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:

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

Exercise: 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.)

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

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

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

$\ket{\psi}$: 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

$$\mathcal{H} \ket{\psi_{N_i}} = E_{N_i} \ket{\psi_{N_i}},$$

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

$$\mathcal{Z} = \text{Tr}(e^{-\beta\mathcal{H}}) = \sum_n \bra{n} e^{-\beta\mathcal{H}} \ket{n}, \qquad \beta = \frac{1}{k_B T},$$

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:

$$\mathcal{Z} = \text{Tr}(e^{-\beta \mathcal{H}}) = \text{Tr}(SS^{-1}e^{-\beta \mathcal{H}}) = \text{Tr}(S^{-1}e^{-\beta \mathcal{H}}S)$$

$$= \sum_n \langle n|S^{-1}e^{-\beta \mathcal{H}}S|n\rangle = \sum_{n'} \langle n'|e^{-\beta \mathcal{H}}|n'\rangle,$$

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

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

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

$$= \frac{1}{\mathcal{Z}} \sum_i \underbrace{\langle N_i|\hat{\mathcal{O}}|N_i\rangle}_{\substack{\text{mean value in} \\ \text{e.g. state}|N_i\rangle}} e^{-\beta E_{N_i}},$$

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" ⇒ "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

$$\lambda = (i,\sigma), \qquad |n_{i,\sigma}\rangle = c_{i,\sigma}^{\dagger}|0\rangle, \qquad \varphi_{i,\sigma} = \phi_w^i(\boldsymbol{r}_i),$$

where i is a lattice point.

1.3 Many-particle states

An N-particle state is given by

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

where

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

This is often called a Fock state.

In the case of fermions we can have <u>maximum one</u> 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

$$\psi^{\dagger}(\boldsymbol{r},t) = \sum_{\lambda} c_{\lambda}^{\dagger}(t)\varphi_{\lambda}^*(\boldsymbol{r}).$$

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

$c_{\lambda}^{\dagger}(t)$: <u>Operator</u> that requires a fermion with a certain quantum number λ at time t.

$\varphi_{\lambda}^*(\boldsymbol{r})$: <u>Function</u> 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.

Orthonormalization

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

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:

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

What commutation relations should be satisfied? In the case of fermions this is the anticommutator relation
$$\left[\psi^\dagger(\boldsymbol{r},t),\psi(\boldsymbol{r}',t)\right]_+ = \delta(\boldsymbol{r}-\boldsymbol{r}') = \sum_{\lambda_1,\lambda_2} \varphi_{\lambda_1}^*(\boldsymbol{r})\varphi_{\lambda_2}(\boldsymbol{r}')\left[c_{\lambda_1}^\dagger, c_{\lambda_2}^\dagger\right]_+.$$

In case that
$$\left[c_{\lambda_1}^\dagger, c_{\lambda_2}\right]_+ = \delta_{\lambda_1,\lambda_2},$$

we get, from completeness:

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

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

In addition it is trivially shown that

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

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

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

Interpretation of the anticommutation relations

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

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

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

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

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:

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

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

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

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:

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

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 <u>distinct</u> pairs.

<u>Example:</u> 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 same 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

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

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

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The latter satisfies the following relations:

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

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

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

But: 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

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

$$= \int d\boldsymbol{r}\, \varphi_{\lambda_1}^*(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right)\varphi_{\lambda_2}(\boldsymbol{r})$$

$$= \varepsilon_{\lambda_2}\int d\boldsymbol{r}\, \varphi_{\lambda_1}^*(\boldsymbol{r})\varphi_{\lambda_2}(\boldsymbol{r})$$

$$= \varepsilon_{\lambda_2}\delta_{\lambda_1,\lambda_2},$$

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 $c_\lambda^\dagger$ that gives the same matrix elements?

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

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

$$|\lambda_2\rangle = c_{\lambda_2}^\dagger|0\rangle$$

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

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

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

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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 $\mathcal{H}_1$.

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

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

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

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

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

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:

<u>Please note:</u> 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.

<u>Example:</u> 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.

<u>Example:</u> 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.

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 good metals (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

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

The basis is given by

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

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

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

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 $\sigma = \downarrow$ ($S_z = +1/2, -1/2$):

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

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:

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

Completeness:

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

where

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

The field operators are now given by

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

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

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

where $c_{\boldsymbol{k},\sigma}^\dagger(t)$ 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):

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

$$\langle \lambda_1|U|\lambda_2 \rangle = \sum_{x} \varphi^*_{\lambda_1}(x) \, U(x) \, \varphi_{\lambda_2}(x)$$

$$= \sum_{s} \int d\boldsymbol{r} \, \chi^*_{\sigma_1}(s) \frac{1}{\sqrt{V}} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} \underbrace{U(\boldsymbol{r})}_{\text{spin-independent potential}} \chi_{\sigma_2}(s) \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}$$

$$= \underbrace{\sum_{s} \chi^*_{\sigma_1}(s)\chi_{\sigma_2}(s)}_{\delta_{\sigma_1,\sigma_2}} \underbrace{\frac{1}{V} \int d\boldsymbol{r} \, U(\boldsymbol{r}) \, e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}}}_{\equiv \tilde{U}(\boldsymbol{k}_1-\boldsymbol{k}_2)},$$

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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

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

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

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

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

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

$$\tag{8}$$

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:

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

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

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 $\quad \Rightarrow \quad$ 2 spin sums remain,

- 1 δ function of $\boldsymbol{k}$ $\quad \Rightarrow \quad$ 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:

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

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. The tunneling represents the electron's kinetic energy. The kinetic energy in the lattice fermion model therefore has its origin in electrostatic interactions! The details are as follows.

Field operators

$$\psi_j^\dagger(\boldsymbol{r}, s, t) = \sum_{n,\sigma} c_{n,\sigma,j}^\dagger(t)\phi_{n,j}^*(\boldsymbol{r})\chi_\sigma^*(s),$$

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

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

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:

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

where $\varepsilon_{n,\sigma,i}$ is the energy of the electron in the isolated 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:

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

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 irregularity 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 regular 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

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

by using the result in equation (6):

$$= \sum_{\substack{n_1,\sigma_1,i_1 \\ n_2,\sigma_2,i_2}} \langle n_1, \sigma_1, i_1 | \underbrace{\sum_{j \neq i} U_a | n_2, \sigma_2, i_2 \rangle}_{\text{No summation over } i \text{ here!}} c_{n_1,\sigma_1,i_1}^\dagger c_{n_2,\sigma_2,i_2} \langle n_1, \sigma_1, i_1 | \underbrace{\sum_{j \neq i} U_a(\boldsymbol{r}_i, \boldsymbol{R}_j) | n_2, \sigma_2, i_2 \rangle}_{\text{Note: } \sum_i \boldsymbol{r}_i \to \int d\boldsymbol{r}}$$

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

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

which gives us

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

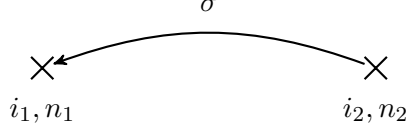This is a "hopping" process <u>from</u> lattice point i_2 <u>to</u> lattice point i_1.

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.

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

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

$$\mathcal{H}_1 = \sum_{n, \sigma, i} \varepsilon_n c_{n, \sigma, i}^{\dagger} c_{n, \sigma, i} + \underbrace{\sum_{\substack{n_1, i_1 \\ n_2, i_2 \\ \sigma}} t_{i_1, i_2}^{n_1, n_2} c_{n_1, \sigma_1, i_1}^{\dagger} c_{n_2, \sigma_2, i_2}}.$$

Contains both intra and interatomic "hopping" processes.

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

i) Assume that

$$t_{i,j}^{n, n'} = t_{i,j} \delta_{n, n'} + \text{"small terms"}.$$

This means that the tunnelling between lattice points mainly occurs from an orbital at one lattice point to the <u>same</u> 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).

$$t_{i_1, i_2}^{n_1, n_2} \rightarrow t_{i_1, i_2}.$$

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:

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

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

$$\frac{1}{2} \sum_{i,j} V(\boldsymbol{r}_i - \boldsymbol{r}_j) \Rightarrow \frac{1}{2} \sum_{\lambda_1, \cdots, \lambda_4} \langle \lambda_1, \lambda_2 | V | \lambda_3, \lambda_4 \rangle c_{\lambda_1}^\dagger c_{\lambda_2}^\dagger c_{\lambda_3} c_{\lambda_4}$$

$$= \frac{1}{2} \sum_{\substack{i_1, \cdots, i_4 \\ \sigma_1, \cdots, \sigma_4}} \langle \sigma_1, i_i; \sigma_2, i_2 | V | \sigma_3, i_3; \sigma_4, i_4 \rangle c_{\sigma_1, i_1}^\dagger c_{\sigma_2, i_2}^\dagger c_{\sigma_3, i_3} c_{\sigma_4, i_4}$$

$$\langle \sigma_1, i_i; \sigma_2, i_2 | V | \sigma_3, i_3; \sigma_4; i_4 \rangle = \sum_{x_1, x_2} \varphi_{\lambda_1}^*(x_1) \varphi_{\lambda_2}^*(x_2) \underbrace{V(x_1, x_2)}_{\text{spin independent}} \varphi_{\lambda_3}(x_2) \varphi_{\lambda_4}(x_1)$$

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

$$\times \int d\boldsymbol{r}_1 \, d\boldsymbol{r}_2 \, \phi_{i_1}^*(\boldsymbol{r}_1) \phi_{i_2}(\boldsymbol{r}_2) V(\boldsymbol{r}_1 - \boldsymbol{r}_2) \phi_{i_3}(\boldsymbol{r}_2) \phi_{i_4}(\boldsymbol{r}_1)$$

$$= \delta_{\sigma_1, \sigma_4} \, \delta_{\sigma_2, \sigma_3} \, V_{i_1, i_2, i_3, i_4},$$

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

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

<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:

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

25

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

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

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 antiferromagnetic 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

$$V_{i_1, \cdots, i_4}, \quad \text{with} \quad \left\{ \begin{array}{l} i_1 = i_4 \\ i_2 = i_3 \end{array} \right. , \quad \text{where } i_1 \text{ and } i_2 \text{ are } \underline{\text{nearest}} \text{ neighbours.}$$

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

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:

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

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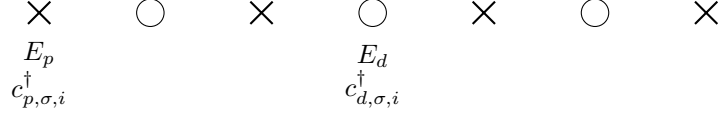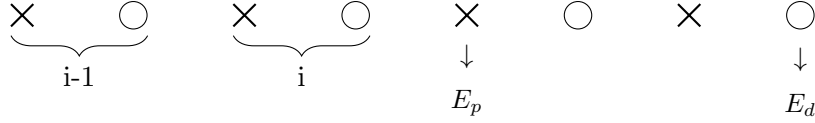
Figure 2: Lattice with two types of lattice points, where $E_p \neq E_d$ and p and d are the orbital indices [].

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

The hopping terms can be written in the form

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

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 <u>phase transitions</u>, 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 <u>boson properties</u>.

> **Fundamental boson properties**
>
>   i) Symmetric under exchange of two single-particle states.
>
>   ii) <u>No</u> limit on the occupation number in single-particle states.

$$|N\rangle = \prod_\lambda |n_\lambda\rangle\,, \qquad a_\lambda^\dagger |0\rangle = |\lambda\rangle\,, \qquad a |0\rangle = 0.$$

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

$$(a_\lambda^\dagger)^n |0\rangle \propto |n_\lambda\rangle\,.$$

Normalizing the above:

$$c_n |n_2 + 1\rangle = a_\lambda^\dagger |n\rangle\,,$$

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

$$a_\lambda^\dagger a_\lambda |n_\lambda\rangle = n_\lambda |n_\lambda\rangle\,,$$

and the following commutation relations apply:

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

Calculating the normalization constant:

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

which means that

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

and

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

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, <u>material</u>, 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:

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

<u>Note:</u> For <u>phonons</u> 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 $t = 0$.

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

$|\psi_0\rangle$ 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. <u>Note!</u> $|\psi_0\rangle$ is degenerate, such that any combination of the 2^N degenerate eigenstates of $\mathcal{H}_0$ are eigenstates. <u>But:</u> From degenerate perturbation theory we know that not <u>all</u> 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

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

First order correction to E_0

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

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

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

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

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

$$|n\rangle : \text{unperturbed excited states},$$

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

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 $E_n = E_0 + U$:

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

$$= \langle \psi_0 | \mathcal{H}_{\text{eff}} | \psi_0 \rangle ,$$

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

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

$$= -\frac{1}{U} \sum_{\substack{i,j,k,l \\ \sigma,\sigma'}} t_{i,j} t_{k,l} c^\dagger_{i,\sigma} c_{j,\sigma} c^\dagger_{k,\sigma'} c_{l,\sigma'}.$$

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:

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

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

This term has the same form as

$$\sum_{i,\sigma} \varepsilon c_{i,\sigma}^\dagger c_{i,\sigma},$$

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

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

<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 $c_{i,\sigma}^\dagger c_{i,\sigma'}$ 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:

$$\sum_{\sigma\sigma'} c_{i,\sigma}^\dagger c_{i,\sigma'} c_{j,\sigma'}^\dagger c_{j,\sigma}$$
$$= \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow$$
$$+ \downarrow \quad \uparrow \quad \uparrow \quad \downarrow$$
$$+ \uparrow \quad \downarrow \quad \downarrow \quad \uparrow$$
$$+ \downarrow \quad \downarrow \quad \downarrow \quad \downarrow$$

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 $c_\uparrow^\dagger c_\uparrow$ etc. becomes irreducible.

$$c_\uparrow^\dagger c_\uparrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \quad ; \quad c_\downarrow^\dagger c_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
$$c_\uparrow^\dagger c_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad ; \quad c_{\downarrow\downarrow}^\dagger c_\downarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

$$
\left.
\begin{array}{l}
\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\[6pt]
\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathbf{0}
\end{array}
\right\}
\quad \Rightarrow \quad c_\uparrow^\dagger c_\uparrow = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}
$$

$$
\left.
\begin{array}{l}
\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbf{0} \\[6pt]
\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\end{array}
\right\}
\quad \Rightarrow \quad c_\downarrow^\dagger c_\downarrow = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}
$$

$$
\left.
\begin{array}{l}
c_\uparrow^\dagger c_\downarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbf{0} \\[6pt]
c_\uparrow^\dagger c_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}
\end{array}
\right\}
\quad \Rightarrow \quad c_\uparrow^\dagger c_\downarrow = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}
$$

$$
\left.
\begin{array}{l}
c_\downarrow^\dagger c_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\[6pt]
c_\downarrow^\dagger c_\uparrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathbf{0}
\end{array}
\right\}
\quad \Rightarrow \quad c_\downarrow^\dagger c_\uparrow = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.
$$

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 $SU(2)$.

$$
\left.
\begin{array}{l}
c_\uparrow^\dagger c_\uparrow = \dfrac{1}{2} \left(1 + \sigma_z\right) \\[8pt]
c_\downarrow^\dagger c_\downarrow = \dfrac{1}{2} \left(1 - \sigma_z\right) \\[8pt]
c_\uparrow^\dagger c_\downarrow = \dfrac{1}{2} \left(\sigma_x + i\sigma_y\right) = \dfrac{1}{2} \sigma^+ \\[8pt]
c_\downarrow^\dagger c_\uparrow = \dfrac{1}{2} \left(\sigma_x - i\sigma_y\right) = \dfrac{1}{2} \sigma^-
\end{array}
\right\}
\quad
\begin{array}{l}
\underline{\text{Note!}} \text{ This connection is independ-} \\
\text{ent of the representation of the Pauli} \\
\text{spin operators (Pauli matrices).}
\end{array}
$$

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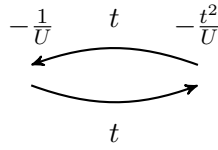
$$\boldsymbol{\sigma} = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}.$$

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:

$$
\begin{array}{ccc}
-\frac{1}{U} & t & -\frac{t^2}{U} \\
& t &
\end{array}
$$

> 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.

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

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 pairwise 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?

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

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

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

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

Note!: 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.

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

$$
\sum_{\substack{i_1 i_2 \\ \sigma_1 \sigma_2}} \langle i_1 i_2|\, V\, |i_2 i_1\rangle\, c^{\dagger}_{i_1\sigma_1} c^{\dagger}_{i_2\sigma_2} c_{i_2\sigma_2} c_{i_1\sigma_1} = \sum_{\substack{ij \\ \sigma\sigma'}} \langle ij|\, V\, |ji\rangle\, c^{\dagger}_{i\sigma} c_{i\sigma} c^{\dagger}_{j\sigma'} c_{j\sigma'}
$$

$$
= \sum_{ij} \langle ij|\, V\, |ji\rangle\, n_i n_j.
$$

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

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

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

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

<u>Note</u>!: 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:

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

Two-center integrals with pairwise equal lattice indices $\left\{ \begin{array}{l} + \displaystyle\sum_{ij} V_{ij} n_i n_j + \displaystyle\sum_{ij\sigma} t^P_{ij} c^\dagger_{i\sigma} c^\dagger_{i-\sigma} c_{j-\sigma} c_{j\sigma} \\[3mm] - \displaystyle\sum_{ij} \tilde{J}_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \quad \begin{array}{l} i, j: \quad \text{Not \ necessarily} \\ \text{nearest neighbours!} \end{array} \end{array} \right.$

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. [**charkravarty1989**] 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:

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

$$S_i^+ |\uparrow\rangle = 0 \ ; \quad S_i^+ |\downarrow\rangle = |\uparrow\rangle$$

$$S_i^- |\uparrow\rangle = |\downarrow\rangle \ ; \quad S_i^- |\downarrow\rangle = 0$$

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

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

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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

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

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.

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

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

This is a spin flip on lattice site i. We obtain energy: $4S^2 J$ 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:

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

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

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:

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

This can be regarded as an expansion in large S.

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

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

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

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

where we have defined $E_0 = -J \sum_{\langle i,j \rangle} S^2 = -JS^2 Nz$ for $N = $ *number of lattice sites* and $z = $ *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 of the form

$$\sum_\lambda \omega_\lambda \underbrace{a_\lambda^\dagger a_\lambda}_{\substack{\text{Same quantum} \\ \text{number}}} \quad : \quad \text{Free boson gas}$$

ω_λ: 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

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

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

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

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

$$= \sum_{\boldsymbol{q}_1} \sum_{\boldsymbol{\delta}} a_{q_1}^\dagger a_{q_2}^\dagger e^{i\boldsymbol{q}_1 \cdot \boldsymbol{\delta}}.$$

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

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

$$= E_0 + \sum_{\boldsymbol{q}} \omega_q a_q^\dagger a_q.$$

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

4.3   2D quadratic lattice

In the

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

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

$$\omega_{\boldsymbol{q}} \approx 2JS \left[4 - 2 \left(1 - \frac{(q_x a)^2}{2} \right) - 2 \left(1 - \frac{(q_y a)^2}{2} \right) \right]$$

$$= 2JS\boldsymbol{q}^2 a^2,$$

$$\boldsymbol{q}^2 = q_x^2 + q_y^2.$$

This behaviour is shown in figure **??**. 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

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

with

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

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 <u>magnons</u>. 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 <u>lattice fermion</u> 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
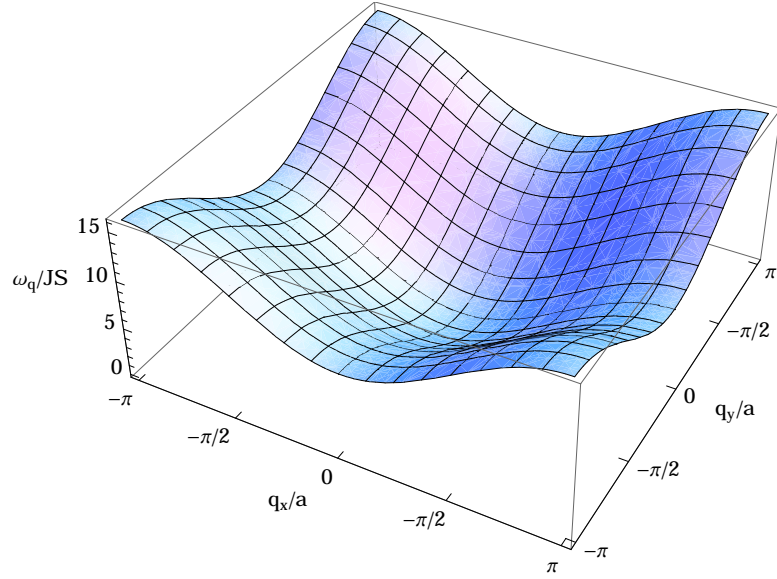
Figure 3: The angular frequency $\omega_{\boldsymbol{q}}$ as a function of the momentum $\boldsymbol{q}$.
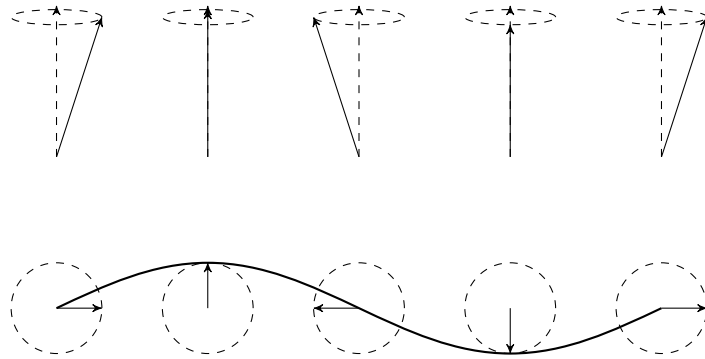

Figure 4: The spins precess slowly in space, creating spin waves.

ferromagnetic case). This gave rise to a free <u>boson theory</u> 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)

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

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

$$\mathcal{H} = NS - N\Omega_d \frac{1}{2\sqrt{\eta}} \left(\frac{1}{\sqrt{\eta}} \right)^{d-1} \underbrace{\int_0^\infty dx \, \frac{x^{d/2-1}}{e^x - 1}}_{A(d)}$$

$$= NS - N\Omega_d \, A(d) \left(\frac{T}{JS} \right)^{d/2}$$

$$= NS \quad \text{for} \quad T = 0.$$

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 <u>many</u> spins. They are therefore collective spin excitations. Note also that $A(d)$ diverges when <u>$d = 1$</u>. What does that mean? And what happens when $d = 2$?

4.4 Antiferromagnets

The contribution to the Hamiltonian from spin interactions is given by

$$\mathcal{H} = -\sum_{i,j} J_{i,j} \vec{S}_i \cdot \vec{S}_j, \qquad J_{i,j} < 0.$$
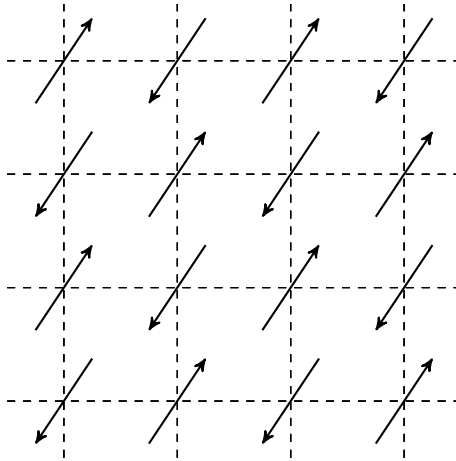
44

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 $J_{i,j}$ <u>stabilises</u> such a spin distribution. Note that next-nearest neighbour spin points in the <u>same</u> direction. That means that a next-nearest neighbour $J_{i,j}$ contributes to <u>destabilise</u> 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 <u>triangular</u> lattice:
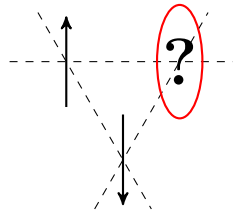
The conclusion is that in antiferromagnets the physics on small scales carries meaning for the physics on larger scales.

Next-nearest neighbour coupling

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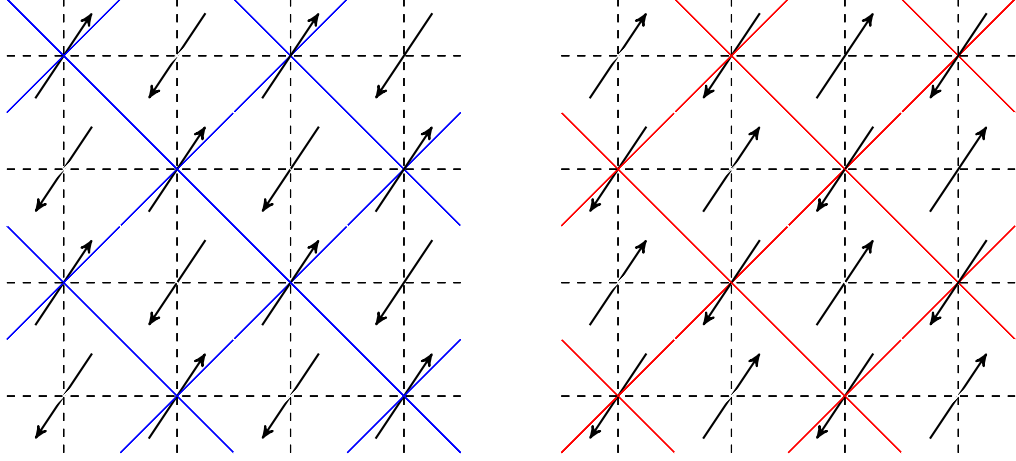

$$\left(\quad \right) \propto \frac{t^4}{u^3}.$$

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 <u>interpenetrating</u> sublattices, A (spin up) and B (spin down). The unit cells in A and B are <u>twice</u> 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.

$$A: \begin{cases} S_{i,z}^A = S - a_i^\dagger a_i, \\[2ex] S_{i,+}^A = \sqrt{2S}\left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2} a_i, \\[2ex] S_{i,-}^A = \sqrt{2S}\, a_i^\dagger \left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2}. \end{cases} \tag{9}$$

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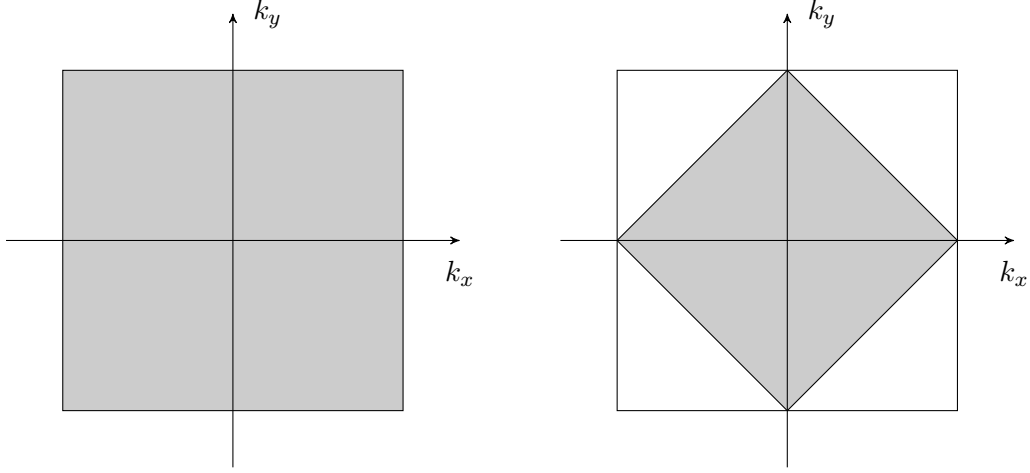
Figure 7:   The Brillouin zones in the original lattice (left) and the sublattices A and B (right).

$$
B : \begin{cases}
S_{i,z}^{B} = -S + b_i^\dagger b_i, \\[2ex]
S_{i,+}^{B} = \sqrt{2S}\left(1 - \dfrac{b_i b_i^\dagger}{2S}\right)^{1/2} b_i^\dagger, \\[2ex]
S_{i,-}^{B} = \sqrt{2S}\, b_i \left(1 - \dfrac{b_i b_i^\dagger}{2S}\right)^{1/2}.
\end{cases}
\tag{10}
$$

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

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

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

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \left(S_{i,z} S_{j,z} + S_{i,+} S_{j,-} \right)$$

$$= -J \sum_{\substack{i \in A \\ j \in B \\ \text{n.n.}}} \left(S_{i,z}^A S_{j,z}^B + S_{i,+}^A S_{j,-}^B \right) - J \sum_{\substack{i \in B \\ j \in A \\ \text{n.n.}}} \left(S_{i,z}^B S_{j,z}^A + S_{i,+}^B S_{j,-}^A \right).$$

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 (9, 9) as

$$A : \begin{cases} S_{i,z}^A = S - a_i^\dagger a_i, \\[2mm] S_{i,+}^A = \sqrt{2S}\, a_i, \\[2mm] S_{i,-}^A = \sqrt{2S}\, a_i^\dagger. \end{cases} \quad , \quad B : \begin{cases} S_{i,z}^B = -S + b_i^\dagger b_i, \\[2mm] S_{i,+}^B = \sqrt{2S}\, b_i^\dagger, \\[2mm] S_{i,-}^B = \sqrt{2S}\, b_i. \end{cases}$$

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

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

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

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

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

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

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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 47). 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

$$\left.\begin{aligned} \sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n. to } i}} a_i^\dagger b_j^\dagger &= \sum_{\boldsymbol{q}} \gamma_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}}^\dagger \\[2em] \sum_{\substack{i\in\mathrm{A}\\ j\in\mathrm{B}\\ \text{n.n. to } i}} a_i b_j &= \sum_{\boldsymbol{q}} \gamma_{\boldsymbol{q}} a_{\boldsymbol{q}} b_{\boldsymbol{q}} \end{aligned}\right\} \qquad \gamma_{\boldsymbol{q}} = \sum_{\boldsymbol{\delta}} e^{+i\boldsymbol{q}\cdot\boldsymbol{\delta}}.$$

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

$$\mathcal{H} = E_0 - 2JSz \sum_{\boldsymbol{q}} \left(a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} + a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} \right) - 2JS \sum_{\boldsymbol{q}} \gamma_{\boldsymbol{q}} \left(a_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}}^\dagger + a_{\boldsymbol{q}} b_{\boldsymbol{q}} \right). \qquad (11)$$

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:

$$\begin{aligned} A_{\boldsymbol{q}} &= u_{\boldsymbol{q}} a_{\boldsymbol{q}} + v_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger, \qquad & a_{\boldsymbol{q}} &= u_{\boldsymbol{q}} A_{\boldsymbol{q}} - v_{\boldsymbol{q}} B_{\boldsymbol{q}}^\dagger, \\[1em] B_{\boldsymbol{q}} &= v_{\boldsymbol{q}} a_{\boldsymbol{q}} + u_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger, \qquad & b_{\boldsymbol{q}} &= u_{\boldsymbol{q}} B_{\boldsymbol{q}} - v_{\boldsymbol{q}} A_{\boldsymbol{q}}^\dagger. \end{aligned} \qquad (12)$$

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

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

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Substituting this back into equation (11) 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

$$\frac{\gamma_{\boldsymbol{q}}}{2} = \cos(q_x) + \cos(q_y), \qquad \tilde{\gamma}_{\boldsymbol{q}} = \frac{1}{2} \sum_{\alpha} \cos(q_{\alpha}),$$

$$\omega_{\boldsymbol{q}} = 4|J|S \left(4 - (\cos(q_x) + \cos(q_y))^2 \right)^{1/2},$$

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

$$\omega_{\boldsymbol{q}} = 4|J|S \left(4 - \left(2 - \frac{\boldsymbol{q}^2}{2} \right)^2 + \cdots \right)^{1/2} = 4|J|S \left(4 - 4 \left(1 - \frac{\boldsymbol{q}^2}{2} \right) + \cdots \right)^{1/2}$$

$$= 4\sqrt{2}|J|S|\boldsymbol{q}|,$$

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

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

Here the expectation value of $a_{\boldsymbol{q}}^{\dagger} a_{\boldsymbol{q}}$ can be calculated using equation (12):

$$\left\langle a_{\boldsymbol{q}}^{\dagger} a_{\boldsymbol{q}} \right\rangle = \left\langle \left(u_{\boldsymbol{q}} A_{\boldsymbol{q}}^{\dagger} - v_{\boldsymbol{q}} B_{\boldsymbol{q}}^{\dagger} \right) \left(u_{\boldsymbol{q}} A_{\boldsymbol{q}} - v_{\boldsymbol{q}} B_{\boldsymbol{q}}^{\dagger} \right) \right\rangle$$

$$= u_{\boldsymbol{q}}^2 \left\langle A_{\boldsymbol{q}}^{\dagger} A_{\boldsymbol{q}} \right\rangle - u_{\boldsymbol{q}} v_{\boldsymbol{q}} \left\langle A_{\boldsymbol{q}}^{\dagger} B_{\boldsymbol{q}}^{\dagger} \right\rangle - u_{\boldsymbol{q}} v_{\boldsymbol{q}} \left\langle B_{\boldsymbol{q}} A_{\boldsymbol{q}} \right\rangle + v_{\boldsymbol{q}}^2 \left\langle B_{\boldsymbol{q}} B_{\boldsymbol{q}}^{\dagger} \right\rangle$$

$$= u_{\boldsymbol{q}}^2 n_{\mathrm{B}}(\omega_{\boldsymbol{q}}) + v_{\boldsymbol{q}}^2 \left[1 + n_{\mathrm{B}}(\omega_{\boldsymbol{q}}) \right].$$

Here we used that

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

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:

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

where

$$\boxed{n_{\mathrm{B}}(\omega_{\boldsymbol{q}}) = \frac{1}{e^{\beta \omega_{\boldsymbol{q}}} - 1}.}$$

What will be the low-temperature form of the T-dependent correction to the magnetization?

4.6 Anharmonicity

A series expansion of $\sum_{n,m} V(R_n - R_{m+n})$ to higher orders than the quadratic term gives anharmonic contributions. We look at the third-order term, which gives the first correction to the ideal boson gas picture.

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

Again we introduce the Fourier transforms of x_n, such that

$$\sum_n x_n^3 = \sum_n \left(\frac{1}{\sqrt{N}} \sum_{k_1} \tilde{x}_{k_1} e^{ik_1 n} \right) \left(\frac{1}{\sqrt{N}} \sum_{k_2} \tilde{x}_{k_2} e^{ik_2 n} \right) \left(\frac{1}{\sqrt{N}} \sum_{k_3} \tilde{x}_{k_3} e^{ik_3 n} \right)$$

$$= \frac{1}{\sqrt{N}} \sum_{k_1, k_2, k_3} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{k_3} \underbrace{\frac{1}{N} \sum_n e^{i(k_1 + k_2 + k_3)n}}_{\delta_{k_1, -k_2 - k_3}}$$

$$= \frac{1}{\sqrt{N}} \sum_{k_1, k_2} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1 - k_2},$$

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

$$\sum_n x_n x_{n+m}^2 = \sum_{n'} x_{n'}^2 x_{n'-m}$$

$$= \frac{1}{\sqrt{N}} \sum_{k_1,k_2} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2} e^{-ik_1 m}.$$

Now the anharmonic third order term is

$$\frac{1}{6} \sum_m \Gamma(-R_m^0) \sum_n (x_n - x_{n+m})^3 = \frac{1}{6} \sum_m \Gamma(-R_m^0) \sum_n (x_n^3 - x_{n+m}^3 - 3x_n^2 x_{n+m} + 3x_n x_{n+m}^2)$$

$$= \frac{1}{6} \sum_m \left(-\Gamma(-R_m^0)\right) \sum_{k_1,k_2} \frac{1}{\sqrt{N}} \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2} \left(e^{ik_1 m} - e^{-ik_1 m}\right)$$

$$= \sum_{k_1,k_2} M(k_1) \tilde{x}_{k_1} \tilde{x}_{k_2} \tilde{x}_{-k_1-k_2},$$

$$\tag{13}$$

where

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

The anharmonic third order term can further be written

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

$$\sum_{k_1,k_2} G(k_1, k_2) \left(a_{-k_1}^\dagger a_{-k_2}^\dagger a_{-q}^\dagger + a_{-k_1}^\dagger a_{-k_2}^\dagger a_q^\dagger + a_{-k_1}^\dagger a_{k_2} a_{-q}^\dagger + a_{-k_1}^\dagger a_{k_2}^\dagger a_q \right.$$

$$\left. + a_{k_1} a_{-k_2}^\dagger a_{-q}^\dagger + a_{k_1} a_{-k_2}^\dagger a_q + a_{k_1} a_{k_2} a_{-q}^\dagger + a_{k_1} a_{k_2} a_q \right).$$

It is possible to do similar calculations for even higher order anharmonic terms.

We notice that the number of phonons are not conserved in the scattering process resulting from the anharmonic term. However; <u>momentum is always conserved in all scattering processes!</u>

Anharmonic 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:

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

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

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

4.7 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.

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

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

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

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

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

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

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

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

The minus sign is just a convention which gives less minus signs in the calculations.

We now write $V_{\text{el-ion}}$ 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

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

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

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

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

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

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

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

Finally,

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

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

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

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

and we want a description of the *quantized* changes which happen as a result of per-turbations 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)
$$V = \sum_{\boldsymbol{k},\boldsymbol{q},\sigma,\lambda} M_{\boldsymbol{q},\lambda}(a_{-\boldsymbol{q},\lambda}^\dagger + a_{\boldsymbol{q},\lambda}) c_{\boldsymbol{k}+\boldsymbol{q},\sigma}^\dagger c_{\boldsymbol{k},\sigma}$$

(Electron-phonon coupling)

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

(Electron-electron interaction)

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 on 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: $\langle\psi(t)|\hat{\mathcal{O}}(0)|\psi(t)\rangle = \langle\psi(0)|e^{i\mathcal{H}t}\hat{\mathcal{O}}(0)e^{-i\mathcal{H}t}|\psi(0)\rangle$
Heisenberg: $\langle\psi(0)|\hat{\mathcal{O}}(t)|\psi(0)\rangle = \langle\psi(0)|e^{i\mathcal{H}t}\hat{\mathcal{O}}(0)e^{-i\mathcal{H}t}|\psi(0)\rangle$

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>

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

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

$U(t)$ 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:

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

$\hat{V}(t)$ 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:

$$
\begin{aligned}
\int_0^t dt' \frac{\partial U(t')}{\partial t'} &= U(t) - U(0) \\
&= -i \int_0^t dt' \hat{V}(t')U(t'),
\end{aligned} \tag{14}
$$

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:

$$\begin{aligned}
\int_{\tilde{t}}^{t} \frac{\partial S(t'', t')}{\partial t''} &= S(t, t') - S(\tilde{t}, t') \\
&= -i\int_{\tilde{t}}^{t} dt''\hat{V}(t'')S(t'', t').
\end{aligned} \tag{15}$$

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.:

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

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

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:

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

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

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

since

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

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

Time ordering of operators

<u>Bosons:</u>
Two boson operators have time-ordered product

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

<u>Fermions:</u>
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:

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

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

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

$$S_2(t, t') = 1 - i \int_{t'}^{t} dt'' \hat{V}(t'') S_1(t'', t')$$

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

$$= 1 + (-i) \int_{t'}^{t} dt'' \hat{V}(t'') + (-i)^2 \int_{t'}^{t} dt'' \int_{t'}^{t''} dt''' \hat{V}(t'') \hat{V}(t'''),$$

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

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

We then look at the expression

$$\frac{1}{2!} \int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 \tilde{T} \left[\hat{V}(t_1) \hat{V}(t_2) \right] = \frac{1}{2} \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 \hat{V}(t_1) \hat{V}(t_2)$$

$$+ \frac{1}{2} \int_{t'}^{t} dt_2 \int_{t'}^{t_2} dt_1 \hat{V}(t_2) \hat{V}(t_1)$$

$$= \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 \hat{V}(t_1) \hat{V}(t_2), \qquad (16)$$

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:

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

$$= 1 + \tilde{T} \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left[\int_{t'}^{t} dt'' \hat{V}(t'') \right]^n, \qquad (17)$$

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 $|t| \ll \epsilon$.