_1} c^\dagger_{i_1\sigma_2}}_{\sigma_2 = -\sigma_1} c_{i_3\sigma_2} c_{i_3\sigma_1} = \sum_{ij\sigma} \langle i\, i |\, V\, | j\, j\rangle\, c^\dagger_{i\sigma} c^\dagger_{i-\sigma} c_{j-\sigma} c_{j\sigma}$$

This describes hopping of pairs as spin-singlet pairs from j to i.

$$\uparrow\times\downarrow \qquad\qquad \uparrow\times\downarrow$$

This does not lead to $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ since the objects that hop are spinless (total $S_z = 0$).

<u>Note</u>!: The tunnelling of pairs on the lattices is a result of the electrostatic pair-potential in the same way that one-electron tunnelling was a result of a electrostatic one-particle potential.

ii) $i_1 = i_4\ ;\quad i_2 = i_3\ ;\quad i_1 \neq i_2$

$$\begin{aligned} \sum_{\substack{i_1 i_2\\ \sigma_1\sigma_2}} \langle i_1 i_2 |\, V\, | i_2 i_1\rangle\, c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} c_{i_2\sigma_2} c_{i_1\sigma_1} &= \sum_{\substack{ij\\ \sigma\sigma'}} \langle ij |\, V\, | ji\rangle\, c^\dagger_{i\sigma} c_{i\sigma} c^\dagger_{j\sigma'} c_{j\sigma'} \\ &= \sum_{ij} \langle ij |\, V\, | ji\rangle\, n_i n_j. \end{aligned}$$

A purely electrostatic interaction between charges. No spin structure. Does <u>not</u> result in $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$.

iii) $i_1 = i_3$; $\quad i_2 = i_4$; $\quad i_1 \neq i_2$

$$\sum_{\substack{i_1 i_2 \\ \sigma_1\sigma_2}} \langle i_1 i_2 | V | i_1 i_2 \rangle c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} c_{i_1\sigma_2} c_{i_2\sigma_1} = -\sum_{\substack{ij \\ \sigma\sigma'}} \langle ij | V | ij \rangle \underbrace{c^\dagger_{i\sigma} c_{i\sigma'} c^\dagger_{j\sigma'} c_{j\sigma}}_{\substack{\text{This we have encountered before} \\ \text{and the result is:}}}$$

$$= -\sum_{ij} 2 \langle ij | V | ij \rangle \boldsymbol{S}_i \boldsymbol{S}_j .$$

Note!: So far we have not used anything about half-filling of the band. By using $i = \cdots i_4$, and $i_1, \cdots, i_4$ pairwise equal we can thus write down a general model for metals that can be magnetic:

$$\mathcal{H} = \sum_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{u}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + \sum_{ij} V_{ij} n_i n_j +$$

$$\underbrace{\sum_{ij\sigma} t^P_{ij} c^\dagger_{i\sigma} c^\dagger_{i-\sigma} c_{j-\sigma} c_{j\sigma} - \sum_{ij} \tilde{J}_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j}_{\text{Two-center integrals with pairwise equal lattice indices.}} .$$

Here i, j are not necessarily nearest neighbours! A completely general model would have included correlated hopping which also is a two-particle process. In the above equation we have defined

$$\begin{aligned} u &= \langle ii | V | ii \rangle , \\ V_{ij} &= \langle ij | V | ji \rangle \quad \text{Electrostatic,} \\ t^P_{ij} &= \langle ii | V | jj \rangle \quad \text{Tunnelling of pairs,} \\ \tilde{J}_{ij} &= 2 \langle ij | V | ij \rangle \quad \text{Spin coupling.} \end{aligned}$$

When we have 1/2 filling, the two first terms is replaced by a spin model, as we have already seen. The third term is uninteresting when there is not dynamic of the charges in the problem, as is the 4th term. In that case what remains is

$$\mathcal{H} = -\sum_{ij} \tilde{\tilde{J}}_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j ; \qquad \tilde{\tilde{J}}_{ij} = 2\left[\tilde{J}_{ij} - \frac{t^2}{u}\right] .$$

It is clear that $\tilde{\tilde{J}}_{ij}$ can give both ferro- and antiferromagnetism!

4.1 Heisenberg model

The model

$$\mathcal{H} = -\sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

is often called the *Heisenberg model*. Here $\boldsymbol{S}$ are dimensionless spin operators and J_{ij} are given by matrix elements that contains a one-particle or two-particle potential.

Even though such models has classical counterparts, we see that interaction of spins is quantum mechanical in nature. With the previously introduced spin operators we have

$$[S_x,\ S_y] = iS_z \quad \text{etc.}$$

by cyclic permutations. It is these non-trivial commutator relations that gives a quantum mechanical spin system. For a classical model the spin operators commute. Because of the non-trivial commutators we get uncertainty in the determination of the spin components. We get *quantum fluctuations.* We could also have generalized the model a bit:

$$\mathcal{H} = -\sum_{ij} \left(J^*_{ij} S^*_i S^*_j + (y) + (z) \right).$$

A possibly cause for such anisotropy could be e.g. anisotropic one-particle hopping in the Hubbard model. The Heisenberg model is solved exactly in one dimension for a general coupling when (i, j) are limited to nearest neighbours [**bethe1931**].

In two dimensions the classical model with $J^x = J^y = 0$ is solved exactly [**onsager1943**]. The two-dimensional quantum mechanical model with isotropic coupling is of great interest lately since quantum fluctuations are assumed to be large in 2D for $S = 1/2$. This can result in interesting "new" types of ground states, completely different from the "classical" ferromagnetic ground states, or antiferromagnetic Néel states, see e.g. [**chakravarty1989**] or [**chubukov1993**].

At Brookhaven National Laboratories and MIT there has recently been initiated large scale experiments to find these new and exotic magnetic ground states in low-dimensional $S = 1/2$ quantum magnets. Finally, let us remark that we started with a *fermion* model, but the effective Hamilton operator at 1/2-filled lattice (the Heisenberg model) is not a fermion model (and neither a boson model). The spin operators do not satisfy the fermion (boson) commutation relations.

4.2 Low temperature properties of magnetic insulators

Generalities

The spin operators ($S = 1/2$) have the following properties

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

where cyclic permutation of spin components applies. The ladder operators for spin:

$$S_i^{\pm} = S_{ix} \pm iS_{iy}$$

$$S_i^+ \left|\uparrow\right\rangle = 0 \ ; \qquad S_i^+ \left|\downarrow\right\rangle = \left|\uparrow\right\rangle$$

$$S_i^- \left|\uparrow\right\rangle = \left|\downarrow\right\rangle \ ; \qquad S_i^- \left|\downarrow\right\rangle = 0$$

$$\left[S_{iz}, S_j^{\pm}\right]_- = \pm\delta_{ij} S_j^{\pm}$$

$$\left[S_i^+, S_j^-\right]_- = 2\delta_{ij} S_{iz}$$

The total spin on the complete lattice is given by

$$\boldsymbol{S}_T = \sum_i \boldsymbol{S}_i, \qquad \text{where} \qquad S_{Tz} = \sum_i S_{iz}.$$

Magnetization: $\langle S_{Tz}\rangle = \sum_i \langle S_{iz}\rangle$, where $\langle\ \cdot\ \rangle$ is the statistical average.

$S_{iz},\ S_i^{\pm}$ are neither fermion or boson operators. What kind of operators are they? Consider e.g. a ferromagnetic ground state

$$|\psi_0\rangle = |\uparrow\uparrow\uparrow\ \ldots\ \uparrow\rangle\,.$$

All the spins point "upwards". This is an eigenstate of S_{iz}.

$$\underbrace{S_{iz}}_{\text{operator}}\ |\psi_0\rangle = \underbrace{S_{iz}}_{\text{number}}\ |\psi_0\rangle$$

Thus it measures the z-component of the spin on lattice site i.

$$S_i^+\,|\psi_0\rangle = 0$$

$$S_i^-\,|\psi_0\rangle = |\uparrow\uparrow\ \ldots\ \underbrace{\downarrow}_{i}\ \ldots\ \uparrow\rangle\,.$$

This is a spin flip on lattice site i. We obtain energy: $4S^2J$ i.e. the process $(\uparrow\uparrow\mapsto\uparrow\downarrow)$ $\Rightarrow\ \ \Delta E = 2JS^2$. The commutator relations for S_z and $S^{\pm}$ show that this excitation neither is a fermion, nor a boson. We shall later see that it is possible to find completely different excitations with much lower energy and that is far "smoother", i.e. they represent less dramatic changes from the ground state. Our aim is to find a description of these low energy excitations in terms of fermion or boson operators and if possible, such that there are no interactions in the theory, i.e. such that the theory is "free". As it turns out it is possible to find such a description using boson operators. It is emphasized here that this description is most useful for low energy fluctuations about the ground state of the magnet, i.e. it is only valid at low temperatures. This description also requires that the ground state is *ordered.* We first consider ferromagnetism (closes neighbour):

$$\mathcal{H} = -\sum_{ij} J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j \quad ; \quad J_{ij} > 0$$

We solve this problem by introducing the *Holstein-Primakoff* transformation for ferromagnets. The Holstein-Primakoff transformation expresses the spin-operators accurately in terms of boson operators. (bosonization of the spin problem)

H-P :

$$S_i^z = S - a_i^\dagger a_i \; ; \quad S \in \mathbb{R} \;\; (= 1/2)$$

$a^\dagger a$: Number operator that causes spin-fluctuations of the ground state at lattice site i. $a_i^\dagger a_i$ reduces the max spin component slightly. The expression for $S_i^\pm$ is a bit more complicated:

$$\begin{aligned} S_i^+ &= \sqrt{2S}\left(1 - \frac{1}{2S} a_i^\dagger a_i\right)^{(1/2)} a_i \\ S_i^- &= \sqrt{2S} a_i^\dagger \left(1 - \frac{1}{2S} a_i^\dagger a_i\right)^{(1/2)} \end{aligned}$$

Holstein and Primakoff discovered that if the boson operators a_i satisfies

$$\left[a_i, a_j^\dagger\right] = \delta_{ij}, \quad \text{etc.}$$

then $S_i^z, S_i^\pm$ satisfy the correct spin commutation relations.

Note!: The expression $(\quad)^{(1/2)}$ is meant to be interpreted as a series expansion in the boson operators.

> Exercise: Verify that the spin commutation relations are satisfied

If we now insert H-P into $\mathcal{H}$ we get an equally difficult problem. The problem is then simplified drastically by assuming that the local fluctuations in the ground state are small:

$$\begin{aligned} \langle\, a_i^\dagger a_i \,\rangle \; \ll \; S \quad &\Rightarrow \\ S_i^+ \simeq \sqrt{2S} a_i &+ \mathcal{O}(a^3) \\ S_i^- \simeq \sqrt{2S} a_i^\dagger &+ \mathcal{O}(a^3) \end{aligned}$$

This can be regarded as an expansion in large S.

$$S_i^z = S - a_i^\dagger a_i$$

$$\begin{aligned} \mathcal{H} &= -J \sum_{\langle\, i,j \,\rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) \\ &= -J \sum_{\langle\, i,j \,\rangle} \left[S_i^z S_j^z + S_i^+ S_j^-\right] \end{aligned}$$

Now we insert the approximations for the S operators and neglect all terms of order 2 or more in a $\Rightarrow$

$$\begin{aligned} \mathcal{H} &= -J \sum_{\langle\, i,j \,\rangle} \left(S^2 - S a_i^\dagger a_i - S a_j^\dagger a_j + 2S a_i a_j^\dagger\right) \\ &= E_0 + JS \sum_{\langle\, i,j \,\rangle} \left(a_i^\dagger a_i + a_j^\dagger a_j - 2 a_i a_j^\dagger\right) \end{aligned}$$

where we have defined

$$E_0 = -J \sum_{\langle\, i,j\, \rangle} S^2 = -JS^2 Nz$$

with N as the number of lattice sites and z as the number of nearest neighbours. Since we have $i \neq j$ in the sum we know $a_i a_j^\dagger = a_j^\dagger a_i$, thus we can write

$$\mathcal{H} = E_0 + 2JS \sum_{\langle\, i,j\, \rangle} \left(a_i^\dagger a_i - a_i^\dagger a_j \right)$$

We wish to write the boson term in the form of a free boson gas:

$$\sum_\lambda \omega_\lambda \qquad \underbrace{a_\lambda^\dagger a_\lambda}_{\text{Same quantum number}}$$

Here ω_λ is the excitation energy of the bosons (spin fluctuations) in the problem. We achieve such a "diagonalization" by introducing the Fourier transformed operators

$$a_{\boldsymbol{q}} = \frac{1}{\sqrt{N}} \sum_j a_j e^{i\boldsymbol{q}\cdot\boldsymbol{r}_j}, \qquad a_{\boldsymbol{q}}^\dagger = \frac{1}{\sqrt{N}} \sum_j a_j^\dagger e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_j}.$$

where $\boldsymbol{q}$ runs over the first Brillouin zone of the reciprocal lattice. Then

$$\sum_i a_i^\dagger a_i = \sum_q a_q^\dagger a_q \qquad \Rightarrow \qquad \sum_{\langle\, i,j\, \rangle} a_i^\dagger a_i = z \sum_{\boldsymbol{q}} a_q^\dagger a_q.$$

$$\sum_{\langle\, i,j\, \rangle} a_i^\dagger a_j = \frac{1}{N} \sum_{\langle\, i,j\, \rangle} \sum_{q_1 q_2} a_{q_1}^\dagger a_{q_2} e^{i(\boldsymbol{q}_2\cdot\boldsymbol{r}_j - \boldsymbol{q}_1\cdot\boldsymbol{r}_i)}.$$

If we now define $\boldsymbol{\delta}$ by

$$\boldsymbol{r}_j = \boldsymbol{r}_j + \boldsymbol{\delta}$$

then $\boldsymbol{\delta}$ is the vector from $\boldsymbol{r}_i$ to nearest neighbour and we can write

$$\begin{aligned}
\sum_i a_i^\dagger a_i &= \frac{1}{N} \sum_i \sum_{\boldsymbol{\delta}} \sum_{q_1 q_2} a_{q_1}^\dagger a_{q_2} e^{-i(\boldsymbol{q}_1 - \boldsymbol{q}_2)\cdot\boldsymbol{r}_i} e^{i\boldsymbol{q}_2\cdot\boldsymbol{\delta}} \\
&= \sum_{\boldsymbol{q}_1} \sum_{\boldsymbol{\delta}} a_{q_1}^\dagger a_{q_2}^\dagger e^{i\boldsymbol{q}_1\cdot\boldsymbol{\delta}}.
\end{aligned}$$

Inserting this into $\mathcal{H}$ we get

$$\begin{aligned}
\mathcal{H} &= E_0 + 2JS \sum_{\boldsymbol{q}} \left\{ \sum_{\boldsymbol{\delta}} \left(1 - e^{i\boldsymbol{q}\cdot\boldsymbol{\delta}} \right) \right\} a_q^\dagger a_q \\
&= E_0 + \sum_{\boldsymbol{q}} \omega_q a_q^\dagger a_q.
\end{aligned}$$

$$\omega_{\boldsymbol{q}} = 2JS \sum_{\boldsymbol{\delta}} \left(1 - e^{i\boldsymbol{q}\cdot\boldsymbol{\delta}}\right)$$

4.3 2D quadratic lattice

In the case of a 2D quadratic lattice we find

$$\omega_{\boldsymbol{q}} = 2JS\big(4 - 2\cos(q_x a) - 2\cos(q_y a)\big), \tag{9}$$

where a is the lattice constant. In the case of small $\boldsymbol{q}$ we get

$$\begin{aligned}
\omega_{\boldsymbol{q}} &\approx 2JS\left[4 - 2\left(1 - \frac{(q_x a)^2}{2}\right) - 2\left(1 - \frac{(q_y a)^2}{2}\right)\right] \\
&= 2JS\boldsymbol{q}^2 a^2, \\
\boldsymbol{q}^2 &= q_x^2 + q_y^2.
\end{aligned}$$

This behaviour is shown in figure 3. In other words: those fluctuations that we have found, have an excitation energy that depends quadratically on the wave number of the fluctuations, when they have long wavelengths. Compare

$$\omega_{\boldsymbol{q}} \approx 2JS\boldsymbol{q}^2 a^2$$

to

$$\Delta E = 4JS^2$$

for a local spin flip with

$$\omega_{\boldsymbol{q}} \ll \Delta E, \qquad |\boldsymbol{q}|a \ll 1.$$

The fluctuations we have found are spin waves, as is shown in figure 4. The operators $a_{\boldsymbol{q}}^\dagger$ and $a_{\boldsymbol{q}}$ are the creation and annihilation operators for the quantized excitations of these waves. The quantized spin waves are called magnons. These are bosons, because they are described by boson operators.

The effective low-energy Hamiltonian for the spin model,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \qquad J > 0,$$

is thus given by a free boson theory:

$$\mathcal{H} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}.$$

We have a lattice fermion model with half-filled bands in the strongly correlated case. This was found to describe a ferromagnetic insulator (we chose to look at it in the

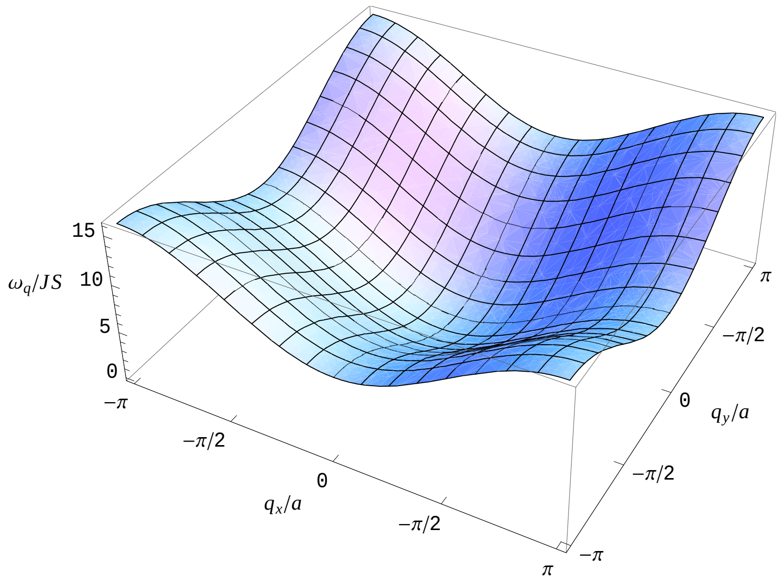


Figure 3: The angular frequency $\omega_{\boldsymbol{q}}$ as a function of the momentum $\boldsymbol{q}$ in the ferromagnetic case as decribed by equation (9).

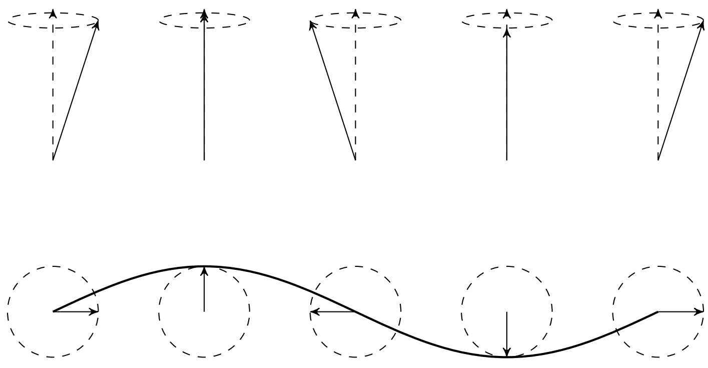


Figure 4: The spins precess slowly in space, creating spin waves.

ferromagnetic case). This gave rise to a free boson theory for ferromagnetic bosons (magnons)! For the ferromagnetic case, see the exercise.

The magnetization of ferromagnets at $T > 0$:

$$\mathcal{H} = \sum_i \left\langle S - a_i^\dagger a_i \right\rangle = NS - \sum_{\boldsymbol{q}} \left\langle a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right\rangle .$$

Using that

$$\mathcal{H} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} \left\langle a_{\boldsymbol{q}}^\dagger c_{\boldsymbol{q}} \right\rangle , \qquad \left\langle a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right\rangle = \frac{1}{e^{\beta\omega_{\boldsymbol{q}}} - 1},$$

(assuming a Bose distribution)

$$\mathcal{H} = NS - N \int \frac{d^d q}{(2\pi)^d} \frac{1}{e^{BJS\boldsymbol{q}^2} - 1}.$$

For low temperatures T, where $\beta \gg \omega_{\boldsymbol{q}}$, only small $\boldsymbol{q}$ will contribute! Performing the angular integration:

$$\mathcal{H} = NS - N\Omega_d \int dq \, \frac{q^{d-1}}{e^{\eta q^2} - 1},$$

where Ω_d is the solid angle in d dimensions and $\eta = \beta JS$. Changing variables to

$$x = \eta q^2 \qquad \Rightarrow \qquad q = \sqrt{\frac{x}{\eta}}, \quad dq = \frac{1}{2\sqrt{\eta}} \frac{dx}{\sqrt{x}},$$

this becomes

$$\begin{aligned}\mathcal{H} &= NS - N\Omega_d \frac{1}{2\sqrt{\eta}} \left(\frac{1}{\sqrt{\eta}}\right)^{d-1} \underbrace{\int_0^\infty dx \, \frac{x^{d/2-1}}{e^x - 1}}_{A(d)} \\ &= NS - N\Omega_d \, A(d) \left(\frac{T}{JS}\right)^{d/2} \\ &= NS \quad \text{for} \quad T = 0.\end{aligned}$$

The corrections to the zero temperature energy go as $T^{d/2}$, or $T^{3/2}$ for $d = 3$. The correction is because of the magnons. Note that magnons involve many spins. They are therefore collective spin excitations. Note also that $A(d)$ diverges when $d = 1$. What does that mean? And what happens when $d = 2$?

4.4 Antiferromagnets

The contribution to the Hamiltonian from spin interactions is given by

$$\mathcal{H} = -\sum_{i,j} J_{i,j} \vec{S}_i \cdot \vec{S}_j, \qquad J_{i,j} < 0.$$

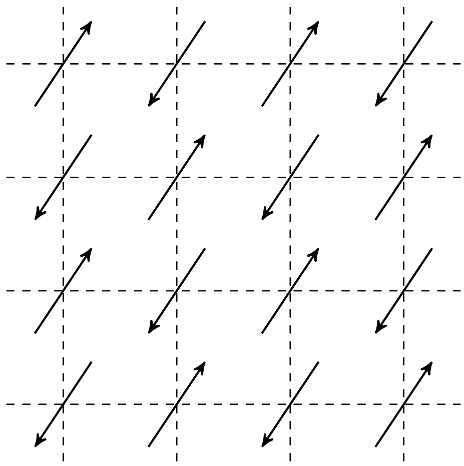
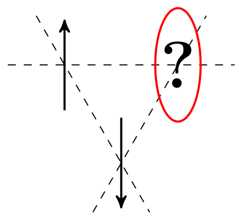


Figure 5: The Néel state, the classical spin distribution in the ground state of a 2D quadratic lattice.

The classical spin distribution in the ground state (2D quadratic lattice) is drawn in figure 5.

Nearest neighbour $J_{i,j}$ stabilises such a spin distribution. Note that next-nearest neighbour spin points in the same direction. That means that a next-nearest neighbour $J_{i,j}$ contributes to destabilise Néel states on a quadratic lattice. The spins become "frustrated". In addition, the lattice structure means a little more now than in ferromagnets. Look for example at a triangular lattice:



The conclusion is that in antiferromagnets the physics on small scales carries meaning for the physics on larger scales.

Next-nearest neighbour coupling

Next-nearest neighbour coupling can come from a "superexchange" described by

$$\left(\begin{tikzcd} 1/u \;\bullet \arrow[r, bend right, "t"'] & \underset{1/u}{\bullet} \arrow[l, bend right, "t"'] \arrow[r, bend right, "t"'] & \bullet\; 1/u \arrow[l, bend right, "t"'] \end{tikzcd} \right) \propto \frac{t^4}{u^3}.$$

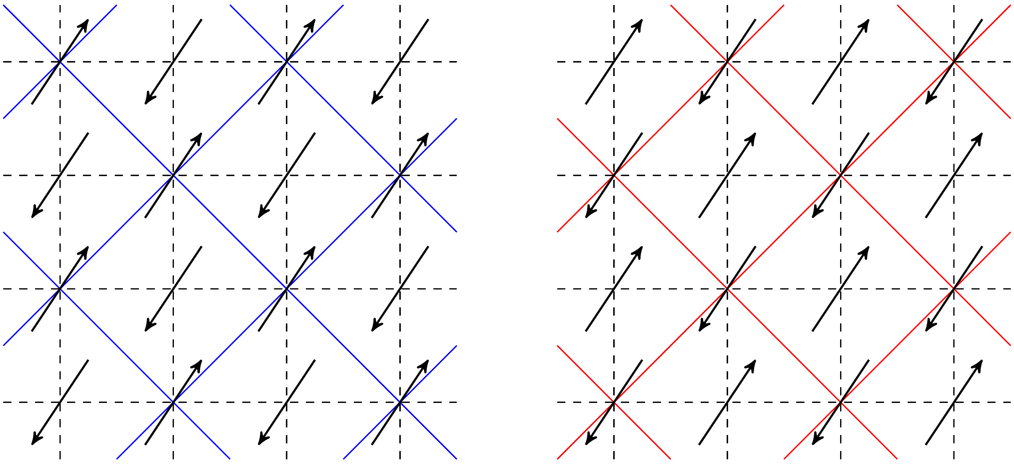


Figure 6: The Néel state with alternating spin directions can be divided into two sublattices with equal spin.

Note that
$$\frac{t^4}{u^3} = t\left(\frac{t}{u}\right)^3 \ll t\left(\frac{t}{u}\right) \quad \text{when} \quad t \ll u.$$
In the Hubbard model and also in general we therefore neglect the next-nearest neighbour coupling.

We will now look at a 2D quadratic lattice, and later generalise it to a d-dimensional hypercubic lattice. Note that the Néel state can be drawn as two sublattices with all spins pointing in the same direction, as drawn in figure 6.

One of the sublattices has all spins "up", the other has all spins "down". The quadratic lattice can therefore be divided up into two interpenetrating sublattices, A (spin up) and B (spin down). The unit cells in A and B are twice as big as those of the original lattice (the Brillouin zones in A and B are therefore half as big as those of the original lattice), as is shown in figure 7.

We now introduce the Holstein-Primakoff transformation for both sublattices.

$$A: \begin{cases} S^A_{i,z} = S - a_i^\dagger a_i, \\ S^A_{i,+} = \sqrt{2S}\left(1 - \dfrac{a_i^\dagger a_i}{2S}\right)^{1/2} a_i, \\ S^A_{i,-} = \sqrt{2S}\, a_i^\dagger \left(1 - \dfrac{a_i^\dagger a_i}{2S}\right)^{1/2}. \end{cases} \tag{10}$$

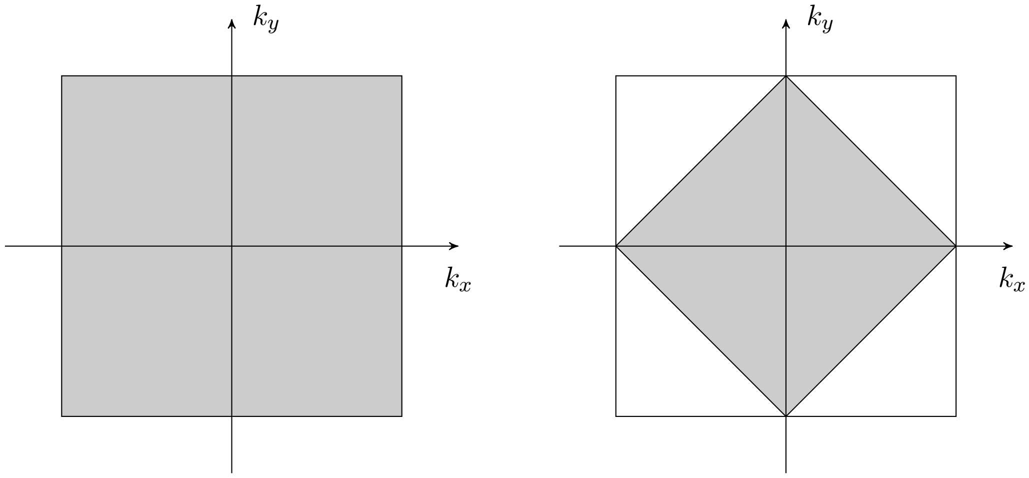


Figure 7: The Brillouin zones in the original lattice (left) and the sublattices A and B (right).

$$B : \begin{cases} S^B_{i,z} = -S + b_i^\dagger b_i, \\ S^B_{i,+} = \sqrt{2S}\left(1 - \dfrac{b_i b_i^\dagger}{2S}\right)^{1/2} b_i^\dagger, \\ S^B_{i,-} = \sqrt{2S}\, b_i \left(1 - \dfrac{b_i b_i^\dagger}{2S}\right)^{1/2}. \end{cases} \tag{11}$$

In the above the operators a_i and $a_i^\dagger$ annihilate and create bosons on A, whereas b_i and $b_i^\dagger$ annihilate and create bosons on B. On each lattice the operators have the normal boson commutation relations. Boson operators on different lattices commute. In the following we will limit ourselves to nearest-neighbour interaction, and write the Hamiltonian in terms of the sublattices.

Splitting the sum in the Hamiltonian using

$$\sum_{\langle i,j\rangle} = \sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \mathrm{n.n.}}} + \sum_{\substack{i\in\mathrm{B}\\ j\in\mathrm{A}\\ \mathrm{n.n.}}},$$

where $\langle i,j\rangle$ is the set of nearest neighbours i and j, we can write

$$\begin{aligned}\mathcal{H} &= -J\sum_{\langle i,j\rangle}\left(S_{i,z}S_{j,z}+S_{i,+}S_{j,-}\right)\\ &= -J\sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n.}}}\left(S^A_{i,z}S^B_{j,z}+S^A_{i,+}S^B_{j,-}\right)-J\sum_{\substack{i\in\mathrm{B}\\ j\in\mathrm{A}\\ \text{n.n.}}}\left(S^B_{i,z}S^A_{j,z}+S^B_{i,+}S^A_{j,-}\right).\end{aligned}$$

With this splitting we now get a certain representation of the spin operators for <u>all</u> i and j involved in the summation. If we now introduce the Holstein-Primakoff transformation for spin operators, we will again get an equally difficult problem as the antiferromagnetic Heisenberg model presented us with. For that reason we'll have a look at the low-temperature case again, where "few" bosons are excited. In that case we can make the approximation that

$$\left(1-\frac{a_i^\dagger a_i}{2S}\right)^{1/2}\approx 1,\qquad \left(1-\frac{b_i^\dagger b_i}{2S}\right)^{1/2}\approx 1.$$

With this we approximate equations (10, 10) as

$$A:\begin{cases} S^A_{i,z}=S-a_i^\dagger a_i,\\ S^A_{i,+}=\sqrt{2S}a_i,\\ S^A_{i,-}=\sqrt{2S}\,a_i^\dagger.\end{cases},\qquad B:\begin{cases} S^B_{i,z}=-S+b_i^\dagger b_i,\\ S^B_{i,+}=\sqrt{2S}b_i^\dagger,\\ S^B_{i,-}=\sqrt{2S}\,b_i.\end{cases}$$

Substitute back into $\mathcal{H}$, and neglect the terms of higher order than quadratic in a, $a^\dagger$, b and $b^\dagger$.

$$\mathcal{H}=\underbrace{2JS^2\sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n.}}}1}_{E_0}-2JS\sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n.}}}\left(\underbrace{a_i^\dagger a_i+b_j^\dagger b_j}_{\substack{\text{independent of}\\ \text{lattices A and B.}}}+\underbrace{a_i^\dagger b_j^\dagger+a_i b_j}_{\substack{\text{coupling between}\\ \text{lattices A and B.}}}\right).$$

In the $b_j^\dagger b_j$ term we use that

$$\sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n.}}}=\sum_{\substack{i\in\mathrm{B}\\ j\in\mathrm{A}\\ \text{n.n.}}}.$$

We call the numbers of lattice points in A and B N_A and N_B, with $N_\mathrm{tot}=N_\mathrm{A}+N_\mathrm{B}$. As we did for ferromagnets, we introduce

$$a_q=\frac{1}{\sqrt{N_\mathrm{A}}}\sum_{i\in\mathrm{A}}a_i\,e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i},\qquad b_q=\frac{1}{\sqrt{N_\mathrm{B}}}\sum_{j\in\mathrm{B}}b_j\,e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_j}$$

and

$$a_i = \frac{1}{\sqrt{N_\mathrm{A}}} \sum_{\boldsymbol{q}} a_{\boldsymbol{q}}\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}, \qquad b_j = \frac{1}{\sqrt{N_\mathrm{B}}} \sum_{\boldsymbol{q}} b_{\boldsymbol{q}}\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_j}.$$

<u>Note!</u> $\boldsymbol{q}$ now iterates over the Brillouin zones of A and B (see page 48). As before, we now get

$$\sum_i a_i^\dagger a_i = \sum_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}, \qquad \sum_j b_j^\dagger b_j = \sum_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}},$$

as well as

$$\left.\begin{aligned} \sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n. to } i}} a_i^\dagger b_j^\dagger &= \sum_{\boldsymbol{q}} \gamma_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}}^\dagger \\ \sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n. to } i}} a_i b_j &= \sum_{\boldsymbol{q}} \gamma_{\boldsymbol{q}} a_{\boldsymbol{q}} b_{\boldsymbol{q}} \end{aligned}\right\} \quad \gamma_{\boldsymbol{q}} = \sum_{\boldsymbol{\delta}} e^{+i\boldsymbol{q}\cdot\boldsymbol{\delta}}.$$

Introducing z as the number of nearest neighbours each lattice point has,

$$\mathcal{H} = E_0 - 2JSz \sum_{\boldsymbol{q}} \left(a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} + a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right) - 2JS \sum_{\boldsymbol{q}} \gamma_{\boldsymbol{q}} \left(a_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}}^\dagger + a_{\boldsymbol{q}} b_{\boldsymbol{q}} \right). \tag{12}$$

The two first terms have the form of a free boson gas, while the last two have a new type of form. As in assignment 2, exercise 1, we will solve this problem by introducing new boson operators:

$$\begin{aligned} A_{\boldsymbol{q}} &= u_{\boldsymbol{q}} a_{\boldsymbol{q}} + v_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger, \qquad & a_{\boldsymbol{q}} &= u_{\boldsymbol{q}} A_{\boldsymbol{q}} - v_{\boldsymbol{q}} B_{\boldsymbol{q}}^\dagger, \\ B_{\boldsymbol{q}} &= v_{\boldsymbol{q}} a_{\boldsymbol{q}} + u_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger, \qquad & b_{\boldsymbol{q}} &= u_{\boldsymbol{q}} B_{\boldsymbol{q}} - v_{\boldsymbol{q}} A_{\boldsymbol{q}}^\dagger. \end{aligned} \tag{13}$$

We demand the $A_{\boldsymbol{q}}$ and $B_{\boldsymbol{q}}$ operators to satisfy the boson commutation rules:

$$\left[A_{\boldsymbol{q}}, A_{\boldsymbol{q}'}^\dagger \right]_- = \delta_{\boldsymbol{q},\boldsymbol{q}'} \qquad \text{etc.},$$

where we take as reference point that

$$\left[a_{\boldsymbol{q}}, a_{\boldsymbol{q}'}^\dagger \right]_- = \delta_{\boldsymbol{q},\boldsymbol{q}'} \qquad \text{etc.}$$

We then get

$$\left[A_{\boldsymbol{q}}, A_{\boldsymbol{q}'}^\dagger \right]_- = \left(u_{\boldsymbol{q}} u_{\boldsymbol{q}'} - v_{\boldsymbol{q}} v_{\boldsymbol{q}'} \right) \delta_{\boldsymbol{q},\boldsymbol{q}'} = \left(u_{\boldsymbol{q}}^2 - v_{\boldsymbol{q}}^2 \right) \delta_{\boldsymbol{q},\boldsymbol{q}'} = \delta_{\boldsymbol{q},\boldsymbol{q}'}.$$

This means that

$$\boxed{u_{\boldsymbol{q}}^2 - v_{\boldsymbol{q}}^2 = 1}, \qquad \text{compare:} \qquad \cosh^2\theta - \sinh^2\theta = 1.$$

We now write

$$u_{\boldsymbol{q}} = \cosh\theta, \qquad v_{\boldsymbol{q}} = \sinh\theta.$$

Substituting this back into equation (12) and choosing θ such that

$$\tanh(2\theta) = \frac{\gamma_{\boldsymbol{q}}}{z},$$

the Hamiltonian becomes

$$\mathcal{H} = \text{ constant } + \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} \left(A_{\boldsymbol{q}}^\dagger A_{\boldsymbol{q}} + B_{\boldsymbol{q}}^\dagger B_{\boldsymbol{q}} \right).$$

(See assignment 3, exercise 2.)

$$\omega_{\boldsymbol{q}} = 4|J|S \left(d^2 - \left(\frac{\gamma_{\boldsymbol{q}}}{2} \right)^2 \right)^{1/2} = 4|J|Sd \left(1 - \tilde{\gamma}_{\boldsymbol{q}}^2 \right)^{1/2}.$$

Here d is the number of dimensions of the system. This now has the form of two free boson gases (A and B-type magnons). On a 2D quadratic lattice we have

$$\begin{aligned} &\frac{\gamma_{\boldsymbol{q}}}{2} = \cos(q_x) + \cos(q_y), \qquad \tilde{\gamma}_{\boldsymbol{q}} = \frac{1}{2} \sum_{\alpha} \cos(q_\alpha), \\ &\omega_{\boldsymbol{q}} = 4|J|S \left(4 - (\cos(q_x) + \cos(q_y))^2 \right)^{1/2}, \end{aligned} \tag{14}$$

which in the case of $q \ll 1$ means that

$$\begin{aligned} \omega_{\boldsymbol{q}} &= 4|J|S \left(4 - \left(2 - \frac{\boldsymbol{q}^2}{2} \right)^2 + \cdots \right)^{1/2} = 4|J|S \left(4 - 4 \left(1 - \frac{\boldsymbol{q}^2}{2} \right) + \cdots \right)^{1/2} \\ &= 4\sqrt{2}|J|S|\boldsymbol{q}|, \end{aligned} \tag{15}$$

which is linear in $\boldsymbol{q}$! *"Feso"/"Fero"/"Fiso"/"Firo"* goes as $\boldsymbol{q}^2$.

4.5 Magnetization on the sublattice A

The total magnetization is given by

$$\mathcal{M}_{\mathrm{A}} = \sum_{i \in \mathrm{A}} \left\langle S_i^{z,\mathrm{A}} \right\rangle = N_{\mathrm{A}} S - \sum_{i \in \mathrm{A}} \left\langle a_i^\dagger a_i \right\rangle = N_{\mathrm{A}} S - \sum_{\boldsymbol{q}} \left\langle a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right\rangle.$$

Here the expectation value of $a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}$ can be calculated using equation (13):

$$\begin{aligned} \left\langle a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right\rangle &= \left\langle \left(u_{\boldsymbol{q}} A_{\boldsymbol{q}}^\dagger - v_{\boldsymbol{q}} B_{\boldsymbol{q}}^\dagger \right) \left(u_{\boldsymbol{q}} A_{\boldsymbol{q}} - v_{\boldsymbol{q}} B_{\boldsymbol{q}}^\dagger \right) \right\rangle \\ &= u_{\boldsymbol{q}}^2 \left\langle A_{\boldsymbol{q}}^\dagger A_{\boldsymbol{q}} \right\rangle - u_{\boldsymbol{q}} v_{\boldsymbol{q}} \left\langle A_{\boldsymbol{q}}^\dagger B_{\boldsymbol{q}}^\dagger \right\rangle - u_{\boldsymbol{q}} v_{\boldsymbol{q}} \left\langle B_{\boldsymbol{q}} A_{\boldsymbol{q}} \right\rangle + v_{\boldsymbol{q}}^2 \left\langle B_{\boldsymbol{q}} B_{\boldsymbol{q}}^\dagger \right\rangle \\ &= u_{\boldsymbol{q}}^2 n_{\mathrm{B}}(\omega_{\boldsymbol{q}}) + v_{\boldsymbol{q}}^2 \left[1 + n_{\mathrm{B}}(\omega_{\boldsymbol{q}}) \right]. \end{aligned} \tag{16}$$

Here we used that

$$\left\langle A_{\boldsymbol{q}}^\dagger B_{\boldsymbol{q}}^\dagger \right\rangle = \left\langle A_{\boldsymbol{q}} B_{\boldsymbol{q}} \right\rangle = 0,$$

because $\mathcal{H}$ is diagonalized, as well as $u_{\boldsymbol{q}}^2 - v_{\boldsymbol{q}}^2 = 1$ and

$$\mathcal{H} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} \left(A_{\boldsymbol{q}}^\dagger A_{\boldsymbol{q}} + B_{\boldsymbol{q}}^\dagger B_{\boldsymbol{q}} \right).$$

We thus conclude:

$$\mathcal{M}_{\mathrm{A}} = N_{\mathrm{A}} S - \sum_{\boldsymbol{q}} v_{\boldsymbol{q}}^2 - \underbrace{\sum_{\boldsymbol{q}} \left(u_{\boldsymbol{q}}^2 + v_{\boldsymbol{q}}^2 \right) n_{\mathrm{B}}(\omega_{\boldsymbol{q}})}_{\substack{\underline{\text{Note!}} \text{ There is a} \\ \text{temperature-dependent} \\ \text{correction to } \mathcal{M}}},$$

where

$$\boxed{n_{\mathrm{B}}(\omega_{\boldsymbol{q}}) = \left\langle B_{\boldsymbol{q}}^\dagger B_{\boldsymbol{q}} \right\rangle = \left\langle A_{\boldsymbol{q}}^\dagger A_{\boldsymbol{q}} \right\rangle = \frac{1}{e^{\beta \omega_{\boldsymbol{q}}} - 1}.}$$

What will be the low-temperature form of the T-dependent correction to the magnetization? <u>Note!</u> In this case we have

$$\left\langle a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right\rangle \neq \frac{1}{e^{\beta \omega_{\boldsymbol{q}}} - 1}.$$

Instead we find, using equation (16):

$$\left\langle a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right\rangle = v_{\boldsymbol{q}}^2 + \left(u_{\boldsymbol{q}}^2 + v_{\boldsymbol{q}}^2 \right) \frac{1}{e^{\beta \omega_{\boldsymbol{q}}} - 1}.$$

This means that we can write $\mathcal{M}_{\mathrm{A}}$ as

$$\mathcal{M}_{\mathrm{A}} = N_{\mathrm{A}} S - \sum_{\boldsymbol{q}} \left[v_{\boldsymbol{q}}^2 + \left(u_{\boldsymbol{q}}^2 + v_{\boldsymbol{q}}^2 \right) \frac{1}{e^{\beta \omega_{\boldsymbol{q}}} - 1} \right].$$

(...) dependent correction (...),

$$\tanh(2\theta) = \frac{2\gamma_{\boldsymbol{q}}}{z} = \frac{2\tanh(\theta)}{1 + \tanh^2(\theta)},$$

where $z = 2d$ on a <u>cubic</u> d-dimensional lattice.

$$\tilde{\gamma}_{\boldsymbol{q}} \equiv \frac{2\gamma_{\boldsymbol{q}}}{z} = \frac{1}{d} \sum_{\alpha=1}^{d} \cos(q_\alpha),$$

or by defining

$$t \equiv \tanh(\theta), \qquad s \equiv \sinh(\theta), \qquad c \equiv \cosh(\theta),$$

$$\tilde{\gamma}_{\boldsymbol{q}} = \frac{2t}{1+t^2} \qquad \Rightarrow \qquad \tilde{\gamma}_{\boldsymbol{q}}^2 = \frac{4t^2}{(1+t^2)^2} = \frac{4s^2c^2}{(c^2+s^2)^2}.$$

Remember: $c^2 - s^2 = 1$, which means that

$$\tilde{\gamma}_{\boldsymbol{q}}^2 = 4\frac{s^2(1+s^2)}{(1+2s^2)^2}.$$

We now introduce $x \equiv s^2$ and $b \equiv \tilde{\gamma}_{\boldsymbol{q}}^2/4$:

$$b = \frac{x(1+x)}{(1+2x)^2} \qquad \xRightarrow{x>0} \qquad x = -\frac{1}{2} + \frac{1}{2}\frac{1}{\sqrt{1-4b}}.$$

This means that we find

$$\sinh^2(\theta) = v_{\boldsymbol{q}}^2 = \frac{1}{2}\left(\frac{1}{\sqrt{1-\tilde{\gamma}_{\boldsymbol{q}}^2}} - 1\right), \qquad u_{\boldsymbol{q}}^2 = 1 + v_{\boldsymbol{q}}^2 = \frac{1}{2}\left(\frac{1}{\sqrt{1-\tilde{\gamma}_{\boldsymbol{q}}^2}} + 1\right).$$

Combining these results:

$$\boxed{u_{\boldsymbol{q}}^2 + v_{\boldsymbol{q}}^2 = \frac{1}{\sqrt{1-\tilde{\gamma}_{\boldsymbol{q}}^2}}.}$$

As was shown in assignment 3,

$$\omega_q = 4|J|Sd\left(1-\tilde{\gamma}_{\boldsymbol{q}}^2\right)^2.$$

For a d-dimensional "cubic" lattice we can write

$$\tilde{\gamma}_{\boldsymbol{q}} = \frac{1}{d}\left(d - \frac{\boldsymbol{q}^2}{2} + \cdots\right) = 1 - \frac{\boldsymbol{q}^2}{2d} + \cdots,$$

$$\tilde{\gamma}_{\boldsymbol{q}}^2 \approx 1 - \frac{\boldsymbol{q}^2}{d} + \cdots,$$

$$1 - \tilde{\gamma}_{\boldsymbol{q}}^2 = \frac{\boldsymbol{q}^2}{d} + \cdots,$$

$$\frac{1}{\sqrt{1-\tilde{\gamma}_{\boldsymbol{q}}^2}} = \frac{\sqrt{d}}{|\boldsymbol{q}|} + \cdots = u_{\boldsymbol{q}}^2 + v_{\boldsymbol{q}}^2. \qquad (|\boldsymbol{q}| \ll 1.)$$

Substituting this back, we get

$$\omega_{\boldsymbol{q}} = 4|J|S\sqrt{d}|\boldsymbol{q}|$$

when $|\boldsymbol{q}| \ll 1$, which in the case of $d = 2$ is in agreement with equation (9). The temperature-dependent correction to the magnetization can now be calculated:

$$\begin{aligned} \Delta\mathcal{M}(T) &= -\sum_{\boldsymbol{q}} \left(u_{\boldsymbol{q}}^2 + v_{\boldsymbol{q}}^2\right) \frac{1}{e^{\beta\omega_{\boldsymbol{q}}} - 1} \\ &\approx -\sum_{\boldsymbol{q}} \frac{\sqrt{d}}{|\boldsymbol{q}|} \frac{1}{e^{\beta|J|\eta|\boldsymbol{q}|} - 1} \qquad \text{(Low T.)} \\ &= -\beta\Omega_d \int_0^\infty d|\boldsymbol{q}| \, \frac{|\boldsymbol{q}|^{d-2}}{e^{\beta|J|\eta|\boldsymbol{q}|} - 1}. \end{aligned} \tag{17}$$

Making a change of variables by introducing

$$x = \beta|J|\eta|\boldsymbol{q}|,$$

the integral is evaluated as

$$\Delta\mathcal{M}(T) \propto \left(\frac{1}{\beta|J|\eta}\right)^{d-2+1} \int_0^\infty dx \, \frac{x^{d-2}}{e^x - 1} \propto \left(\frac{T}{|J|}\right)^{d-1}.$$

In the case where $d = 3$ this means that

$$\Delta\mathcal{M}(T) \propto \left(\frac{T}{|J|}\right)^2 \qquad (\underline{\text{Antiferromagnetic}}).$$

Recall the ferromagnetic case, in which for $d = 3$ we got (equation reference needed)

$$\Delta\mathcal{M}(T) \propto \left(\frac{T}{|J|}\right)^{3/2}.$$

Comparing the two, we can say that

$$\Delta\mathcal{M}_{\text{AF}}(T) = \Delta\mathcal{M}_{\text{Ferro}}(T) \cdot \left(\frac{T}{|J|}\right)^{1/2} \ll \Delta\mathcal{M}_{\text{Ferro}}(T). \qquad (T/J \ll 1.)$$

The corrections to $\mathcal{M}$ due to temperature effects are weaker in antiferromagnets than in ferromagnets. This can be seen from the magnon spectrum (compare figures 3 and 8). It is easier to thermically excite ferromagnetic magnons than antiferromagnetic ones. We thus find a bigger temperature correction for the magnetization in a ferromagnet than in an antiferromagnet.

But! Note that ferromagnets don't have quantum fluctuations, while antiferromagnets do.

There are fluctuations even at zero temperature:

$$\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}^2 = \frac{1}{2} \sum_{\boldsymbol{q}} \left(\frac{1}{\sqrt{1 - \tilde{\gamma}_{\boldsymbol{q}}^2}} - 1 \right) = \frac{\sqrt{d}}{2} \sum_{\boldsymbol{q}} \frac{1}{|\boldsymbol{q}|} - \left(\frac{N_{\text{A}}}{2}\right),$$

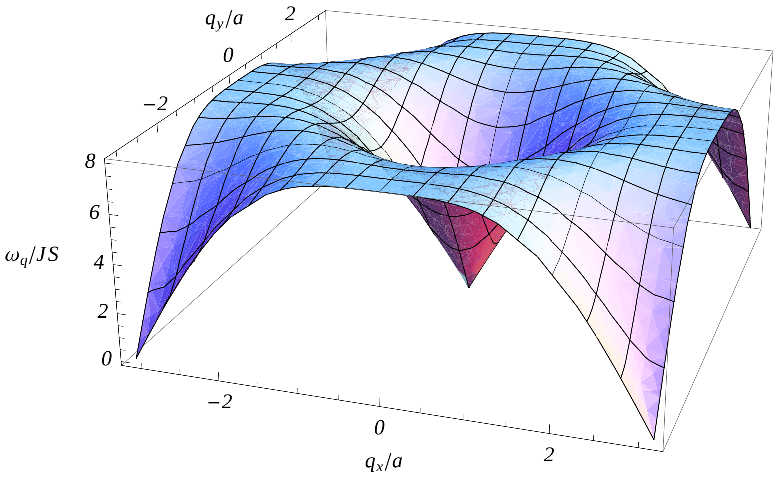


Figure 8: The angular frequency $\omega_{\boldsymbol{q}}$ as a function of the momentum $\boldsymbol{q}$ for the antiferromagnetic case described by equation (15).

which for $T = 0$ gives

$$\mathcal{M}_{\mathrm{A}} = N_{\mathrm{A}}\left(S + \frac{1}{2}\right) - \sum_{\boldsymbol{q}} \frac{\sqrt{d}}{2}\frac{1}{|\boldsymbol{q}|}.$$

For large $|\boldsymbol{q}|$ (Brillouin zone) no problem with integers. For small $|\boldsymbol{q}|$ the integral in equation (17) becomes

$$\Omega_d \int dq\, q^{d-2},$$

which for $d = 2$ is ok for small $|\boldsymbol{q}|$, but for $d = 1$ we get

$$\int_{1/L}^{1} dq\, \frac{1}{q} \propto \ln L,$$

a divergent function with weak divergence when $L \to \infty$. For $T = 0$ the quantum fluctuations are large when $d = 1$.

As can be seen from figure 6 the corners of the Brillouin zone are not involved. This is why only small $|\boldsymbol{q}|$ contribute.

4.6 Quantization of lattice vibrations: phonons

First look at a 1D lattice model (only look at the ion vibrations). The Hamiltonian for such a lattice system has the classical form

$$\mathcal{H} = \sum_i \sum \boldsymbol{P}_i^2 2M + \sum_{n=1}^{N} \sum_{m=1}^{\#\text{ neighbours}} V(R_n - R_{n+m}).$$

Here $V(x)$ is a microscopic pair potential that works between the ions. This is not limited to nearest-neighbour interaction. We can write

$$R_n = R_n^0 + x_n,$$

with R_n for the equilibrium position of lattice point n and x_n for the small deviation from it. For small fluctuations around the equilibrium position, the lattice will exhibit <u>harmonic</u> oscillations.

Taylor expanding $V(R_n - R_{n+m})$ to second order, we find

$$\sum_{n,m} V(R_n - R_{n+m}) = \underbrace{\sum_{n,m} V(R_n^0 - R_{n+m}^0)}_{\text{constant}} + \underbrace{\sum_{n,m} \left.\frac{\partial V}{\partial x}\right|_{x=R_n^0 - R_{n+m}^0} (x_n - x_{n+m})}_{=0 \text{ since we expand around a minimum}}$$

$$+ \frac{1}{2} \sum_{n,m} \left.\frac{\partial^2 V}{\partial x^2}\right|_{x=R_n^0 - R_{n+m}^0} (x_n - x_{n+m})^2 + \cdots$$

Defining now

$$\Phi(R_n^0 - R_{n+m}^0) \equiv \left.\frac{\partial^2 V}{\partial x^2}\right|_{x=R_n^0 - R_{n+m}^0} > 0,$$

the significant term becomes

$$\frac{1}{2} \sum_{n,m} \Phi(R_n^0 - R_{n+m}^0)(x_n^2 + x_{n+m}^2 - 2x_n x_{n+m}).$$

Since

$$\Phi(R_n^0 - R_{n+m}^0) = \Phi(R_m^0)$$

and

$$\left.\begin{aligned} R_n^0 &= an \\ R_{n+m} &= a(n+m) \end{aligned}\right\} \quad \Rightarrow \quad R_n^0 - R_{n+m}^0 = -R_m^0,$$

we find

$$\Phi(x) = \Phi(-x),$$

with which we get

$$\sum_{n,m} V(R_n^0 - R_{n+m}^0) = \frac{1}{2} \sum_m \Phi(R_m^0) \sum_n \left(x_n^2 + x_{n+m}^2 - 2x_n x_{n+m}\right).$$

We wish to write this in the form of harmonic oscillations, to which end we introduce new variables that "decouple" the potential term. This will be done, as we did in assignment 2, exercise 1, with Fourier-transformed variables:

$$x_n = \frac{1}{\sqrt{N}} \sum_k \tilde{x}_k \, e^{ikn}, \qquad \tilde{x}_k = \frac{1}{\sqrt{N}} \sum_n x_n \, e^{-ikn}.$$

With this we get:

$$\sum_n x_n x_{n+m} = \sum_k \tilde{x}_k \tilde{x}_{-k}\, e^{-ikn},$$

which means that the potential term becomes

$$\sum_{n,m} V(R_n - R_{n+m}) = \sum_k \underbrace{\left(\sum_{m \in \text{neighbours}} \Phi(R_m^0)\, [1 - \cos(km)] \right)}_{\equiv \frac{1}{2}\omega_k^2 M} \tilde{x}_k \tilde{x}_{-k}.$$

We can also Fourier transform the momentum:

$$p_n = \frac{1}{\sqrt{N}} \sum_k \tilde{p}_k\, e^{-ikn},$$

$$\tilde{p}_k = \frac{1}{\sqrt{N}} \sum_n p_n\, e^{ikn},$$

$$\sum_n \frac{p_n^2}{2M} = \sum_k \frac{\tilde{p}_k \tilde{p}_{-k}}{2M}.$$

The Hamiltonian for a one-dimensional lattice, in the harmonic approximation, then becomes:

$$\boxed{\mathcal{H} = \sum_k \left(\frac{\tilde{p}_k \tilde{p}_{-k}}{2M} + \frac{M\omega_k^2}{2}\, \tilde{x}_k \tilde{x}_{-k} \right).}$$

This is the standard form of a harmonic oscillator, the sum of 1D harmonic, <u>independent</u> oscillators. We will second quantize this by introducing creation and annihilation operators exactly as for a single 1D harmonic oscillator, for each k value.

$$\tilde{x}_k = \sqrt{\frac{\hbar}{2m\omega_k}} \left(a_{-k}^\dagger + a_k \right)$$

$$\tilde{p}_k = i\sqrt{\frac{m\omega_k \hbar}{2}} \left(a_k^\dagger - a_{-k} \right),$$

$$\left[a_k, a_{k'}^\dagger \right]_- = \delta_{k,k'},$$

$$[\tilde{x}_k, \tilde{p}_{k'}]_- = i\hbar\delta_{k,k'},$$

$$[x_n, p_{n'}]_- = i\hbar\delta_{n,n'}.$$

Substituting back into the Hamiltonian,

$$\boxed{\mathcal{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right),}$$

as one would have guessed. The last term is a "zero point" energy, which we will drop hereafter. The (harmonic) lattice vibrations will we quantized to a free boson gas. The quantized excitations of the sound field are called phonons, and have creation/annihilation operators $a_k^\dagger$, a_k. This is entirely analogous to the quantized excitations of spin waves, which we called magnons.

4.7 Non-harmonics

The series expansion of

$$\sum_{n,m} V(R_n - R_{n+m})$$

to higher order than quadratic gives non-harmonic fluctuations. We will look at the third order term, which gives the first corrections to the ideal boson gas picture.

$$\frac{1}{3!} \sum_{n,m} \underbrace{\left. \frac{\partial^3 V}{\partial x^3} \right|_{x=R_n^0 - R_{n+m}^0}}_{\Gamma(R_n^0 - R_{n+m}^0) = \Gamma(R_{m^0}} (x_n - x_{n+m})^3 = \frac{1}{6} \sum_m \Gamma(R_m^0) \sum_n (x_n - x_{n+m})^3.$$

We again introduce the Fourier modes to the fluctuations:

$$\begin{aligned}
\sum_n x_n^3 &= \sum_n \left(\frac{1}{\sqrt{N}} \sum_{k_1} \tilde{x}_{k_1} \, e^{ik_1 n} \right) \left(\frac{1}{\sqrt{N}} \sum_{k_2} \tilde{x}_{k_2} \, e^{ik_2 n} \right) \left(\frac{1}{\sqrt{N}} \sum_{k_3} \tilde{x}_{k_3} \, e^{ik_3 n} \right) \\
&= \frac{1}{\sqrt{N}} \sum_{k_{1,2,3}} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{k_3} \underbrace{\frac{1}{N} \sum_n e^{i(k_1+k_2+k_3)n}}_{\delta_{k_1-k_2-k_3}} \\
&= \boxed{\frac{1}{\sqrt{N}} \sum_{k_1,k_2} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2}}
\end{aligned}$$

while

$$\sum_n x_n^2 x_{n+m} = \frac{1}{\sqrt{N}} \sum_{k_1,k_2} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2} e^{ik_1 m},$$

and by introducing $n' = n + m$ then

$$\begin{aligned}\sum_n x_n x_{n+m}^2 =& \sum_{n'} x_{n'}^2 x_{n'-m} \\ =& \frac{1}{\sqrt{N}} \sum_{k_1,k_2} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2} e^{-ik_1 m}.\end{aligned}$$

Now the non-harmonic third order term is

$$\frac{1}{6} \sum_m \Gamma(-R_m^0) \sum_n (x_n - x_{n+m})^3$$

$$\begin{aligned}&= \frac{1}{6} \sum_m \Gamma(-R_m^0) \sum_n (x_n^3 - x_{n+m}^3 - 3x_n^2 x_{n+m} + 3x_n x_{n+m}^2) \\ &= \frac{1}{6} \sum_m \left(-\Gamma(-R_m^0)\right) \sum_{k_1,k_2} \frac{1}{\sqrt{N}} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2} \left(e^{ik_1 m} - e^{-ik_1 m}\right) \\ &= \sum_{k_1,k_2} M(k_1) \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2},\end{aligned}$$

where

$$M(k_1) = \frac{-i}{3} \frac{1}{\sqrt{N}} \sum_m \Gamma(-R_m^0) \sin(k_1 m).$$

The non-harmonic third order term can further be written

$$\sum_{k_1,k_2} M(k_1) \left(\frac{\hbar}{2M}\right)^{\frac{3}{2}} \frac{1}{\sqrt{\omega_{k_1} \omega_{k_2} \omega_{k_1+k_2}}} \left(a_{-k_1}^\dagger + a_{k_1}\right) \left(a_{-k_2}^\dagger + a_{k_2}\right) \left(a_{-k_3}^\dagger + a_{k_3}\right)$$

$$\begin{aligned}= \sum_{k_1,k_2} G(k_1,k_2) \Big(& a_{-k_1}^\dagger a_{-k_2}^\dagger a_{-q}^\dagger + a_{-k_1}^\dagger a_{-k_2}^\dagger a_q^\dagger + a_{-k_1}^\dagger a_{k_2} a_{-q}^\dagger + a_{-k_1}^\dagger a_{k_2}^\dagger a_q \\ &+ a_{k_1} a_{-k_2}^\dagger a_{-q}^\dagger + a_{k_1} a_{-k_2}^\dagger a_q + a_{k_1} a_{k_2} a_{-q}^\dagger + a_{k_1} a_{k_2} a_q \Big)\end{aligned}$$

It is possible to do similar calculations for even higher order non-harmonic terms. We notice that the number of phonons are not conserved in the scattering process resulting from the non-harmonic term. However; momentum is always conserved in all scattering processes! Non-harmonic effects are most important in crystals with small atom masses, M, and large lattice constants.

We can generalize our method by looking at two- or three-dimensional lattices and introduce more than one mode, labelled by an index λ. For the *harmonic* case we get

$$\mathcal{H} = \sum_{\boldsymbol{q},\lambda} \hbar \omega_{\boldsymbol{q},\lambda} a_{\boldsymbol{q},\lambda}^\dagger a_{\boldsymbol{q},\lambda}.$$

Now the oscillations are described by vectors:

$$\boldsymbol{x}_{\boldsymbol{q},\lambda} = \sqrt{\frac{\hbar}{2M\omega_{\boldsymbol{q},\lambda}}}\boldsymbol{\xi}_{\boldsymbol{q},\lambda}\left(a^{\dagger}_{-\boldsymbol{q},\lambda} + a_{\boldsymbol{q},\lambda}\right),$$

$$\boldsymbol{p}_{\boldsymbol{q},\lambda} = i\sqrt{\frac{\hbar M\omega_{\boldsymbol{q},\lambda}}{2}}\boldsymbol{\xi}_{\boldsymbol{q},\lambda}\left(a^{\dagger}_{\boldsymbol{q},\lambda} - a_{-\boldsymbol{q},\lambda}\right),$$

where $\boldsymbol{\xi}_{\boldsymbol{q},\lambda}$ is the excitation direction for mode λ with wave vector $\boldsymbol{q}$.

4.8 Electron-phonon coupling

Up to now we have looked at the second quantized form of the electron gas and lattice vibrations. We now want to couple these degrees of freedom.

$$\mathcal{H}_{\text{phonon}} = \sum_{\boldsymbol{q},\lambda} \omega_{\boldsymbol{q},\lambda} a^{\dagger}_{\boldsymbol{q},\lambda} a_{\boldsymbol{q},\lambda},$$

$$\mathcal{H}_{\text{electron}} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \frac{1}{2}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\sigma,\sigma'} V(\boldsymbol{q}) c^{\dagger}_{\boldsymbol{k},\sigma} c^{\dagger}_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k}'+\boldsymbol{q},\sigma'} c_{\boldsymbol{k}-\boldsymbol{q},\sigma}$$

Here we have used the plane wave representation for electrons, which is suitable for good metals. Earlier we looked at the second-quantized form of the one-particle operator

$$H_{\text{el}-\text{ion}} = \sum_i U(\boldsymbol{r}_i) = \sum_{i,j} V_{\text{el}-\text{ion}}\left(\boldsymbol{r}_i; \boldsymbol{R}_j\right)$$

Previously we ignored the dynamics of the ion lattice when we second-quantized this term. When lattice excitations are included in $H_{\text{el}-\text{ion}}$, this results in electron-phonon coupling.

$$V_{\text{el}-\text{ion}}\left(\boldsymbol{r}_i; \boldsymbol{R}_j\right) = V_{\text{el}-\text{ion}}\left(\boldsymbol{r}_i - \boldsymbol{R}_j\right)$$

The equilibrium postion for lattice points are given by $\boldsymbol{R}^0_j$, such that

$$\boldsymbol{R}_j = \boldsymbol{R}^0_j - \sum_{\lambda} \boldsymbol{x}_{j,\lambda}.$$

The minus sign is just a convention which gives less minus signs in the calculations. We now write $V_{\text{el}-\text{ion}}$ in a Taylor series in terms of small lattice excitations.We only use the lowest order term which has a non-zero contribution, and this is expected to be a good approximation for *weak electron-phonon coupling*. The series is

$$V_{\text{el}-\text{ion}}(\boldsymbol{r}_i - \boldsymbol{R}_j) = V_{\text{el}-\text{ion}}(\boldsymbol{r}_i - \boldsymbol{R}^0_j) + \sum_{\lambda} \boldsymbol{x}_{j,\lambda} \cdot \nabla V_{\text{el}-\text{ion}}\Big|_{\boldsymbol{r}_i - \boldsymbol{R}^0_j} + ...$$

We have already looked at the first term, which results in

$$\mathcal{H}^{(1)}_{\text{el}-\text{ion}} = \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \tilde{U}(\boldsymbol{q}) c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma}$$

where $\tilde{U}(\boldsymbol{q})$ is the Fourier transform of $U(\boldsymbol{r}) = \sum_j V_{\text{el-ion}}\left(\boldsymbol{r} - \boldsymbol{R}_j^0\right)$. This is the contribution from the *static* ion lattice. We now look at

$$\sum_{i,j,\lambda} \boldsymbol{x}_{j,\lambda} \cdot \nabla V_{\text{el-ion}}(\boldsymbol{r}_i - \boldsymbol{R}_j^0),$$

and by introducing

$$V_{\text{el-ion}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{q}} \tilde{V}_{\text{e-i}}(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}},$$

then

$$\nabla V_{\text{el-ion}} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{q}} i\boldsymbol{q}\tilde{V}_{\text{e-i}}(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}}.$$

We want to find the second-quantized form of the second term

$$\begin{aligned}
H^{(2)}_{\text{el-ion}} =& \frac{1}{\sqrt{N}} \sum_{i,j,\lambda} \boldsymbol{x}_{j,\lambda} \cdot \sum_{\boldsymbol{q}} i\boldsymbol{q}\tilde{V}_{\text{e-i}}(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{R}_j^0)} \\
=& \sum_i \sum_{\boldsymbol{q},\lambda} \left(\frac{1}{\sqrt{N}} \sum_j \boldsymbol{x}_{j,\lambda} e^{-i\boldsymbol{q}\cdot\boldsymbol{R}_j^0} \right) i\boldsymbol{q}\tilde{V}_{\text{e-i}}(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i} \\
=& \sum_i \sum_{\boldsymbol{q},\lambda} \tilde{\boldsymbol{x}}_{\boldsymbol{q},\lambda} \cdot i\boldsymbol{q}\tilde{V}_{\text{e-i}}(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i} \\
\equiv& \sum_i F(\boldsymbol{r}_i),
\end{aligned}$$

where

$$F(\boldsymbol{r}_i) = \sum_q \tilde{F}(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}$$

and

$$\tilde{F}(\boldsymbol{q}) = \sum_\lambda \boldsymbol{x}_{\boldsymbol{q},\lambda} \cdot i\boldsymbol{q}\tilde{V}_{\text{e-i}}(\boldsymbol{q}).$$

When $H^{(2)}_{\text{el-ion}} = \sum_i F(\boldsymbol{r}_i)$, we know that the second-quantized form in the plane wave basis is

$$\mathcal{H}^{(2)}_{\text{el-ion}} = \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \tilde{F}(\boldsymbol{q}) c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma},$$

since $F(\boldsymbol{r})$ is independent of spin. We now introduce the quantized phonon-gas:

$$\boldsymbol{x}_{\boldsymbol{q},\lambda} = \sqrt{\frac{\hbar}{2M\omega_{\boldsymbol{q},\lambda}}} \boldsymbol{\xi}_{\boldsymbol{q},\lambda} \left(a^\dagger_{-\boldsymbol{q},\lambda} + a_{\boldsymbol{q},\lambda} \right),$$

such that

$$\tilde{F}(\boldsymbol{q}) = \sum_\lambda M_{\boldsymbol{q},\lambda} \left(a^\dagger_{-\boldsymbol{q},\lambda} + a_{\boldsymbol{q},\lambda} \right),$$

where

$$\boxed{M_{\boldsymbol{q},\lambda} = i\left(\boldsymbol{q}\cdot\boldsymbol{\xi}_{\boldsymbol{q},\lambda}\right)\sqrt{\frac{\hbar}{2M\omega_{\boldsymbol{q},\lambda}}}\tilde{V}_{\mathrm{e-i}}(\boldsymbol{q})}$$

Finally,

$$\begin{aligned}\mathcal{H}_{\mathrm{el-ion}} =& \mathcal{H}_{\mathrm{el-phonon}}\\ =& \sum_{\boldsymbol{k},\boldsymbol{q},\sigma,\lambda} M_{\boldsymbol{q},\lambda}\left(a^\dagger_{-\boldsymbol{q},\lambda} + a_{\boldsymbol{q},\lambda}\right) c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma}.\end{aligned}$$

The quantity $M_{\boldsymbol{q},\lambda}$ is the coupling constant between electrons and phonons. One important feature is that $M_{\boldsymbol{q},\lambda} \propto \boldsymbol{q}$, which means that

$$\boxed{\boldsymbol{q} \to 0, \Rightarrow M_{\boldsymbol{q},\lambda} \to 0.}$$

The case of $\boldsymbol{q} = 0$ is equivalent with that the whole lattice is translated uniformly, which does not affect the electrons due to Galilean invariance. Another important fact is that the coupling $M_{\boldsymbol{q},\lambda}$ is independent of both $\boldsymbol{k}$ and σ. The σ-independence comes naturally since the lattice potential is spin independent. The coupling is independent of k <u>only because we use the plane wave basis</u>. Also, $M_{\boldsymbol{q},\lambda} \propto 1/\sqrt{M}$, such that the coupling is weaker for heavy ions.

5 Many-particle perturbation theory

5.1 Zero temperature

Let us assume we can describe a system with a known Hamilton operator, for example

$$\mathcal{H}_0^{\mathrm{F}} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}, \qquad \text{(fermions)}$$

$$\mathcal{H}_0^{\mathrm{B}} = \sum_{\boldsymbol{q},\lambda} \omega_{\boldsymbol{q},\lambda} a^\dagger_{\boldsymbol{q},\lambda} a_{\boldsymbol{q},\lambda}, \qquad \text{(bosons)}$$

and we want a description of the *quantized* changes which happen as a result of perturbations of $\mathcal{H}_0$, i.e. $\mathcal{H}_0 \to \mathcal{H}_0 + V$. Usually, the perturbated Hamiltonian can not be diagonalized exactly. Examples of perturbations are:

i) Electron-phonon coupling:

$$V = \sum_{\boldsymbol{k},\boldsymbol{q},\sigma,\lambda} M_{\boldsymbol{q},\lambda}(a^\dagger_{-\boldsymbol{q},\lambda} + a_{\boldsymbol{q},\lambda}) c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma}$$

ii) Electron-electron interaction:

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

iii) The U-term in the Hubbard model.

5.2 Time-evolution of states

Hamilton-operator

$$\mathcal{H} = \mathcal{H}_0 + V.$$

$\mathcal{H}_0$: One-particle operator. V: Perturbation, such that we can not solve the problem exact.

Schrödinger picture

Operators are independent of time: $\hat{\mathcal{O}}(t) = \hat{\mathcal{O}}(0)$.
States are time-dependent:

$$i\frac{\partial}{\partial t}|\psi\rangle = \mathcal{H}|\psi\rangle$$

Formally:

$$|\psi(t)\rangle = e^{-i\mathcal{H}t}|\psi(0)\rangle$$

$e^{-i\mathcal{H}t}$: Evolution operator which takes the system from the state $|\psi(0)\rangle$ at time $t = 0$ to the state $|\psi(t)\rangle$ at time t.

Heisenberg picture

States are time-independent: $|\psi(t)\rangle = |\psi(0)\rangle$.
Operators are time-dependent:

$$\frac{d\hat{\mathcal{O}}}{dt} = -i\left[\hat{\mathcal{O}}, \mathcal{H}\right]$$

Formally:

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

Schrödinger:

$$\left\langle \psi(t) \middle| \hat{\mathcal{O}}(0) \middle| \psi(t) \right\rangle = \left\langle \psi(0) \middle| e^{i\mathcal{H}t}\hat{\mathcal{O}}(0)e^{-i\mathcal{H}t} \middle| \psi(0) \right\rangle.$$

Heisenberg:

$$\left\langle psi(0) \middle| \hat{\mathcal{O}}(t) \middle| \psi(0) \right\rangle = \left\langle \psi(0) \middle| e^{i\mathcal{H}t}\hat{\mathcal{O}}(0)e^{-i\mathcal{H}t} \middle| \psi(0) \right\rangle$$

We get the same matrix elements in both pictures!

There is a third picture, which is used in perturbation theory:

Interaction picture

Some time dependence in *both* the states and the operators.

$$|\psi(t)\rangle = e^{i\mathcal{H}_0 t}e^{-i\mathcal{H}t}|\psi(0)\rangle,$$

$$\hat{\mathcal{O}}(t) = e^{i\mathcal{H}_0 t}\hat{\mathcal{O}}(0)e^{-i\mathcal{H}_0 t}.$$

<u>NB:</u> In general, $[\mathcal{H}_0, V] \neq 0$, such that $e^{i\mathcal{H}_0 t}e^{-i\mathcal{H}t}$ is much more complicated than e^{-iVt}!

For $V = 0$ the interaction picture coincides with the Heisenberg picture. Since we assume that the components of V is much smaller than the components of $\mathcal{H}_0$ for the perturbation theory to work, it follows that most of the time development lies in the operators, while the states has a slow time-variation.

<u>**Evolution operator for a state $|\psi(t)\rangle$ in the interaction picture:**</u>

$$\begin{aligned} |\psi(t)\rangle &= U(t)|\psi(0)\rangle, \\ U(t) &= e^{i\mathcal{H}_0 t}e^{-i\mathcal{H}t} \neq e^{i(\mathcal{H}_0 - \mathcal{H}_0 - V)t} \quad (!!) \end{aligned}$$

$\boxed{V = 0 : U(t) = .\, [\mathcal{H}_0, \mathcal{H}_0] = .e^{i\mathcal{H}_0 t}e^{-i\mathcal{H}_0 t} = 1.}$

$U(t)$ have a non-trivial time-dependence only when $V \neq 0$, and we want to find U as a functional of V. (A functional is a number which depends on a function, i.e. a mapping from a space of functions onto the complex numbers.) We find $U(t)$ from $V(t)$ like this:

$$\begin{aligned} \frac{\partial U}{\partial t} &= \frac{\partial}{\partial t}\left(e^{i\mathcal{H}_0 t}e^{-i\mathcal{H}t}\right) \\ &= i\mathcal{H}_0 e^{i\mathcal{H}_0 t}e^{-i\mathcal{H}t} - e^{i\mathcal{H}_0 t}i\mathcal{H}e^{-i\mathcal{H}t} \\ &= ie^{i\mathcal{H}_0 t}\left(\mathcal{H}_0 - \mathcal{H}\right)e^{-i\mathcal{H}t} \\ &= ie^{i\mathcal{H}_0 t}Ve^{-i\mathcal{H}t} \\ &= -\, i\,\underbrace{e^{i\mathcal{H}_0 t}Ve^{-i\mathcal{H}_0 t}}_{\hat{V}(t)}\underbrace{e^{i\mathcal{H}_0 t}e^{-i\mathcal{H}t}}_{U(t)} \\ &= -\, i\hat{V}(t)U(t). \end{aligned}$$

$\hat{V}(t)$ explisitly time-dependent, such that $U(t) \neq e^{-i\hat{V}t}U(0)$. When $V = 0$ then $\partial U/\partial t = 0$, such that $U(t) = U(0) = 1$. We integrate over t:

$$\begin{aligned} \int_0^t dt' \frac{\partial U(t')}{\partial t'} &= U(t) - U(0) \\ &= -i\int_0^t dt' \hat{V}(t')U(t'), \end{aligned} \tag{18}$$

such that

$$\boxed{U(t) = 1 - i\int_0^t dt'\hat{V}(t')U(t')}$$

This is a (linear) integral equation for $U(t)$. We want to solve this by iteration, but first we introduce a more general evolution operator.

The S-matrix

The scattering matrix, S, is the central quantity in many-particle perturbation theory. With a perturbation theory for S then we will almost automatically have a method to write a perturbation series for **any physical quantity**. The S-matrix is defined as:

$$|\psi(t)\rangle = S(t,t')|\psi(t')\rangle,$$

such that $S(t,0) = U(t)$, by recalling that $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. The state can be written as

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

such that

$$U(t) = S(t,t')U(t'),$$

or in other words

$$S(t,t') = U(t)U^{-1}(t').$$

We utilize the unitarity of U, which we find from

$$U^{-1}(t) = e^{i\mathcal{H}t}e^{-i\mathcal{H}_0 t} = U^\dagger(t),$$

such that the scattering matrix is written as

$$\boxed{S(t,t') = U(t)U^\dagger(t').}$$

We want to find an integral equation for S:

$$\begin{aligned}\frac{\partial S(t,t')}{\partial t} &= \frac{\partial U(t)}{\partial t}U^\dagger(t') \\ &= -i\hat{V}(t)U(t)U^\dagger(t') \\ &= -i\hat{V}(t)S(t,t').\end{aligned}$$

We integrate over time:

$$\begin{aligned}\int_{\tilde{t}}^t \frac{\partial S(t'',t')}{\partial t''} =& S(t,t') - S(\tilde{t},t') \\ =& -i\int_{\tilde{t}}^t dt''\hat{V}(t'')S(t'',t'). \qquad (19)\end{aligned}$$

In the special case of $\tilde{t} = t'$, then $S(t',t') = 1 = U(t')U^\dagger(t')$. The integral equation for the scattering matrix then follows:

$$\boxed{S(t,t') = 1 - i\int_{t'}^{t} dt''\hat{V}(t'')S(t'',t')}$$

The time evolution of S is given by $\hat{V}(t) = e^{i\mathcal{H}_0 t}Ve^{-i\mathcal{H}_0 t}$, and in a similar way as for $U(t)$ we can construct a perturbation theory for $S(t,t')$ by solving the integral equation by iteration.

0'th approx.:

$$S_0(t,t') = 1.$$

1st approx.:

$$S_1(t,t') = 1 - i\int_{t'}^{t} dt''\hat{V}(t'').$$

Now we can see what it means that V should be small, i.e.

$$\left|\int_{t'}^{t} dt''\hat{V}(t'')\right| \ll 1.$$

Properties of the S-matrix:

$$S(t,t) = 1,$$

$$\begin{aligned}(S(t,t'))^{\dagger} &= \left(U(t)U^{\dagger}(t')\right)^{\dagger} = U(t')U^{\dagger}(t)\\ &= S(t't),\end{aligned}$$

$$S(t,t'') = S(t,t')S(t',t''),$$

since

$$|\psi(t)\rangle =$$

To find an exact expression for S we introduce the time ordering operator: $\tilde{T}$.

Time ordering of operators

Bosons: Two boson operators have time-ordered product

$$\tilde{T}[A(t_1)B(t_2)] = \begin{cases} A(t_1)B(t_t); & t_1 > t_2. \\ B(t_2)A(t_1); & t_2 > t_1. \end{cases}$$

Fermions: Two fermion operators have time-ordered product

$$\tilde{T}[A(t_1)B(t_2)] = \begin{cases} A(t_1)B(t_t); & t_1 > t_2. \\ -B(t_2)A(t_1); & t_2 > t_1. \end{cases}$$

The operator $\tilde{T}$ orders the operator with the earliest time to the right, such that it operates first on a ket, $|\psi\rangle$.

We look further at the equation for S:

$$S(t,t') = 1 - i\int_{t'}^{t} dt''\hat{V}(t'')S(t'',t'),$$

<u>0.:</u>

$$S_0(t,t') = 1,$$

<u>1.:</u>

$$S_1(t,t') = 1 - i\int_{t'}^{t} dt''\hat{V}(t''),$$

<u>2.:</u>

$$\begin{aligned} S_2(t,t') &= 1 - i\int_{t'}^{t} dt''\hat{V}(t'')S_1(t'',t') \\ &= 1 - i\int_{t'}^{t} dt''\hat{V}(t'')\left(1 - i\int_{t'}^{t''} dt'''\hat{V}(t''')\right) \\ &= 1 + (-i)\int_{t'}^{t} dt''\hat{V}(t'') + (-i)^2\int_{t'}^{t} dt''\int_{t'}^{t''} dt'''\hat{V}(t'')\hat{V}(t'''), \end{aligned}$$

This can be done infinitly, such that

$$S(t,t') = 1 + \sum_{n=1}^{\infty}(-i)^n\int_{t'}^{t} dt_1\int_{t'}^{t_1} dt_2 ... \int_{t'}^{t_{n-1}} dt_n \left(\hat{V}(t_1)\hat{V}(t_2)...\hat{V}(t_n)\right).$$

This expression is such that all the integrations have the same lower bound, t', while the upper bounds are different. We use time ordering of the operators to get all the upper integration bounds the same. Let us consider a $\hat{V}$ consisting of a combination of fermion and/or boson operators in a way such that

$$\tilde{T}\left[V(t_1)V(t_2)\right] = \begin{cases} V(t_1)V(t_2); & t_1 > t_2 \\ V(t_2)V(t_1); & t_2 > t_1. \end{cases}$$

We then look at the expression

$$\begin{aligned} \frac{1}{2!}\int_{t'}^{t} dt_1\int_{t'}^{t} dt_2\tilde{T}\left[\hat{V}(t_1)\hat{V}(t_2)\right] = \quad & \frac{1}{2}\int_{t'}^{t} dt_1\int_{t'}^{t_1} dt_2\hat{V}(t_1)\hat{V}(t_2) \\ & + \frac{1}{2}\int_{t'}^{t} dt_2\int_{t'}^{t_2} dt_1\hat{V}(t_2)\hat{V}(t_1) \\ = & \int_{t'}^{t} dt_1\int_{t'}^{t_1} dt_2\hat{V}(t_1)\hat{V}(t_2), \end{aligned} \tag{20}$$

by interchanging the labels $t_1 \leftrightarrow t_2$ in the second term. In the same way:

$$\frac{1}{n!}\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 ... \int_{t'}^{t} dt_n \tilde{T}\left[\hat{V}(t_1)...\hat{V}(t_n)\right] = \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 ... \int_{t'}^{t_{n-1}} dt_n \hat{V}(t_1)...\hat{V}(t_n).$$

We then get an expression for S:

$$\begin{aligned} S(t,t') &= 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} dt_1 ... \int_{t'}^{t} dt_n \tilde{T}\left[\hat{V}(t_1)...\hat{V}(t_n)\right] \\ &= 1 + \tilde{T}\sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left[\int_{t'}^{t} dt'' \hat{V}(t'')\right]^n, \end{aligned} \tag{21}$$

which can be written formally as

$$\boxed{S(t,t') = \tilde{T}\left[\exp\left(-i\int_{t'}^{t} dt'' \hat{V}(t'')\right)\right]}$$

Typically, we want to calculate expectation values on the form

$$\langle \psi(0)|\hat{O}(t)|\psi(0)\rangle.$$

Here, the state $|\psi(0)\rangle$ is the exact ground state for the interacting system. The problem is that $|\psi(0)\rangle$ is unknown, since $\mathcal{H} = \mathcal{H}_0 + V$ is such that we cannot solve the problem exact. Can we relate $|\psi(0)\rangle$ formally to the groundstate $|\phi\rangle_0$ of $\mathcal{H}_0$?

The Gell-Mann-Low relations solves this. The trick is to introduce the perturbation V adiabatically, i.e. the potential is turned on really slowly. We can use

$$\mathcal{H} = \mathcal{H}_0 + V e^{-|t|\epsilon},$$

where ϵ is very small, and we assume that we study the system for times $|t| \ll \epsilon$.

pp.121-140 (Dag-Vidar)

We see that we have simplified the expectation value of one two-particle operator (4 fermion operators) to a sum of products of two one-particle propagators.

$$\begin{aligned}
&\langle\Phi_0|T\big[c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2,\sigma_2}(t_2)c_{k_3,\sigma_3}(t_3)c^\dagger_{k_4,\sigma_4}(t_4)\big]|\Phi_0\rangle \\
&= \quad i^2G_0(k_1,t_1-t_2)G_0(k_3,t_3-t_4)\delta_{k_1,k_2}\delta_{k_3,k_4}\delta_{\sigma_1,\sigma_2}\delta_{\sigma_3,\sigma_4} \\
&\quad - i^2G_0(k_1,t_1-t_4)G_0(k_3,t_3-t_2)\delta_{k_1,k_4}\delta_{k_2,k_3}\delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3}
\end{aligned}$$

As we will see, the expectation value of one three-particle operator is reduced to a sum of products of three one-particle propagators.

Equivalently: The expectation value of N-particle operator is reduced to a sum of products of $N/2$ one-particle propegators. The number of terms in the sum grows dramatically with N: $\sim (N/2)!$ (rough estimate).

We now go back to the second order expectation value. For the second order term we must look at the following contractions:

$$\begin{aligned}
&1) \quad \langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)\big]\,|\Phi_0\rangle \\
&2) \quad \langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)\big]\,|\Phi_0\rangle \\
&3) \quad \langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)\big]\,|\Phi_0\rangle \\
&4) \quad \langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)\big]\,|\Phi_0\rangle \\
&5) \quad \langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)\big]\,|\Phi_0\rangle \\
&6) \quad \langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)\big]\,|\Phi_0\rangle
\end{aligned}$$

This gives a sum of 6 terms, where each term is a product of three one-particle operators. The contracted operators must be placed together, and we therefore have to use the anti-commutation relations several times in order to get the correct sign for each term.

1:

$$\begin{aligned}
&\langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')\big]\,|\Phi_0\rangle\,\langle\Phi_0|\,T\big[\underbrace{c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)}_{-c_{k_1,\sigma_1}(t_1)c^\dagger_{k_1+q_1,\sigma_1}(t_1)}\big]\,|\Phi_0\rangle\,\langle\Phi_0|\,T\big[\underbrace{c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)}_{-c_{k_2,\sigma_2}(t_2)c^\dagger_{k_2+q_2,\sigma_2}(t_2)}\big]\,|\Phi_0\rangle \\
&= \underline{(-1)^2i^3G_0(k,t-t')G_0(k_1,t_1-t_1)G_0(k_2,t_2-t_2)\delta_{k,k}\delta_{k_1+q_1,k_1}\delta_{k_2+q_2,k_2}\delta_{\sigma,\sigma}\delta_{\sigma_1,\sigma_1}\delta_{\sigma_2,\sigma_2}}
\end{aligned}$$

2:

$$\begin{aligned}
&(-1)\,\langle\Phi_0|\,T\big[c_{k,\sigma}(t)c^\dagger_{k_1+q_1,\sigma_1}(t_1)\big]\,|\Phi_0\rangle\,\langle\Phi_0|\,T\big[\underbrace{c^\dagger_{k,\sigma}(t')c_{k_1,\sigma_1}(t_1)}_{-c_{k_1,\sigma_1}(t_1)c^\dagger_{k,\sigma}(t')}\big]\,|\Phi_0\rangle\,\langle\Phi_0|\,T\big[\underbrace{c^\dagger_{k_2+q_2,\sigma_2}(t_2)c_{k_2,\sigma_2}(t_2)}_{-c_{k_2,\sigma_2}(t_2)c^\dagger_{k_2+q_2,\sigma_2}(t_2)}\big]\,|\Phi_0\rangle \\
&= \underline{(-1)^3i^3G_0(k,t-t_1)G_0(k,t_1-t')G_0(k_2,t_2-t_2)\delta_{k,k_1}\delta_{k,k_1+q_1}\delta_{k_2+q_2,k_2}\delta_{\sigma,\sigma_1}\delta_{\sigma,\sigma_1}\delta_{\sigma_2,\sigma_2}}
\end{aligned}$$

3:

$$(-1)^2 \langle\Phi_0| T\big[c_{k,\sigma}(t)c^\dagger_{k,\sigma}(t')\big] |\Phi_0\rangle \langle\Phi_0| T\big[\underbrace{c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_2,\sigma_2}(t_2)}_{-c_{k_2,\sigma_2}(t_2)c^\dagger_{k_1+q_1,\sigma_1}(t_1)}\big] |\Phi_0\rangle \langle\Phi_0| T\big[c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)\big] |\Phi_0\rangle$$

$$= \underline{(-1)^3 i^3 G_0(k,t-t')G_0(k_2,t_2-t_1)G_0(k_1,t_1-t_2)\delta_{k_1+q_1,k_2}\delta_{k_2+q_2,k_1}\delta_{\sigma_1,\sigma_2}}$$

4:

$$(-1)^3 \langle\Phi_0| T\big[c_{k,\sigma}(t)c^\dagger_{k_1+q_1,\sigma_1}(t_1)\big] |\Phi_0\rangle \langle\Phi_0| T\big[\underbrace{c^\dagger_{k,\sigma}(t')c_{k_2,\sigma_2}(t_2)}_{-c_{k_2,\sigma_2}(t_2)c^\dagger_{k,\sigma}(t')}\big] |\Phi_0\rangle \langle\Phi_0| T\big[c_{k_1,\sigma_1}(t_1)c^\dagger_{k_2+q_2,\sigma_2}(t_2)\big] |\Phi_0\rangle$$

$$= \underline{i^3 G_0(k,t-t_1)G_0(k,t_2-t')G_0(k_1,t_1-t_2)\delta_{k,k_1+q_1}\delta_{k,k_2}\delta_{k_1,k_2+q_2}\delta_{\sigma,\sigma_2}\delta_{\sigma_1,\sigma_2}\delta_{\sigma,\sigma_1}}$$

5:

$$(-1)^5 \langle\Phi_0| T\big[c_{k,\sigma}(t)c^\dagger_{k_2+q_2,\sigma_2}(t_2)\big] |\Phi_0\rangle \langle\Phi_0| T\big[\underbrace{c^\dagger_{k,\sigma}(t')c_{k_2,\sigma_2}(t_2)}_{-c_{k_2,\sigma_2}(t_2)c^\dagger_{k,\sigma}(t')}\big] |\Phi_0\rangle \langle\Phi_0| T\big[\underbrace{c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_1,\sigma_1}(t_1)}_{-c_{k_1,\sigma_1}(t_1)c^\dagger_{k_1+q_1,\sigma_1}(t_1)}\big] |\Phi_0\rangle$$

$$= \underline{(-1) i^3 G_0(k,t-t_2)G_0(k,t_2-t')G_0(k_1,t_1-t_1)\delta_{k_1,k_1+q_1}\delta_{k,k_2+q_2}\delta_{k,k_2}\delta_{\sigma,\sigma_2}\delta_{\sigma,\sigma_2}\delta_{\sigma_1,\sigma_1}}$$

6:

$$(-1)^4 \langle\Phi_0| T\big[c_{k,\sigma}(t)c^\dagger_{k_2+q_2,\sigma_2}(t_2)\big] |\Phi_0\rangle \langle\Phi_0| T\big[\underbrace{c^\dagger_{k,\sigma}(t')c_{k_1,\sigma_1}(t_1)}_{-c_{k_1,\sigma_1}(t_1)c^\dagger_{k,\sigma}(t')}\big] |\Phi_0\rangle \langle\Phi_0| T\big[\underbrace{c^\dagger_{k_1+q_1,\sigma_1}(t_1)c_{k_2,\sigma_2}(t_2)}_{-c_{k_2,\sigma_2}(t_2)c^\dagger_{k_1+q_1,\sigma_1}(t_1)}\big] |\Phi_0\rangle$$

$$= \underline{i^3 G_0(k,t-t_2)G_0(k,t_1-t')G_0(k_2,t_2-t_1)\delta_{k,k_2+q_2}\delta_{k,k_1}\delta_{k_2,k_1+q_1}\delta_{\sigma,\sigma_2}\delta_{\sigma,\sigma_1}\delta_{\sigma_1,\sigma_2}}$$

We will now insert these terms into the double integral (NB: Equation reference). Remember that all six terms must be multiplied by M_{q_1}, M_{q_2} and $iD_0(q_1,t_1-t_2)\delta_{q_1,-q_2}$. Finally we must sum over k_1, k_2, q_1, q_2, σ_1 and σ_2. Remember that

$$M_q = i\sqrt{\frac{\hbar}{2MN\omega_q}}\left(\vec{\xi}\cdot\vec{q}\right)\tilde{V}(\vec{q}) \to 0$$

as $\vec{q} \to 0$. This means that three of the terms are zero:
First term:

$$\begin{aligned} & \delta_{k_1+q_1,k_1}\delta_{k_2+q_2,k_2} \\ \Rightarrow\quad & q_1 = q_2 = 0 \quad \Rightarrow \quad M_{q_1} = M_{q_2} = 0 \\ & \underline{\text{First term} = 0} \end{aligned}$$

Second term:

$$\begin{aligned}
&\delta_{k_2+q_2,k_2} \\
\Rightarrow\quad & q_2 = 0 \quad \Rightarrow \quad M_{q_2} = 0 \\
& \underline{\text{Second term} = 0}
\end{aligned}$$

Fifth term:

$$\begin{aligned}
&\delta_{k_1,k_1+q_1} \\
\Rightarrow\quad & q_1 = 0 \quad \Rightarrow \quad M_{q_1} = 0 \\
& \underline{\text{Fifth term} = 0}
\end{aligned}$$

We have two q-summations, $\sum\limits_{q_1,q_2}$. However, since the free phonon-propagator is multiplied with $\delta_{q_1,-q_2}$, one of the summations is used to set $q_1 = -q_2$. Hence $M_{q_1}M_{q_2} = M_{q_1}M_{-q_1} = |M_{q_1}|^2$. For the remaining terms we then get:
Third term:

$$\begin{aligned}
&\delta_{k_1+q_1,k_2}\delta_{k_2+q_2,k_1} = \delta_{k_1+q_1,k_2}\delta_{k_2-q_1,k_1} \\
\Rightarrow\quad & k_2 = k_1 + q_1 \\
& \underline{\text{One } k\text{-summation left}}
\end{aligned}$$

Fourth term:

$$\begin{aligned}
&\delta_{k,k_1+q_1}\delta_{k,k_2}\delta_{k_1,k_2-q_1} = \delta_{k,k_2}\delta_{k_1,k_2-q_1} \\
& \underline{\text{No } k\text{-summation}}
\end{aligned}$$

Sixth term:

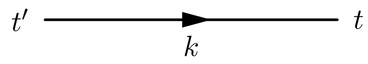
$$\begin{aligned}
&\delta_{k,k_1}\delta_{k,k_2-q_1}\delta_{k_2,k_1+q_1} = \delta_{k,k_1}\delta_{k_2,k_1+q_1} \\
& \underline{\text{No } k\text{-summation}}
\end{aligned}$$

Inserting these results we get

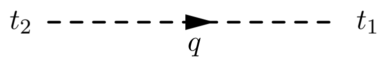
$$\begin{aligned}
G(k,t-t') = {} & \frac{G_0(k,t-t')}{\langle\Phi_0|\, S(\infty,-\infty)\,|\Phi_0\rangle} \\
& + \frac{(-i)^2}{2!}\frac{(-i)}{\langle\Phi_0|\, S(\infty,-\infty)\,|\Phi_0\rangle}\sum_q \int\limits_{-\infty}^{\infty} \mathrm{d}t_1 \int\limits_{-\infty}^{\infty} \mathrm{d}t_2\, |M_q|^2\, iD_0(q,t_1-t_2) \\
& \times \sum_{\sigma_1,\sigma_2} \Big\{ \delta_{\sigma_1,\sigma_2}(-i)^3 G_0(k,t-t') \sum_{k_1} G_0(k_1,t_1-t_2)G_0(k_1+q,t_2-t_1) \\
& + \delta_{\sigma,\sigma_1}\delta_{\sigma,\sigma_2} i^3 G_0(k,t-t_1)G_0(k-q,t_1-t_2)G_0(k,t_2-t') \\
& + \delta_{\sigma,\sigma_1}\delta_{\sigma,\sigma_2} i^3 G_0(k,t-t_2)G_0(k,t_1-t')G_0(k+q,t_2-t_1)\Big\}.
\end{aligned}$$

In the third term there is one spin summation left, while in the fourth and sixth terms the spin summations disappear. In order to give a diagrammatic representation of the previous equation, we define the following symbols for the propagators:

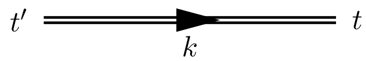
- Free electron propagator:

$G_0(k, t - t') =$ 

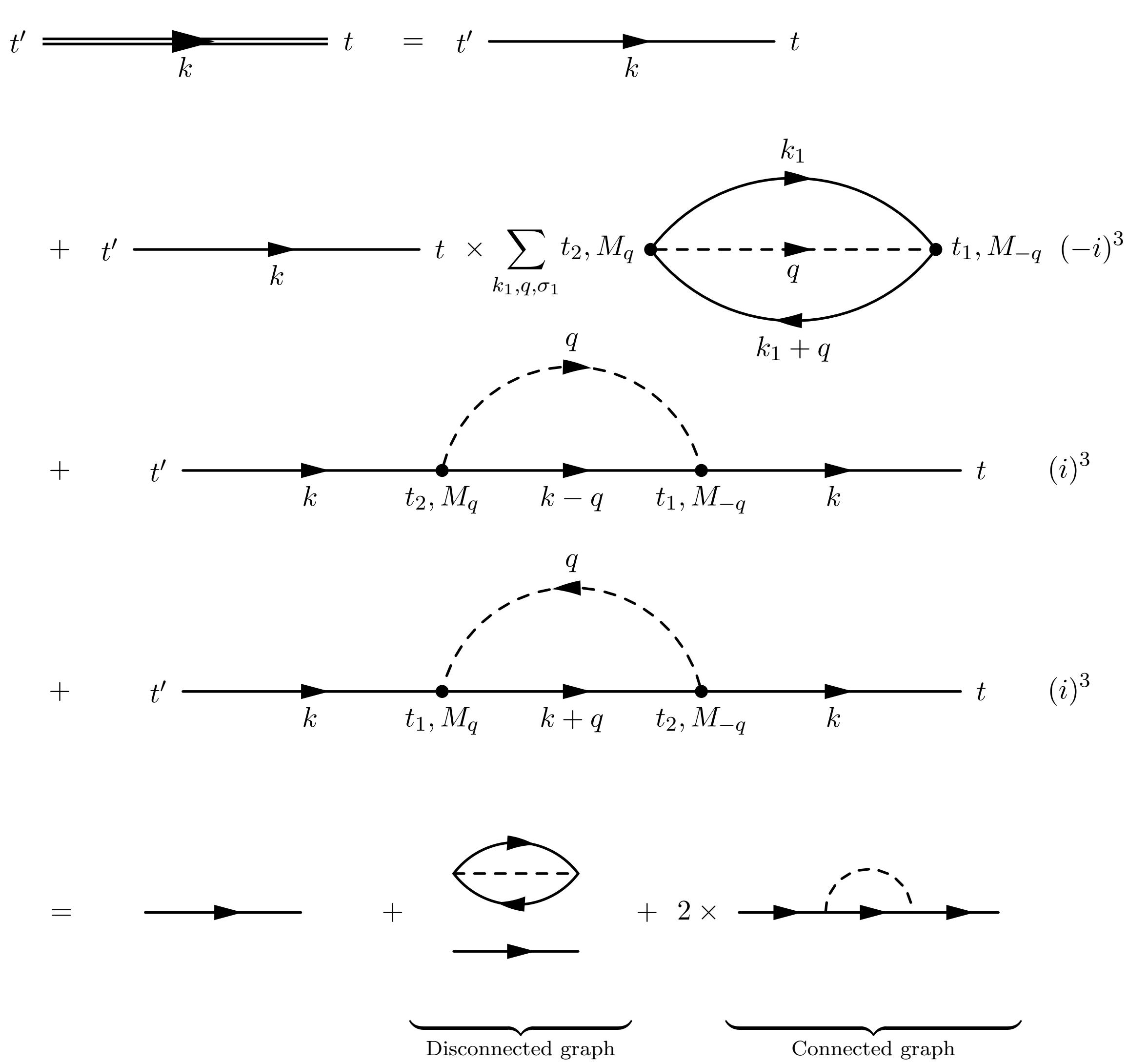
- Free phonon propagator:

$D_0(q, t_1 - t_2) =$ 

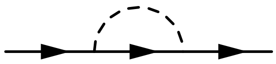
- Exact electron propagator:

$G(k, t - t') =$ 

Using this we get the diagrammatic representation of $G(k, t - t')$:

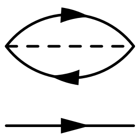


In general the correction to at each order consists of connected and disconnected graphs. The fourth and sixth terms give the same contribution, as seen by renaming the integration variables, $t_1 \leftrightarrow t_2$, $q \to -q$. This gives the connected graph to second order:

 $\equiv F_2$

$$= \frac{(-i)^2}{2!} \cdot 2(-i)i^3 i \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \sum_q |M_q|^2 D_0(q, t_1 - t_2)$$
$$\times G_0(k, t - t_1) G_0(k - q, t_1 - t_2) G_0(k, t_2 - t')$$

We see that the factor $1/2!$ is cancelled! For the unconnected graphs to second order we get:

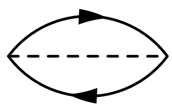
 $= G_0 F_1$

$$F_1 = \frac{(-i)^2}{2!} \cdot (-i^3)(-i) \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \sum_q |M_q|^2 \, i D_0(q, t_1 - t_2)$$
$$\times \sum_{k'} G_0(k' + q, t_2 - t_1) G_0(k', t_1 - t_2)$$

Hence to second order we have:

$$G = \frac{1}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle} \{ G_0(1 + F_1) + F_2 \}$$

But what about $\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle$? To second order (see exercise 5)

$\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle = 1 + F_1 = 1 +$ 

To higher orders one can always write (we will not show the proof here, but it follows directly from Wick's theorem)

$$G = \frac{1}{\langle\Phi_0| S(\infty,-\infty) |\Phi_0\rangle} \{G_0(1+F_1+A) + F_2(1+F_1+A) + B(1+F_1+A)\},$$

$\langle\Phi_0| S(\infty,-\infty) |\Phi_0\rangle = 1 + F_1 + A,$

A: the sum of distinct higher order unconnected graphs,

B: the sum of distinct higher order connected graphs.

Hence

$$G = G_0 + F_2 + B$$

B: Contains graphs of 4th, 6th, 8th,... order in M_q. Terms of odd order in the electron-phonon vertex gives zero.

We can now write

$$\begin{aligned}
&G(\mathbf{k}, t-t') \\
&= G_0(\mathbf{k}, t-t') - i \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 ... \int_{-\infty}^{\infty} dt_n \underbrace{\langle\Phi_0| T\left[c_{k\sigma}(t) c_{k\sigma}^{\dagger}(t') V(t_1)...V(t_n)\right] |\Phi_0\rangle_c}_{\text{Connected graphs}} \\
&= G_0(\mathbf{k}, t-t') - i \sum_{n=1}^{\infty} (-i)^n \int_{-\infty}^{\infty} dt_1 ... \int_{-\infty}^{\infty} dt_n \underbrace{\langle\Phi_0| T\left[c_{k\sigma}(t) c_{k\sigma}^{\dagger}(t') V(t_1)...V(t_n)\right] |\Phi_0\rangle_{dc}}_{\text{Distinct, connected graphs}}
\end{aligned}$$

We have now achieved a considerable reduction of the number of contributions we need to calculate in the perturbation expansion, since there is far fewer connected graphs than the total number of graphs to each order. Similarily, the fraction of distinct connected graphs to each order is $1/n!$.

It is possible to further reduce the number of contributions we need to calculate: We introduce the Fourier-transformed Green's function

$$G(k,\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G(k,t)$$

$$G(k,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} G(k,\omega)$$

Exactly the same transformations are used for the phonon-propagators. To second order we have (with $t' = 0$)

$$\begin{aligned}
G(k,t) = G_0(k,t) + i(-i) \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \sum_q |M_q|^2 \, iD_0(q, t_1 - t_2) \\
\times G_0(k, t-t_1) G_0(k-q, t_1-t_2) G_0(k, t_2)
\end{aligned}$$

Fourier-transforming the above, we get

$$G(k,\omega) = G_0(k,\omega) + i(-i) \int\limits_{-\infty}^{\infty} dt_1 \int\limits_{-\infty}^{\infty} dt_2 \sum_q |M_q|^2 \int\limits_{-\infty}^{\infty} dt\ e^{i\omega t}$$
$$\times \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} d\omega_1 D_0(q,\omega_1) e^{-i\omega_1(t_1-t_2)}$$
$$\times \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} d\omega_2 G_0(k,\omega_2) e^{-i\omega_2(t-t_1)}$$
$$\times \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} d\omega_3 G_0(k-q,\omega_3) e^{-i\omega_3(t_1-t_2)}$$
$$\times \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} d\omega_4 G_0(k,\omega_4) e^{-i\omega_4 t_2}$$

$$\begin{aligned} G(k,\omega) &= G_0(k,\omega) \\ &+ i \sum_q |M_q|^2 \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} ... \int\limits_{-\infty}^{\infty} \frac{d\omega_4}{2\pi} i D_0(q,\omega_1) G_0(k,\omega_2) G_0(k-q,\omega_3) G_0(k,\omega_4) \\ &\times \int\limits_{-\infty}^{\infty} dt_1\ e^{-it_1(\omega_1+\omega_2+\omega_3)} \cdot \int\limits_{-\infty}^{\infty} dt_2\ e^{-it_2(-\omega_1-\omega_3+\omega_4)} \cdot \int\limits_{-\infty}^{\infty} dt\ e^{it(\omega-\omega_2)} \end{aligned}$$

We use

$$\int\limits_{-\infty}^{\infty} dt\ e^{it\omega} = 2\pi\delta(\omega)$$

which sets

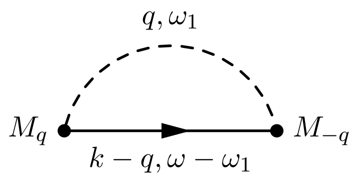
$$\begin{aligned} \omega_2 &= \omega \\ \omega_2 &= \omega_1 + \omega_3 \\ \omega_4 &= \omega_1 + \omega_3 = \omega_2 = \omega \\ \omega_3 &= \omega_2 - \omega_1 = \omega - \omega_1 \end{aligned}$$

We are then left with one ω_1-integration,

$$\begin{aligned} G(k,\omega) &= G_0(k,\omega) \\ &\quad + i \sum_q |M_q|^2 \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} i D_0(q,\omega_1) G_0(k,\omega) G_0(k-q,\omega-\omega_1) G_0(k,\omega) \\ &= G_0(k,\omega) + G_0(k,\omega)\Sigma^{(2)}(k,\omega) G_0(k,\omega) \end{aligned}$$

where

$$\Sigma^{(2)}(k,\omega) = i\sum_q |M_q|^2 \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} iD_0(q,\omega_1)G_0(k-q,\omega-\omega_1)$$

$=$ 

We have momentum and energy conservation at each vertex.

To second order we now have

$$\begin{aligned} G &= G_0 + G_0\Sigma^{(2)}G_0 + ... \\ &= G_0(1+\Sigma^{(2)}G_0 + ...) \\ G^{-1} &= G_0^{-1}(1-G_0\Sigma^{(2)}) + ...) \\ &= G_0^{-1} - \Sigma^{(2)} + ... \end{aligned}$$

5.3 The Dyson Equation

We could have continued the perturbation expansion for G and arrived at

$$\begin{aligned} G &= G_0 + G_0\Sigma^{(2)}G_0 + G_0\tilde{\Sigma}^{(4)}G_0 + ... \\ &= G_0(1+G_0\Sigma^{(2)} + G_0\tilde{\Sigma}^{(4)} + ...) \\ G^{-1} &= G_0^{-1}(1-G_0\Sigma^{(2)} - G_0\Sigma^{(4)} - ...) \\ &= G_0^{-1} - (\Sigma^{(2)} + \Sigma^{(4)} + ...) \end{aligned}$$

From this we get

$$G^{-1} = G_0^{-1} - \Sigma \qquad \text{(The Dyson equation)}$$

This is an exact expression for the Green's function.

The simplification is due to the fact that the perturbation expansion for Σ is far simpler than the expansion for G!

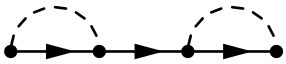
Σ : Is calculated from one-particle irreducible diagrams.

A one-particle irreducible diagram is a diagram which does not split into two pieces if one "cuts" a one-particle propagator.

$$G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + ...$$

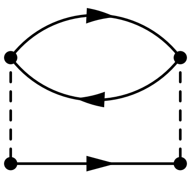
We look at the fourth order terms:
One-particle reducible diagram:

$$\left(\Sigma^{(2)}\right)^2 G_0 =$$

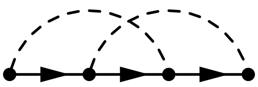


One-particle irreducible fourth order graphs:

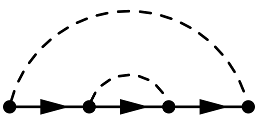
$$\Sigma_a^{(4)} =$$



$$\Sigma_b^{(4)} =$$

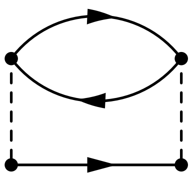


$$\Sigma_c^{(4)} =$$



We now use

$$\Sigma^{(4)} =$$



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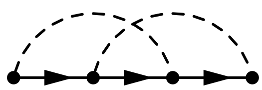

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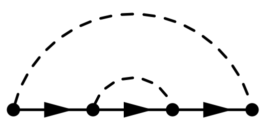
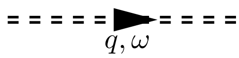
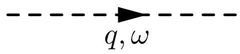


in the Dyson equation to fourth order in M_q.

> We see that the perturbation expansion for G can be reduced to a perturbation expansion for Σ with the help of the Dyson equation. This gives fewer contributions to consider.

We could have done the same thing for the phonon-propagator.

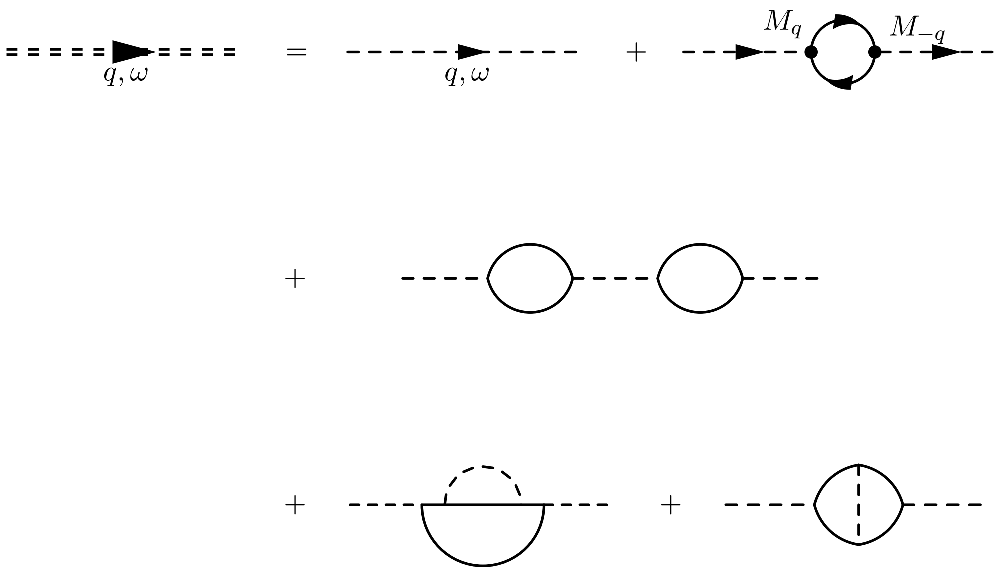
$D(q, \omega) =$ 

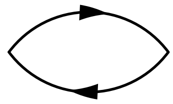
$D_0(q, \omega) =$ 

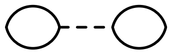
The Dyson equation for the phonon-propagator reads

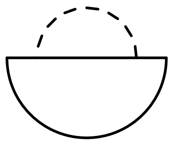
$$D^{-1}(q, \omega) = D_0^{-1} - \Pi$$

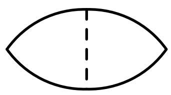
$\Pi(q, \omega)$ contains only irreducible one-phonon diagrams:



$\Pi^{(2)} =$  Irreducible

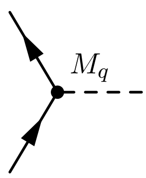
$\Pi_a^{(4)} =$  Reducible

$\Pi_b^{(4)} =$  Irreducible

$\Pi_c^{(4)} =$  Irreducible

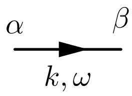
How did we get the diagrams for Π? We used the Feynman rules: For diagrams of order $2m$

1. Draw all topologically distinct diagrams with $2m$ vertices



   To every vertex, we associate a factor M_q.

2. With every free electron line, we associate a factor

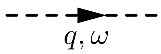
$G_0(k,\omega) =$ 

$= \dfrac{\delta_{\alpha\beta}}{\omega - \epsilon_k + i\delta_k}$

where $\delta_k = \delta \mathrm{sign}(\epsilon_k - \mu)$. This is a combined particle and hole propagator.

3. With each phonon line we associate a factor

$$D_0(q,\omega) =$$

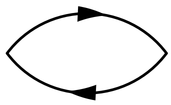


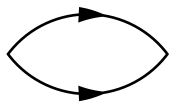
$$= \frac{2\omega_q}{\omega^2 - \omega_q^2 + i\delta}.$$

4. Make sure that momentum and energy is conserved at each vertex.

5. Prefactor for each distinct diagram:

   $i^m(-1)^F(2s+1)^F$
   s : spinn ($= 1/2$ for electrons)

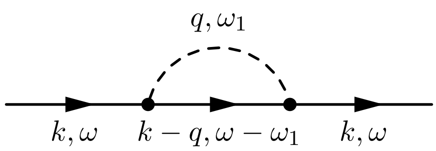
   F : the number of closed fermion loops in the diagram: 

   NB: this is not a closed loop: 

6. Integrate over independent momenta and frequencies.

Examples

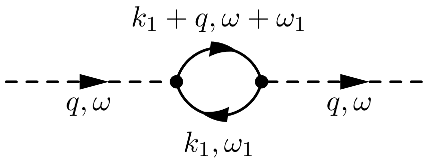
Σ to Second order in M_q The diagram is



which yields

$$\Sigma^{(2)}(k,\omega) = i \sum_q \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} |M_q|^2 D_0(q,\omega_1) G_0(k-q,\omega-\omega_1)$$

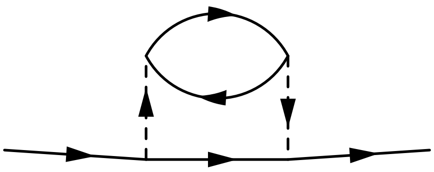
Π to Second order in M_q The diagram is



which yields

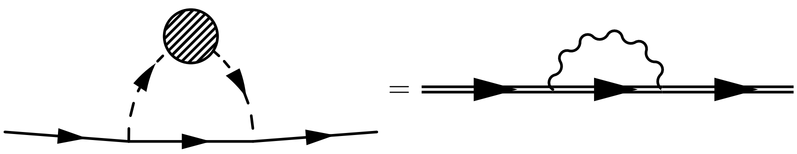
$$\Pi^{(2)}(q,\omega) = i(-1)^1 \left(2 \cdot \frac{1}{2} + 1\right) \sum_{k_1} \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \left|M_q\right|^2 G_0(k_1,\omega_1) G_0(k_1 - q, \omega+\omega_1),$$

where $|M_q|^2$ can be moved outside the sum and integration. The advantage here is that the diagrams can be given a physical interpretation, in contrast to the associated mathematical expressions. Let's look at a more complicated example.



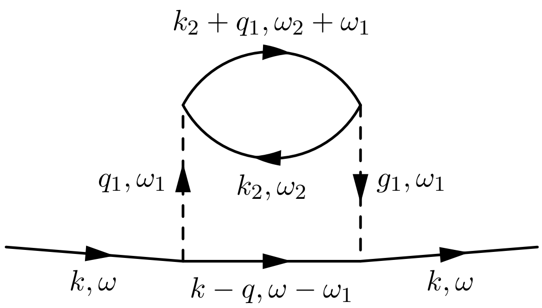
$\sim |M|^4$ Fourth order

The diagram describes an electron which comes in, excites a phonon and continues to propagate as a free electron. However, the phonon does <u>not</u> propagate freely, it excites a particle-hole excitation along its way. Finally, the phonon and electron collide. Therefore, the process is a version of



where the blob indicates that something happens with the phonon. We here see the traces of complicated effects. Let's look at the above diagram in more detail, where

$m = 2$, $F = 1$:



$\sim |M|^4$

From this we get the mathematical expression

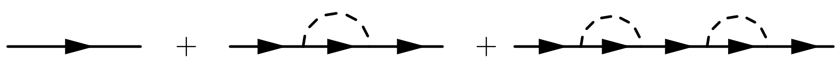
$$i^2(-1)^1 \left(2 \cdot \frac{1}{2} + 1\right)^1 G_0(k,\omega)^2 \sum_{q_1} \sum_{k_2} \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega_2}{2\pi} |M_{q_1}|^4$$
$$\times D_0(q_1,\omega_1)^2 G_0(k_2,\omega_2) G_0(k - q_1, \omega - \omega_1) G_0(k_2 + q_1, \omega_1 + \omega_2)$$

We here see that the expressions quickly become complicated.

i) Small quantitative changes $\Rightarrow$ use perturbation theory to low order (second order).

ii) If we expect large changes, we can sum classes of simple () diagrams.

Example:

$G \approx$  $+ \ldots$

$$= G_0 \left(1 + \Sigma^{(2)} G_0 + (\Sigma^{(2)} G_0)^2 + \ldots\right)$$
$$= \frac{G_0}{1 - G_0 \Sigma^{(2)}} = \frac{1}{G_0^{-1} - \Sigma^{(2)}}$$

We use

$$G_0(k,\omega) = \frac{\theta(\epsilon_k - \epsilon_F)}{\omega - \epsilon_k + i\delta} + \frac{\theta(\epsilon_F - \epsilon_k)}{\omega - \epsilon_k - i\delta}$$
$$= \frac{1}{\omega - \epsilon_k + i\delta_k}$$
$$\delta_k = \delta \operatorname{sign}(\epsilon_k - \epsilon_F)$$

to get an approximate expression for G,

$$G(k,\omega) \approx \frac{1}{\omega - \epsilon_k + i\delta_k - \Sigma^{(2)}}$$
$$\Sigma^{(2)} = \Sigma_R^{(2)} + i\Sigma_I^{(2)}$$

$$G = \frac{1}{\omega - \tilde{\epsilon}_k + i/\tau}$$

$$\tilde{\epsilon}_k = \epsilon_k + \Sigma_R^{(2)}$$

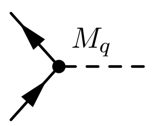
$$\tau^{-1} = -\Sigma_I^{(2)}$$

From this we see that $G_0 \sim \exp(-i\epsilon_k t - \delta t)$, while $G_0 \sim \exp(-i\tilde{\epsilon}_k t - t/\tau)$. This means that $\Sigma_R^{(2)}$ renormalizes the energy, $\epsilon_k \to \tilde{\epsilon}_k$, while $\Sigma_I^{(2)}$ leads to a damping due to the spreading of plane waves.

5.4 Effective Interaction Between Electrons due to Phonons

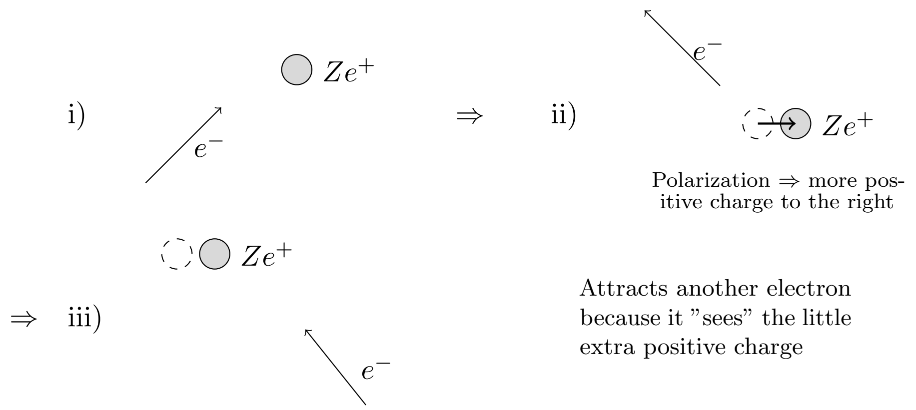
$$V = \sum_{kq\sigma} M_q \left(a_{-q}^\dagger + a_q \right) c_{k+q,\sigma}^\dagger c_{k,\sigma}$$

This is a scattering process which gives rise to



Electron-phonon interaction

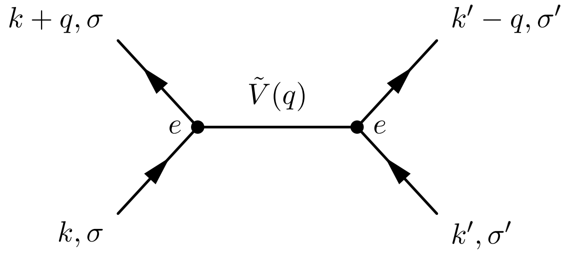
which we call a vertex. This gives rise to a electron-phonon-electron interaction, or alternatively: An effective interaction between two electrons mediated by phonons.
Classical picture:



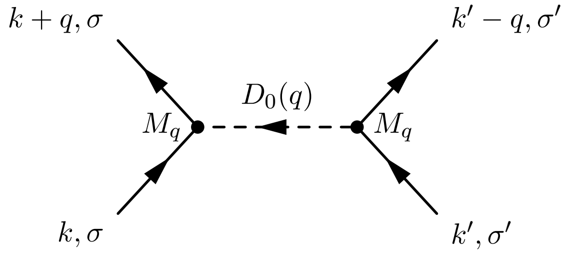
NB! If the ion relaxes slowly enough, the little extra positive charge "lives" around the lattice point for a long time. Then the electron that caused the lattice fluctuation is long gone. **Another** electron is then allowed to be pulled towards the positive charge, without the original electron pushing it away, as the repulsive and strong Coulomb interaction is weakened when the distance between the electrons become large. In other words: by using lattice fluctuations, and by "waiting a little",

> two electrons interact attractively, even if the Coulomb-force (that is repulsive), is taken into account!

This is quite astonishing, as one naively expects that the Coulomb-forces are **much** stronger than the weak connection between electrons and phonons. Remember the Coulomb-potential, we drew it like this:



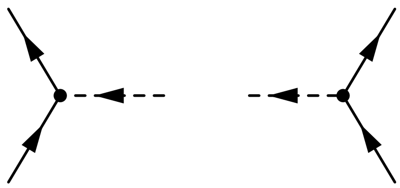
Coulomb-interaction between the electrons is looked at as an effective interaction between electrons, caused by photons, after an electron-photon-electron interaction. The photon-propagator: $\sim \frac{1}{q^2}$. There is **no** frequency dependency for **non**-relativistic electrons: electrons at the Fermi-level have a velocity of $\sim 1.0 \times 10^5$ m/s. Photons have a velocity of $\sim 3 \times 10^8$ m/s. The interaction between electrons, caused by photons (= Coulomb) is therefore instantaneous: $\delta(t-t')$. The Fourier-transform of a δ function is a constant. For the phonons it is different, the ions relax with velocities much smaller than the electron's, because it has a much greater mass. Therefore the interaction between the electrons caused by phonons is far from instantaneous, it is actually retarded. This means that it takes a long time before the phonon that is emitted from an electron hits another. The diagram, however, stays the same as for the Coulomb-interaction. **NB!** We know this from our general considerations around the general form (in a plane-wave basis) of the second quantized form any two-particle operator.



This is an effective interaction between electrons caused by **phonons**.

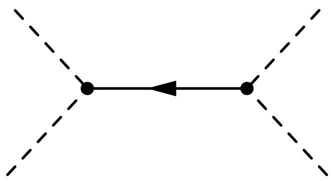
$$\tilde{V}_{\text{eff}} = |M_q|^2 D_0(q,\omega) = \frac{2|M_q|^2\omega_q}{\omega^2-\omega_q^2}. \tag{22}$$

When $|\omega| < \omega_q$: $\tilde{V}_{eff} < 0$! The diagram consists of

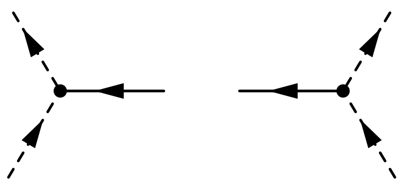


(23)

) : the two vertexes we have in $\underline{V}$. What becomes the effective interaction between phonons, caused by electrons, with V? The diagram would have to look something like this:



But something like this does not exist with our V, as the vertex



(24)

does not exist. Generally: if we have a potential that couples fermions to a boson, of the type

$$\sum_{k,q,\sigma} \lambda_q B_q c^\dagger_{k+q,\sigma} c_{k,\sigma} \tag{25}$$

where the corresponding propagator for the bosons being given by

$$D_0(q,t) = -i\ {}_0\langle\phi| T\left[B_q(t) B_q(0)^\dagger\right] |\phi\rangle_0 \tag{26}$$

then the effective b_ω (?) interaction between the fermions is given by

$$V_{eff} = |\lambda_q|^2 D_0(q,\omega) + \tilde{V}_{Coulomb}(\vec{q}). \tag{27}$$

Examples of bosons that have such a link: photons, phonons, magnons (ferromagnetic and antiferromagnetic). (How does a free magnon-propagator look like? Can magnons cause attraction between electrons?) We look a little closer at $\tilde{V}_{\text{eff}}$ in (22). A plot of this potential as a function of ω is shown in Figure 9. If we add the Coulomb-interaction, we

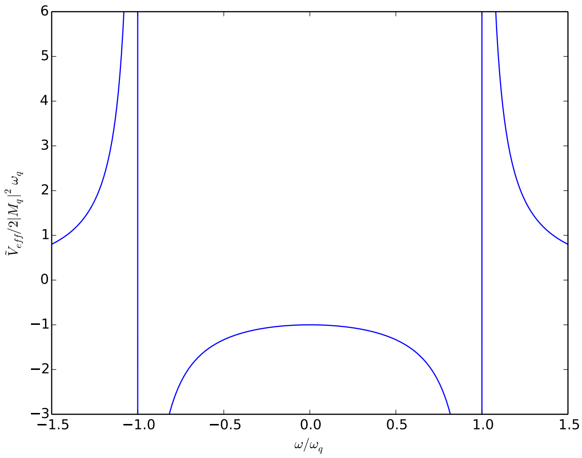


Figure 9

get a schematical increase $\sim 1/q^2$, which is independent of ω. This is shown in Figure 10. As one can see, there is a small region close to $\pm\omega_q$ where the electrons can only interact attractively. Still we **always** have a small frequency region where the interaction between the electrions become attractive. ω: the energy that is transferred from one electron to another when they collide via phonons (corresponding for other electrons). The electrons that can scatter must be close to the Fermi-level: $\omega \sim \omega_q$ makes $\tilde{V}_{eff}$ large. $\omega_q \sim \omega_D$, the Debye-frequency, which has an order og magnitude $\sim 1.0 \times 10^{-1}\,\text{eV} \sim 1.00 \times 10^{2}\,\text{K}$. Compared to ε_F, ω_q is very small. Therefore the involved electrons can only be close to ε_F. The energy transfer ω is small $\implies$ only electrons in a **thin shell** $\sim \omega_q \sim \omega_D$ around the Fermi-level can interact attractively via phonons.

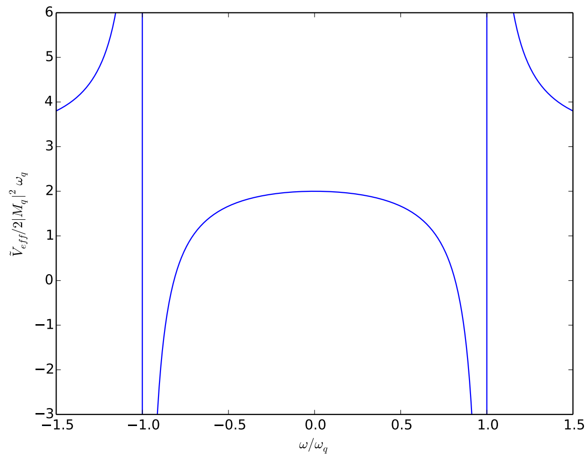


Figure 10

NB! A small frequency corresponds to a long time. The thin shell around the Fermi-level reflects that the second electron must "wait a little" (long time) for the first electron to get away, for the interaction to get attractive.

NB! The electrons cannot wait too long either, then the lattice has relaxed and there is no positive charge anymore.

6 Screening of Coulomb-interaction

Why does the "free-electron" approximation work well in many metals? That is due to screening, as we will now calculate using Feynman diagrams. Remember Dyson's equation for the **phonon-propagator:**

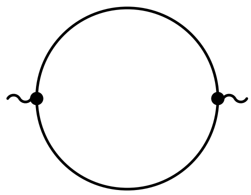
$$D^{-1} = D_0^{-1} - \Pi \implies D = \frac{D_0}{1 - D_0 \Pi}. \tag{28}$$

Entirely analogously, we find a Dyson's equation for the photon-propagator, which is the Coulomb-interaction:
$D_0(\vec{q}) = \frac{4\pi e^2}{q^2} = V_0$: "Naked" Coulomb-interacton): Coulomb-interaction between two isolated electrons.
D: Renormalized photon-propagator): renormalized Coulomb-potential.

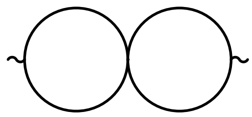
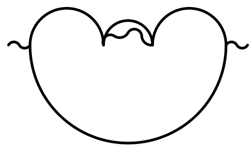
Diagrammatically:

$D =$ 

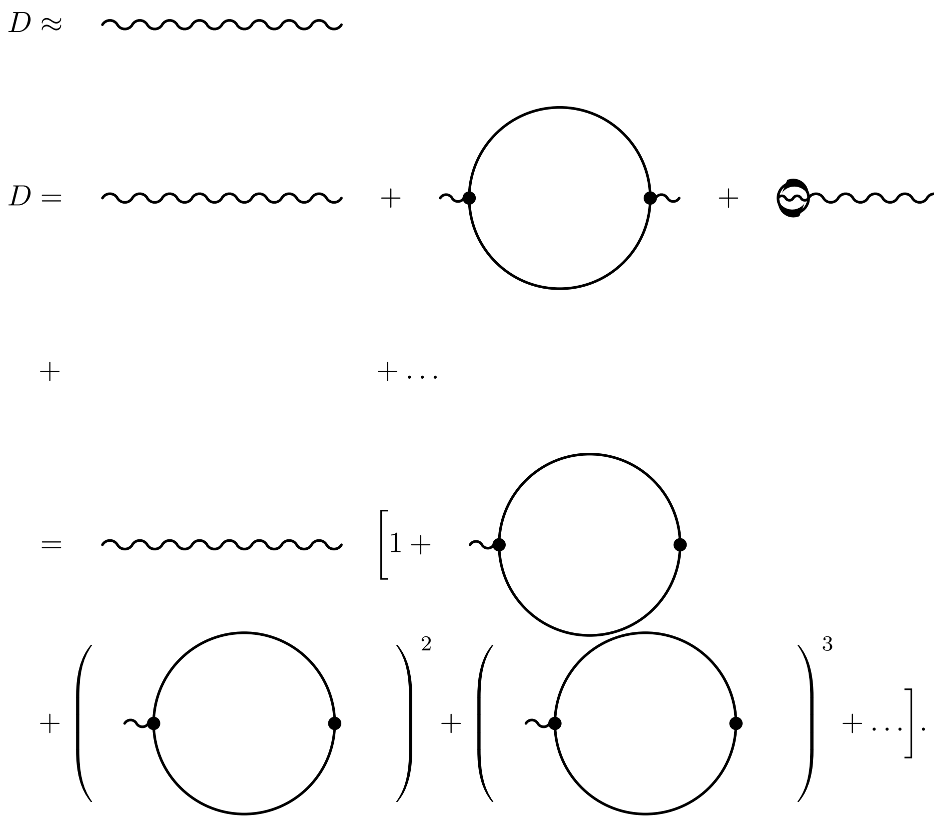
$D_0 =$

$D =$ $+$ 

$+$ 

$+$  $+$  $+ \dots$

We now make the following approximation: instead of doing *pure* perturbation theory, we sum all the diagrams of one particular type to the order of infinity:

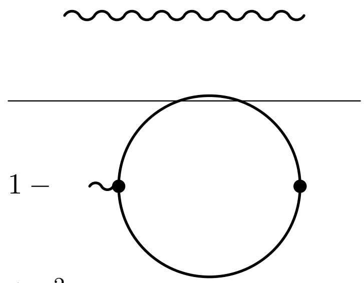


The content between the brackets is recognized as a geometric series, the sum of which is known as

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}. \tag{29}$$

This gives us

$D(q,\omega) =$



$1 -$

$$= \frac{V_0(q)}{1 - V_0(q)\Pi^2(q,\omega)}$$

$$= \frac{4\pi e^2}{q^2}\frac{1}{\varepsilon(q,\omega)}.$$

Here $\varepsilon(q,\omega) = 1 - V_0(q)\Pi^{(2)}(q,\omega)$ is the dielectric constant. This we have to calculate, which means we have to calculate the feynman diagram

.

6.1 Calculation of $\Pi^{(2)}(q,\omega)$

Use the Feynman rules. $F = 1$: number of vertexes $= 2 \implies m = 1$. The prefactor is

$$i(-1)^1(2 \cdot \frac{1}{2} + 1)^1 \sum_{k,q} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} G_0(k+q, \omega+\omega') \cdot G(k,\omega'). \tag{30}$$

Remember that

$$G_0(k,\omega) = \frac{\theta(\varepsilon_k - \varepsilon_F)}{\omega - \varepsilon_k + i\delta} + \frac{\theta(\varepsilon_F - \varepsilon_k)}{\omega - \varepsilon_k - i\delta}. \tag{31}$$

We do the frequency integral first by contour-integration and residue calculation. $\int_{-\infty}^{\infty} \mathrm{d}x \to \int_C \mathrm{d}z$, with C being a curve in the complex plane that closes the integral over x. Whether we close the integral in the upper or lower part of the complex plane is up to us. We have the freedom to choose whether to close the contour in the lower or upper complex plane. Let's first look at terms in (EQ p. 170) on the form

$$\int_{-\infty}^{\infty} dx \frac{1}{x - A + i\delta}\frac{1}{x - B + i\delta}. \tag{32}$$

We chose to close the contour in the upper complex half-plane, and we get

$$\int_{upper} dz \frac{1}{z - A + i\delta}\frac{1}{z - B + i\delta} = \frac{1}{A - B}\int_{upper} dz \{\frac{1}{z - A + i\delta} - \frac{1}{z - B + i\delta}\}. \tag{33}$$

Both $z - A + i\delta$ and $z - B + i\delta$ have their pole in the lower complex half-plane, and the integral is accordingly zero. We next look at terms on the form

$$\int_{-\infty}^{\infty} \frac{1}{x - A - i\delta} \frac{1}{x - B - i\delta}. \tag{34}$$

We choose to close the contour in the upper complex half-plane, and we get

$$\int_{upper} dz \frac{1}{z - A - i\delta} \frac{1}{z - B - i\delta} = \frac{1}{A - B} \int_{upper} dz \{ \frac{1}{z - A - i\delta} - \frac{1}{z - B - i\delta} \} \tag{35}$$

$$= \frac{1}{A - B}(2\pi i - 2\pi i) \tag{36}$$

$$= 0. \tag{37}$$

Both $z - A - i\delta$ and $z - B - i\delta$ have their pole in the upper complex half-plane, but the negative sign between the two terms in the integral cancel the residues. Finally we look at the cross-terms

$$\int_{-\infty}^{\infty} \frac{1}{x - A + i\delta} \frac{1}{x - B - i\delta}. \tag{38}$$

We choose to close the contour in the upper complex half-plane, and we get

$$\int_{upper} dz \frac{1}{z - A + i\delta} \frac{1}{z - B - i\delta} = \frac{1}{A - B - 2i\delta} \int_{upper} dz \{ \frac{1}{z - A + i\delta} - \frac{1}{z - B - i\delta} \} \tag{39}$$

$$= \frac{1}{A - B - 2i\delta}(0 - 2\pi i) \tag{40}$$

$$= \frac{-2\pi i}{A - B - 2i\delta}. \tag{41}$$

The only contribution here comes from the pole of $z = B + i\delta$. Similarly

$$\int_{upper} dz \frac{1}{z - A - i\delta} \frac{1}{z - B + i\delta} = \frac{2\pi i}{A - B - 2i\delta}. \tag{42}$$

Since the particle-propagator and the hole-propagator have poles in opposite half-planes, only the cross-terms between particle- and hole-propagators contribute to the diagram. We then have

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} G_0(k+q, \omega + \omega') G_0(k, \omega') &= \theta(\epsilon_k - \epsilon_F)\theta(\epsilon_F - \epsilon_{k+q}) \\
&\times \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{1}{\omega' - \epsilon_k + i\delta} \frac{1}{\omega + \omega' - \epsilon_{k+q} - i\delta} \\
&+ \theta(\epsilon_F - \epsilon_k)\theta(\epsilon_{k+q} - \epsilon_F) \\
&\times \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{1}{\omega + \omega' - \epsilon_{k+q} + i\delta} \frac{1}{\omega' - \epsilon_k - i\delta} \\
&= -2\pi i \frac{\theta(\epsilon_k - \epsilon_F)\theta(\epsilon_F - \epsilon_{k+q})}{\epsilon_k - \epsilon_{k+q} + \omega + 2i\delta} + 2\pi i \frac{\theta(\epsilon_F - \epsilon_k)\theta(\epsilon_{k+q} - \epsilon_F)}{\omega + \epsilon_k - \epsilon_{k+q} - 2i\delta}.
\end{aligned}$$

We have here used in the first term $A = \epsilon_k$, $B = \epsilon_{k+q} - \omega$, and in the second term $A = \epsilon_{k+q} - \omega$, $B = \epsilon_k$. In total we get

$$\Pi^{(2)}(q,\omega) = -2i\frac{2\pi i}{2\pi}(-1)\sum_k\{\frac{\theta(\epsilon_F - \epsilon_k)\theta(\epsilon_{k+q} - \epsilon_F)}{\omega + \epsilon_k - \epsilon_{k+q} - 2i\delta} - \frac{\theta(\epsilon_k - \epsilon_F)\theta(\epsilon_F - \epsilon_{k+q})}{\epsilon_k - \epsilon_{k+q} + \omega + 2i\delta}\}. \quad (43)$$

This expression is in general difficult to calculate. To illustrate how one carries out such a calculation we will take as an example a static screened Coulomb potential. We then have $\omega = 0$ and start out with $q > 0$, which we will take to zero later. We introduce $n(\epsilon_k) = \theta(\epsilon_k - \epsilon_F)$, i.e. the Fermi distribution at $T = 0$. We get

$$\Pi^{(2)}(q,0) = 2\sum_k\{\frac{n(\epsilon_k)\big[1 - n(\epsilon_{k+q})\big]}{\epsilon_k - \epsilon_{k+q} - 2i\delta} - \frac{n(\epsilon_{k+q})\big[1 - n(\epsilon_k)\big]}{\epsilon_k - \epsilon_{k+q} + 2i\delta}\}. \quad (44)$$

One can easily check that $Im(\Pi^{(2)}(q,0)) = 0$, and the real part is

$$Re(\Pi^{(2)}(q,0)) = 2\sum_k \frac{n(\epsilon_k) - n(\epsilon_{k+q})}{\epsilon_k - \epsilon_{k+q}} \overset{q\to 0}{\to} 2\sum_k \frac{\partial n(\epsilon_k)}{\partial \epsilon_k}. \quad (45)$$

Furthermore $\frac{\partial n(\epsilon_k)}{\partial \epsilon_k} = -\delta(\epsilon_k - \epsilon_F)$, and letting

$$\sum_k \to \int N(\epsilon)d\epsilon \approx N(\epsilon_F)\int d\epsilon \quad (46)$$

yields

$$\Pi^{(2)}(q,0) \overset{q\to 0}{\to} -2N(\epsilon_F), \quad (47)$$

where $N(\epsilon_F)$ is the density of states (DOS) at the Fermi level. With a Coulomb potential, $V_0 = \frac{4\pi e^2}{q^2}$, we now have

$$\begin{aligned} V &= \frac{V_0}{1 - V_0\Pi^{(2)}} \\ &= \frac{4\pi e^2}{q^2(1 - \frac{4\pi e^2}{q^2}(-2N(\epsilon_F)))} \\ &= \frac{4\pi e^2}{q^2 + \widetilde{q}^2}, \end{aligned}$$

where we have defined $\widetilde{q}^2 = 8\pi e^2 N(\epsilon_F)$. $\widetilde{q}$ here represents the inverse screening length. The $V(q)$ we have found represents a static, screened Coulomb potential. In real-space we now have

$$V(r) \approx \frac{e^2}{r}e^{-r\widetilde{q}} = \frac{e^2}{r}e^{-r/\lambda}.$$

If the screening length $\lambda = \widetilde{q}^{-1}$ is small, the screening of the Coulomb potential is strong. Increasing λ, reduces the Coulomb potential in strength. To illustrate this a little more, lets look at good metals and semiconductors. A good metal has a large density of states at the Fermi level, and since $\lambda \sim (N(\epsilon_F))^{-1/2}$ then is small the Coulomb potential is screened. For a semiconductor on the other hand the Fermi level lies above the topmost filled states, such that $N(\epsilon_F) = 0$, and the Coulomb potential is not screened.

6.2 Quasi Particles in Interacting Electron Systems

In a free electron system we have seen that the propagator has the form

$$G_0(k,\omega) = \frac{1}{\omega - \epsilon_k + i\delta_k}, \tag{48}$$

where we have defined $\delta_k = \delta \mathrm{sgn}(\epsilon_k - \epsilon_F)$. The simple poles means that the system has well defined single particle excitations, $\omega = \epsilon_k$, with an infinite lifetime. This is because δ is infinitesimal. In an interacting system, Dysons equation yields

$$G = \frac{1}{\omega - \epsilon_k - \Sigma(k,\omega)}. \tag{49}$$

We wish to investigate if we can write this on the form

$$G \sim \frac{1}{\omega - \widetilde{\epsilon}_k - \frac{1}{\tau_k}}. \tag{50}$$

$\widetilde{\epsilon}_k$ is here the renormalized dispersion realation, and τ_k is the lifetime of a single particle excitation. If this is possible, the interacting system is said to have quasi particles, which we consider as renormalized electrons (with for instance an effective mass $m^* > m$. Generally we can write

$$\Sigma = \Sigma_R + i\Sigma_I. \tag{51}$$

We assume that the imaginary part is small, i.e. that damping effects in our system are negligible

$$\frac{\mid \Sigma_I \mid}{\mid \Sigma_R \mid} \ll 1. \tag{52}$$

The quasi particle poles are found from

$$\omega - \epsilon_k - \Sigma_R(k,\omega) - i\Sigma_I(k,\omega) = 0. \tag{53}$$

The solution, ω, to this equation will give the quasi particle excitation energies. To 0th order we ignore Σ_I and get

$$\omega = \widetilde{\epsilon_k} = \epsilon_k + \Sigma_R(k,\omega), \tag{54}$$

where

$$\Sigma_R = \Sigma_R(k,\widetilde{\epsilon_k}) + (\omega - \widetilde{\epsilon_k})\frac{\partial \Sigma_R}{\partial \omega}. \tag{55}$$

We can set $\omega = \widetilde{\epsilon_k} + \omega_1$, where ω_1 is a correction to $\widetilde{\epsilon_k}$ caused by $\Sigma_I \neq 0$. Inserting this yields

$$\omega_1 - \omega_1 \Sigma_R' - i\Sigma_I(k,\widetilde{\epsilon_k}) = 0, \tag{56}$$

with

$$\Sigma_R' = \frac{\partial \Sigma_R(k,\omega)}{\partial \omega} \mid_{\omega=\widetilde{\epsilon_k}} . \tag{57}$$

We finally get

$$\omega_1 = \frac{i\Sigma_I(k, \widetilde{\epsilon_k})}{1 - \Sigma'_R}. \tag{58}$$

With $\omega = \widetilde{\epsilon_k} - \frac{i}{\tau_k} = \widetilde{\epsilon_k} + \omega_1$ we find the quasi particle lifetime

$$\frac{1}{\tau_k} = -\frac{\Sigma_I(k, \widetilde{\epsilon_k})}{1 - \Sigma'_R}, \tag{59}$$

and the quasi particle excitation energy

$$\widetilde{\epsilon_k} = \epsilon_k + \Sigma_R(k, \widetilde{\epsilon_k}). \tag{60}$$

Inserting all this into the expression for G of the interacting system yields

$$\begin{aligned} G(k, \omega) &= \frac{1}{\omega - \epsilon_k - \Sigma_R(k, \omega) - i\Sigma_I(k, \omega)} && (61) \\ &\approx \frac{1}{\omega - \widetilde{\epsilon_k} - (\omega - \widetilde{\epsilon_k})\Sigma'_R + \frac{i}{\tau_k}(1 - \Sigma'_R)} && (62) \\ &= \frac{1/(1 - \Sigma'_R)}{\omega - \widetilde{\epsilon_k} + \frac{1}{\tau_k}}. && (63) \end{aligned}$$

We now define

$$Z_k = 1 - \Sigma'_R \tag{64}$$

, which is the weight to our quasi particle pole, or the quasi particle residue. We then get the wanted quasi particle form for G

$$G(k, \omega) = \frac{Z_k}{\omega - \widetilde{\epsilon_k} + \frac{1}{\tau_k}}. \tag{65}$$