Introduction to the microscopic theory of superconductors

Frank Schindler[1]

[1] Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

frankschindler.github.io
Please reach out if you find errors! :)

These are the notes for the second half of the course "Quantum Theory of Matter", taught at Imperial College London in early 2026. They give a brief overview of the microscopic theory of superconductivity. As much as possible, I tried to derive the theory following a series of logical steps, starting from basic assumptions and without quoting too many nontrivial results without derivation. There are, however, still bound to be some jumps in the logic. This reflects the history of the field where important discoveries were made only after lengthy periods of trial-and-error exploration and incremental progress. Nevertheless, these notes are meant to be read in sequence, as every section may rely on content developed in previous sections.

Contents

1 Conventions

These notes assume a working knowledge of undergraduate quantum mechanics. We set Planck's constant to $\hbar = 1$.

We mostly work in 3 spatial dimensions, where we denote vectors by bold symbols: $\boldsymbol{v}$ is a vector with components v_i, $i = x, y, z$. Unit vectors look like this: $\hat{\boldsymbol{e}}_i$, *e.g.* $\hat{\boldsymbol{e}}_x = (1,0,0)^{\mathrm{T}}$.[1] Integrals over space will be simply denoted by[2]

$$\int \mathrm{d}\boldsymbol{x} \equiv \int_{-L/2}^{L/2} \mathrm{d}x \int_{-L/2}^{L/2} \mathrm{d}y \int_{-L/2}^{L/2} \mathrm{d}z. \tag{1.1}$$

Here we work in a box of volume $V = L^3$ and periodic boundary conditions: particles leaving on one side come out again at the opposite side, like in the videogame Pac-Man. This means that all momenta are quantised to take on discrete values $p_i \in 2\pi\mathbb{Z}/L$,[3] however, in the thermodynamic limit $L \to \infty$ they will become arbitrarily close and fill out the whole of the (infinitely large) momentum space. We denote sums (and products) over *all* allowable momenta simply by $\sum_{\boldsymbol{p}}$ (by $\prod_{\boldsymbol{p}}$). To be explicit, for $\boldsymbol{n}$ a vector of integers $\boldsymbol{n} \in \mathbb{Z}^3$,

$$\sum_{\boldsymbol{p}} f(\boldsymbol{p}) \equiv \sum_{n_x=-\infty}^{\infty} \sum_{n_y=-\infty}^{\infty} \sum_{n_z=-\infty}^{\infty} f\left(\frac{2\pi}{L}\boldsymbol{n}\right). \tag{1.2}$$

In the thermodynamic limit, the momenta are ever closer spaced and the sum over momentum space can be approximated by an integral:

$$\sum_{\boldsymbol{p}} \quad \xrightarrow{L\to\infty} \quad V \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3} \equiv V \int_{-\infty}^{\infty} \frac{\mathrm{d}p_x}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_y}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_z}{2\pi}. \tag{1.3}$$

The extra factor $V/(2\pi)^3$ is necessary so that we don't overcount momenta.[4]

We usually use σ as a label for the z-component of electron spin, so that it ranges over the two values $\sigma = \uparrow, \downarrow$ (spin up, $S_z = +1/2$, or spin down, $S_z = -1/2$). A sum of the form $\sum_\sigma$ indicates summation over both values of spin, so that

$$\sum_{\sigma} \equiv \sum_{\sigma=\uparrow,\downarrow}. \tag{1.4}$$

Often we sum over both momenta and spin and abbreviate this by $\sum_{\boldsymbol{p}\sigma} = \sum_{\boldsymbol{p}} \sum_\sigma$. The same is true for products such as $\prod_{\boldsymbol{p}\sigma}$.

Sometimes we will be a bit lazy with the sums and products, and we will write down expressions like $\sum_{\boldsymbol{p}}^{\epsilon_{\boldsymbol{p}}>0}$. What this means is that we use a function $\epsilon_{\boldsymbol{p}} \in \mathbb{R}$ that depends on momentum $\boldsymbol{p}$, and the sum is *over all momenta* for which the condition $\epsilon_{\boldsymbol{p}} > 0$ is satisfied.[5] To reiterate, this is still a sum over (a subset of) momenta $\boldsymbol{p}$, *not* a

[1] To be a bit pedantic, I'm using T here to denote the transpose: $(1,0,0)^{\mathrm{T}} = \begin{pmatrix}1\\0\\0\end{pmatrix}$.

[2] Note that I'm using $\boldsymbol{x}$ for the position vector so that, rather awkwardly, $x_x = x$ is the coordinate x, $x_y = y$, $x_z = z$.

[3] This is so that momentum eigenfunctions of the form $\Psi_{\boldsymbol{p}}(\boldsymbol{x}) \sim e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}$ come out periodic in the box: $\Psi_{\boldsymbol{p}}(\boldsymbol{x} + L\hat{\boldsymbol{e}}_j) = \Psi_{\boldsymbol{p}}(\boldsymbol{x})$, where $\hat{\boldsymbol{e}}_j$ is the unit vector in j-direction ($j = x, y, z$).

[4] A momentum-space cube of volume $(2\pi)^3/L$ contains only *a single* momentum that satisfies the quantisation rule $p_i \in 2\pi\mathbb{Z}/L$, $i = x, y, z$.

[5] In practice, $\epsilon_{\boldsymbol{p}}$ will be the kinetic energy of a single electron with momentum $\boldsymbol{p}$.

sum over the different values of $\epsilon_{\boldsymbol{p}}$. More explicitly,

$$\sum_{\boldsymbol{p}}^{\epsilon_{\boldsymbol{p}}>0} \equiv \sum_{\boldsymbol{p}} \int_0^\infty \mathrm{d}\epsilon\, \delta(\epsilon - \epsilon_{\boldsymbol{p}}), \tag{1.5}$$

where $\delta(x)$ is the Dirac delta function.

In most practical situations we will encounter, the quantities being summed over will only depend on the value of the scalar function $\epsilon_{\boldsymbol{p}}$, rather than on the full vector $\boldsymbol{p}$. In this special case, and in the thermodynamic limit, we can replace the sum by an integral *over* ϵ:

$$\sum_{\boldsymbol{p}}^{\epsilon_{\boldsymbol{p}}>0} \quad \xrightarrow{L\to\infty} \quad V \int_0^\infty \mathrm{d}\epsilon\, \rho(\epsilon). \tag{1.6}$$

Here, the function $\rho(\epsilon)$ must be chosen such that $V\mathrm{d}\epsilon\,\rho(\epsilon)$ is the number of momenta $\boldsymbol{p}$ for which the function $\epsilon_{\boldsymbol{p}}$ lies in the interval $\mathrm{d}\epsilon$.[6] By comparing with Eqs. (1.3) and (1.5), we find

$$\rho(\epsilon) = \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3} \delta(\epsilon - \epsilon_{\boldsymbol{p}}). \tag{1.7}$$

[6] In practice, when $\epsilon_{\boldsymbol{p}}$ is the kinetic energy, $\rho(\epsilon)$ is called the *density of states*.

2 Fermions

To describe a system of many electrons, which are fermions, we'll be using a bit of a different formalism from what you're used to in undergraduate quantum mechanics.

2.1 Exchange statistics

Quantum matter is composed of a multitude ($\sim 10^{23}$) of identical particles. As soon as we talk about more than one particle in quantum mechanics and the particles are indistinguishable[1], it becomes important to ask what their *exchange statistics* is, *i.e.*, how the wavefunction behaves under the exchange of two particles.

[1] The fact that electrons, the main actors in quantum matter, are identical, comes from quantum field theory. Microscopically, electrons are excitations of the *electron field*. Multiple electrons are obtained from the *same* excitation of the *same* field at *different* locations in space, and are therefore indistinguishable in all their inherent properties such as mass, spin, magnetic moment, *etc.*

Consider a wavefunction of two particles in position space, $\Phi(\boldsymbol{x_1}, \boldsymbol{x_2})$ that assigns a quantum amplitude $\Phi(\boldsymbol{x_1}, \boldsymbol{x_2}) \in \mathbb{C}$ to the configuration where particle 1 is located at position $\boldsymbol{x_1} \in \mathbb{R}^3$ and particle 2 is located at position $\boldsymbol{x_2} \in \mathbb{R}^3$. Since the two particles are indistinguishable, the corresponding quantum state should be the same if the situation were reversed, and therefore

$$\Phi(\boldsymbol{x_2}, \boldsymbol{x_1}) \stackrel{!}{=} e^{i\alpha}\Phi(\boldsymbol{x_1}, \boldsymbol{x_2}). \tag{2.1}$$

Here, $e^{i\alpha}$ with $\alpha \in \mathbb{R}$ is some phase factor – recall that quantum mechanical states have a gauge degree of freedom, in that complex phase factors do not change any physical properties of a state. Doing a double exchange by plugging Eq. (2.1) into itself, we obtain

$$\Phi(\boldsymbol{x_2}, \boldsymbol{x_1}) = e^{i\alpha}\Phi(\boldsymbol{x_1}, \boldsymbol{x_2}) = e^{2i\alpha}\Phi(\boldsymbol{x_2}, \boldsymbol{x_1}), \tag{2.2}$$

so that $e^{2i\alpha} = 1$ with solutions $\alpha = 0, \pi$.[2] Since these solutions are *discrete* (they can not be continuously connected to each other, as all solutions where α is between 0 and π are disallowed), there are two allowed types of particles that compose all matter:

[2] This argument glosses over some subtle topological considerations that become relevant in two spatial dimensions and give rise to *anyons*, particles characterised by a general $\alpha \in \mathbb{R}$. However, in our three-dimensional universe, all known microscopic particles that appear in the standard model of particle physics satisfy either $\alpha = 0$ or $\alpha = \pi$.

- **Bosons ($\alpha = 0$):** The wavefunction of two bosons does not change under exchange, $\Phi(\boldsymbol{x_2}, \boldsymbol{x_1}) = \Phi(\boldsymbol{x_1}, \boldsymbol{x_2})$. This means that multiple bosons can occupy the same quantum state, e.g.

  $$\Phi(\boldsymbol{x_1}, \boldsymbol{x_2}) = \phi(\boldsymbol{x_1})\phi(\boldsymbol{x_2}), \tag{2.3}$$

  where $\phi(\boldsymbol{x})$ is some single-particle wavefunction. For a macroscopic system of bosons, such a state describes a Bose-Einstein condensate. In our universe, the force-carrying particles are bosons (photons, gluons, gravitons, ...).

- **Fermions ($\alpha = \pi$):** The wavefunction of two fermions is multiplied by a minus sign under exchange, $\Phi(\boldsymbol{x_2}, \boldsymbol{x_1}) = -\Phi(\boldsymbol{x_1}, \boldsymbol{x_2})$.

This implies that a state of the form of Eq. (2.3) is impossible for fermions, meaning that two fermions can never occupy the same single-particle wavefunction. This result is known as the *Pauli exclusion principle*. In our universe, matter particles are usually fermions (electrons, protons, neutrons, quarks ...), but it is possible to obtain a boson by combining an even number of fermions (so that the minus sign cancels). The Pauli exclusion principle is the basic reason for why different elements behave differently, giving rise to the surprising complexity of the periodic table.

In these notes, **we will exclusively work with electrons**, which are fermions.

2.2 Creation and annihilation operators

Recall that a quantum wavefunction of a single particle, in the position space basis, is a function of the form $\Phi(\boldsymbol{x})$ where $\boldsymbol{x} \in \mathbb{R}^3$ ranges over all possible coordinates the particle can occupy in space. Introducing a basis of position operator eigenstates $|\boldsymbol{x}\rangle$, which satisfy $\hat{\boldsymbol{x}}\,|\boldsymbol{x}\rangle = \boldsymbol{x}\,|\boldsymbol{x}\rangle$ where $\hat{\boldsymbol{x}}$ is the (single-particle) position operator, we can write

$$\Phi(\boldsymbol{x}) = \langle \boldsymbol{x}|\Phi\rangle\,. \tag{2.4}$$

Here, we have introduced the basis-independent quantum *state* $|\Phi\rangle$ that corresponds to the wavefunction $\Phi(\boldsymbol{x})$, it is alternatively expressed as

$$|\Phi\rangle = \int \mathrm{d}\boldsymbol{x}\ \langle \boldsymbol{x}|\Phi\rangle\,|\boldsymbol{x}\rangle = \int \mathrm{d}\boldsymbol{x}\,\Phi(\boldsymbol{x})\,|\boldsymbol{x}\rangle\,, \tag{2.5}$$

where we have used the resolution of the identity in terms of position eigenstates, $\int \mathrm{d}\boldsymbol{x}\ |\boldsymbol{x}\rangle\,\langle \boldsymbol{x}| = \mathbb{1}$. For our purposes, it will be much more convenient to work with abstract states $|\Phi\rangle$ rather than basis-dependent wavefunctions $\Phi(\boldsymbol{x})$. How do we write down a *state*, rather than a wavefunction, for two fermions?

Consider the two-fermion wavefunction

$$\Psi(\boldsymbol{x_1}, \boldsymbol{x_2}) = \phi_A(\boldsymbol{x_1})\phi_B(\boldsymbol{x_2}) - \phi_A(\boldsymbol{x_2})\phi_B(\boldsymbol{x_1}) = -\Psi(\boldsymbol{x_2}, \boldsymbol{x_1}), \tag{2.6}$$

where $\phi_A(\boldsymbol{x}) \neq \phi_B(\boldsymbol{x})$ must be *orthogonal* single-particle wavefunctions to satisfy the Pauli exclusion principle. Naively, and following Eq. (2.5), we can write the corresponding state as follows:

$$|\Psi\rangle = \int \mathrm{d}\boldsymbol{x_1}\mathrm{d}\boldsymbol{x_2}\,\Psi(\boldsymbol{x_1}, \boldsymbol{x_2})\,|\boldsymbol{x_1}\rangle \otimes |\boldsymbol{x_2}\rangle\,, \tag{2.7}$$

where $\otimes$ is the tensor product. However, for a large number of fermions, it will be very cumbersome to work with this such states. This is because due to the anti-symmetric nature of the wavefunctions these states will contain a very large number of terms, all essentially the same up to the exchange of two fermions.

To avoid this problem, we would like a formalism that directly incorporates fermionic exchange statistics, so that we do not have to explicitly work with anti-symmetric wavefunctions all the time. The trick is to introduce a set of *creation* ($c_x^\dagger$) and *annihilation* (c_x) operators and that satisfy the **canonical anti-commutation relations**[3]

$$\begin{aligned}\{c_x, c_y^\dagger\} &\equiv c_x c_y^\dagger + c_y^\dagger c_x = \delta(\boldsymbol{x}-\boldsymbol{y}),\\ \{c_x^\dagger, c_y^\dagger\} &\equiv c_x^\dagger c_y^\dagger + c_y^\dagger c_x^\dagger = 0,\\ \{c_x, c_y\} &\equiv c_x c_y + c_y c_x = 0,\end{aligned} \tag{2.8}$$

[3] This formalism is sometimes called "second quantisation" for historical reasons.

where $\boldsymbol{x}$ and $\boldsymbol{y}$ are positions in real space. The important point is that $c_x^\dagger$ (c_x) has the interpretation of creating (destroying) a fermion at position $\boldsymbol{x}$. We also introduce a *vacuum state* $|0\rangle$ that is normalised such that $\langle 0|0\rangle = 1$ and is defined by the condition

$$c_x |0\rangle = 0, \tag{2.9}$$

so that destroying (= annihilating) a particle is not possible and results in the zero vector (rather than any normalisable state). We can then write the two-fermion state as

$$\begin{aligned}|\Psi\rangle &= \int \mathrm{d}\boldsymbol{x_1}\mathrm{d}\boldsymbol{x_2}\, \Psi(\boldsymbol{x_1},\boldsymbol{x_2}) c_{x_1}^\dagger c_{x_2}^\dagger |0\rangle\\ &= \frac{1}{2}\int \mathrm{d}\boldsymbol{x_1}\mathrm{d}\boldsymbol{x_2}\, \Psi(\boldsymbol{x_1},\boldsymbol{x_2})(c_{x_1}^\dagger c_{x_2}^\dagger - c_{x_2}^\dagger c_{x_1}^\dagger)|0\rangle\\ &= \frac{1}{2}\int \mathrm{d}\boldsymbol{x_1}\mathrm{d}\boldsymbol{x_2}\, [\Psi(\boldsymbol{x_1},\boldsymbol{x_2}) - \Psi(\boldsymbol{x_2},\boldsymbol{x_1})] c_{x_1}^\dagger c_{x_2}^\dagger |0\rangle\,,\end{aligned} \tag{2.10}$$

where we have used Eq. (2.8) in the second line, and then exchanged integration variables $\boldsymbol{x_1} \leftrightarrow \boldsymbol{x_2}$ for the second term only in the third line. Crucially, this result implies that we can choose $\Psi(\boldsymbol{x_1},\boldsymbol{x_2})$ to be any function we want – it does not need to be anti-symmetric – and the resulting state $|\Psi\rangle$ will be the same as if we had properly anti-symmetrised it. To see this, note that *any* function of two variables can be split up into a symmetric plus an anti-symmetric function as follows:

$$\Psi(\boldsymbol{x_1},\boldsymbol{x_2}) = \underbrace{\frac{1}{2}[\Psi(\boldsymbol{x_1},\boldsymbol{x_2}) + \Psi(\boldsymbol{x_2},\boldsymbol{x_1})]}_{\text{symmetric}} + \underbrace{\frac{1}{2}[\Psi(\boldsymbol{x_1},\boldsymbol{x_2}) - \Psi(\boldsymbol{x_2},\boldsymbol{x_1})]}_{\text{anti-symmetric}}, \tag{2.11}$$

and only the anti-symmetric contribution survives Eq. (2.10).

It is now straightforward to show that a general N-fermion state of the form

$$|\Psi\rangle = \int \mathrm{d}\boldsymbol{x_1}\mathrm{d}\boldsymbol{x_2}\cdots\mathrm{d}\boldsymbol{x_N}\, \Psi(\boldsymbol{x_1},\boldsymbol{x_2},\ldots,\boldsymbol{x_N}) c_{x_1}^\dagger c_{x_2}^\dagger \cdots c_{x_N}^\dagger |0\rangle \tag{2.12}$$

will be automatically properly anti-symmetrised on account of the fermionic anti-commutation relations in Eq. (2.8), no matter what the

form of the function $\Psi(\boldsymbol{x_1}, \boldsymbol{x_2}, \ldots, \boldsymbol{x_N})$ is. This means that as long as we keep the algebraic properties of the creation and annihilation operators encoded in Eq. (2.8) in mind, we do not need to worry about anti-symmetrisation and can work with simple wavefunctions. We will see that this formalism tremendously simplifies the treatment of fermionic quantum systems, especially in the case of a macroscopic number of fermions.

2.3 Kinetic energy Hamiltonian

We can build all operators acting on the fermionic Hilbert space from the elementary creation and annihilation operators $c_{\boldsymbol{x}}^\dagger$ and $c_{\boldsymbol{x}}$. For example, the operator creating a fermion *at a fixed momentum* $\boldsymbol{p}$ is obtained by a Fourier transform:[4]

$$c_{\boldsymbol{p}}^\dagger = \frac{1}{\sqrt{V}} \int \mathrm{d}\boldsymbol{x}\, e^{\mathrm{i}\boldsymbol{p}\boldsymbol{x}} c_{\boldsymbol{x}}^\dagger, \tag{2.13}$$

where V is the volume of the system. Correspondingly, the operator destroying a fermion at a fixed momentum is given by

$$c_{\boldsymbol{p}} = \frac{1}{\sqrt{V}} \int \mathrm{d}\boldsymbol{x}\, e^{-\mathrm{i}\boldsymbol{p}\boldsymbol{x}} c_{\boldsymbol{x}}. \tag{2.14}$$

You can check that the momentum-space operators also satisfy the canonical anti-commutation relations, in that

$$\{c_{\boldsymbol{p}}, c_{\boldsymbol{q}}\} = 0, \quad \{c_{\boldsymbol{p}}^\dagger, c_{\boldsymbol{q}}^\dagger\} = 0, \quad \{c_{\boldsymbol{p}}, c_{\boldsymbol{q}}^\dagger\} = \delta_{\boldsymbol{p}\boldsymbol{q}}. \tag{2.15}$$

Moreover, the vacuum still satisfies $c_{\boldsymbol{p}} |0\rangle = 0$ also in the momentum basis, which follows directly from the fact that $c_{\boldsymbol{p}}$ only contains annihilation operators.

We now introduce the *occupation number operator* in momentum space, $n_{\boldsymbol{p}} = c_{\boldsymbol{p}}^\dagger c_{\boldsymbol{p}}$. This operator has eigenvalues 0 or 1, depending on whether the fermionic mode at momentum $\boldsymbol{p}$ is occupied or empty. In particular,

$$\begin{aligned} n_{\boldsymbol{p}} |0\rangle &= 0, && \text{the vacuum is empty} \\ n_{\boldsymbol{p}} c_{\boldsymbol{p}}^\dagger |0\rangle &= c_{\boldsymbol{p}}^\dagger |0\rangle, && \text{this state has the fermion occupied} \\ n_{\boldsymbol{p}} c_{\boldsymbol{q}}^\dagger |0\rangle &= \delta_{\boldsymbol{p}\boldsymbol{q}} c_{\boldsymbol{p}}^\dagger |0\rangle, && \text{this is only nonzero when } \boldsymbol{p} = \boldsymbol{q}. \end{aligned} \tag{2.16}$$

You can derive these equations using the canonical anti-commutation relations in Eq. (2.15). Note that unlike for bosons, $n_{\boldsymbol{p}}$ cannot be larger than 1, because of the Pauli exclusion principle (no more than 1 fermion per single-particle state). In addition to the single-particle number operators $n_{\boldsymbol{p}}$, we can define the many-body number operator[5]

[4] In an abuse of notation, we call this operator $c_{\boldsymbol{p}}^\dagger$ where we really should give it another letter such as $d_{\boldsymbol{p}}^\dagger$ to show that it is not simply obtained from $c_{\boldsymbol{x}}^\dagger$ by replacing $\boldsymbol{x} \to \boldsymbol{p}$. However, in these notes, we will only ever use letters x, y, z to denote positions while letters such as p, q, k denote momenta.

[5] Note that the definition of $\hat{N}$ involves a sum, and not an integral, over momentum $\boldsymbol{p}$. The reason is that we work in a box of volume V and with periodic boundary conditions, so that momentum is discrete. To review this please re-read the section on Conventions.

$$\hat{N} = \sum_{p} n_p = \sum_{p} c_p^\dagger c_p, \tag{2.17}$$

which counts the total number of fermions in a given state. For instance, for a collection of 4 momenta $\boldsymbol{p_1} \neq \boldsymbol{p_2} \neq \boldsymbol{p_3} \neq \boldsymbol{p_4}$ that are all different,

$$\begin{aligned} \hat{N} c_{p_1}^\dagger c_{p_2}^\dagger c_{p_3}^\dagger c_{p_4}^\dagger |0\rangle &= 4 c_{p_1}^\dagger c_{p_2}^\dagger c_{p_3}^\dagger c_{p_4}^\dagger |0\rangle , \\ \hat{N} c_{p_2}^\dagger c_{p_3} c_{p_3}^\dagger c_{p_4}^\dagger |0\rangle &= 2 c_{p_2}^\dagger c_{p_3} c_{p_3}^\dagger c_{p_4}^\dagger |0\rangle , \\ &\cdots , \end{aligned} \tag{2.18}$$

which follows directly from the canonical anti-commutation relations in Eq. (2.15) and the fact that $c_p |0\rangle = 0$.

We are now in a position to write down the Hamiltonian for a free fermion system with translational symmetry. Recall from classical physics that translational symmetry implies that momentum is conserved, meaning that the Hamiltonian should be diagonal in momentum. In particular, for a free system where the fermions do not interact with each other, the Hamiltonian should preserve the momentum of each individual fermion and can therefore only contain operators of the form n_p.[6] Consider a collection of fermions with fixed momenta $\boldsymbol{p}$, each of which has a single-particle energy ϵ_p that depends on $\boldsymbol{p}$. For example, in the case of non-relativistic electrons, we have

$$\epsilon_p = \frac{|\boldsymbol{p}|^2}{2m}, \tag{2.19}$$

where m is the electron mass. The total (= many-body, rather than single-particle) energy is then given by the Hamiltonian

$$\hat{H} = \sum_{p} \epsilon_p n_p = \sum_{p} \epsilon_p c_p^\dagger c_p. \tag{2.20}$$

In practical terms, this operator goes over each momentum $\boldsymbol{p}$, checks that it is occupied, and only then adds the corresponding energy ϵ_p (and otherwise adds 0 if there is no fermion with momentum $\boldsymbol{p}$). Using Eq. (2.15) you can confirm that H commutes with total particle number $\hat{N}$,

$$[\hat{H}, \hat{N}] = 0, \tag{2.21}$$

which is to be expected as each term in $\hat{H}$ contains an equal number of creation and annihilation operators.

So far, we have considered the simplest kind of fermions, which are only characterised by a position or momentum variable. We know from our universe that real fermions also have a spin degree of freedom. In particular, electrons are spin-$\frac{1}{2}$ particles and their spin projection along the z-axis can be either up $\uparrow$ or down $\downarrow$, or a superposition thereof. To describe electrons, we therefore need creation ($c_{p\sigma}^\dagger$) and annihilation ($c_{p\sigma}$) operators that include spin, where

[6] This is because n_p measures but does not change the number of occupied fermions at a fixed single-particle momentum $\boldsymbol{p}$.

$\sigma = \uparrow, \downarrow$ in addition to momentum $\boldsymbol{p}$.[7] In analogy to Eq. (2.15), these fulfil the canonical anti-commutation relations

$$\{c_{p\sigma}, c_{q\sigma'}\} = 0, \quad \{c^\dagger_{p\sigma}, c^\dagger_{q\sigma'}\} = 0, \quad \{c_{p\sigma}, c^\dagger_{q\sigma'}\} = \delta_{\sigma\sigma'}\delta_{pq}. \tag{2.22}$$

The Hamiltonian for a system of free electrons with translational symmetry then becomes

$$\hat{H} = \sum_{p\sigma} \epsilon_{p\sigma} n_{p\sigma} = \sum_{p} \epsilon_{p\sigma} c^\dagger_{p\sigma} c_{p\sigma}. \tag{2.23}$$

Unless there is a magnetic field, the energy of $\sigma = \uparrow$ is the same as that of $\sigma = \downarrow$ due to time-reversal symmetry, which means that it is usually safe to assume that the single-particle energy (= dispersion relation) $\epsilon_{p\sigma} = \epsilon_p$ is spin-independent. In analogy to Eq. (2.17), the total number of electrons then becomes

$$\hat{N} = \sum_{p\sigma} n_{p\sigma} = \sum_{p\sigma} c^\dagger_{p\sigma} c_{p\sigma}, \tag{2.24}$$

and again satisfies $[\hat{H}, \hat{N}] = 0$.

2.4 Electron-electron interaction

While the kinetic energy for electrons is most easily expressed in momentum space, see Eq. (2.23), interactions between different electrons are simpler in real space because they are local – we expect the interaction between two electrons to become negligible in the limit where they are far apart from one another.

A simple class of interactions only depends on the *density* of electrons at a given point $\boldsymbol{x}$ in space. In analogy to the electron number operator $n_{p\sigma}$ in momentum space, we define the electron *density* operator at a position $\boldsymbol{x}$ and for a given spin σ via

$$n_{x\sigma} = c^\dagger_{x\sigma} c_{x\sigma}. \tag{2.25}$$

Here, we have straightforwardly generalised the real space creation and annihilation operators to include spin, so that they satisfy the canonical anti-commutation relations

$$\{c_{x\sigma}, c_{y\sigma'}\} = 0, \quad \{c^\dagger_{x\sigma}, c^\dagger_{y\sigma'}\} = 0, \quad \{c_{x\sigma}, c^\dagger_{y\sigma'}\} = \delta_{\sigma\sigma'}\delta(\boldsymbol{x} - \boldsymbol{y}). \tag{2.26}$$

The real-space and momentum-space operators are again related to each other via a Fourier transform, *e.g.*,

$$c^\dagger_{p\sigma} = \frac{1}{\sqrt{V}} \int \mathrm{d}\boldsymbol{x}\, e^{\mathrm{i}p\boldsymbol{x}} c^\dagger_{x\sigma}. \tag{2.27}$$

To see that $n_{x\sigma}$ is a density, note that

$$\hat{N} = \sum_{p\sigma} c^\dagger_{p\sigma} c_{p\sigma} = \sum_{\sigma} \int \mathrm{d}\boldsymbol{x}\, c^\dagger_{x\sigma} c_{x\sigma} = \sum_{\sigma} \int \mathrm{d}\boldsymbol{x}\, n_{x\sigma}, \tag{2.28}$$

[7] You can also define theses operators in real space as $c^\dagger_{x\sigma}$ and $c_{x\sigma}$, the relation to the momentum space operators is still the same Fourier transform as in Eq. (2.13) where the spin variable σ simply stays along for the ride [see Eq. (2.27) below].

which you can derive using Eq. (2.27) and the canonical anti-commutation relations in Eq. (2.26). Using the density operators, we can now write the standard Coulomb interaction between electrons as follows:

$$\hat{H}_{\text{Coulomb}} = \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y}\,\frac{e^2}{4\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{y}|}n_{x\sigma}n_{y\sigma'}, \tag{2.29}$$

where the factor $1/2$ in front makes sure that we count every pair of electrons only once.

3 Cooper instability

In this section, we'll introduce the starting point for the microscopic theory of superconductivity: a metal in its ground state, also known as the *Fermi sea*. We'll then have a look at the effective interaction between electrons above the Fermi sea. Following Leon Cooper's seminal work in 1956, we will show that any arbitrarily small attractive interaction leads to bound states, so-called *Cooper pairs*.

3.1 Effective electron interaction

Consider a metal. Our cartoon picture of the metal only involves two ingredients: the conduction (valence) electrons, and the left-over lattice of atomic ions[1], which we'll often just call "atoms". Since the atoms are much heavier than the electrons, they don't move as much. For all practical purposes, we can assume that they only move about their equilibrium positions in small lattice vibrations, so-called *phonons*. To simplify things further, we'll assume that the valence electrons roam freely through the metal and basically do not notice the lattice, with one important exception: due to the phonon background, their interaction is not of the usual Coulomb type. Recall that in vacuum, electrons repel as they have an equal elementary charge e, and their Hamiltonian reads

$$\hat{H}^{\text{vac}} = \underbrace{\sum_{p\sigma} \frac{|\boldsymbol{p}|^2}{2m} c^\dagger_{p\sigma} c_{p\sigma}}_{\hat{H}^{\text{vac}}_{\text{kin}}} + \underbrace{\frac{1}{2} \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{x}-\boldsymbol{y}|} n_{x\sigma} n_{y\sigma'}}_{\hat{H}^{\text{vac}}_{\text{int}}}, \tag{3.1}$$

where we have abbreviated the kinetic part of the Hamiltonian by $\hat{H}^{\text{vac}}_{\text{kin}}$ and the interaction part by $\hat{H}^{\text{vac}}_{\text{int}}$. Here, m is the electron mass in vacuum, and ϵ_0 is the electric permittivity in vacuum. Don't worry if this expression looks horrible, we will never have to solve it in this class, and we will instead look at more simplified models. In fact, it is near impossible to diagonalise this kind of Hamiltonian for a realistic number of electrons, say an Avogadro's number $N \sim 10^{23}$ worth of electrons, even numerically![2]

It turns out that due to the background of an ionic lattice and phonon vibrations, the electrons in a metal – at least at low energies – *attract* rather than repel. This is possible because of two main reasons: (1) In any material at equilibrium, the overall charge density is neutral. The net negative charge of an electron is cancelled by a background of positively charged atomic ions in the surrounding material. This effect neutralises the Coulomb repulsion between electrons at long distances. (2) However, at short distances, electrons do have a noticeably negative charge that distorts the positively charged crys-

[1] The atoms potentially contain further lower-shell electrons that we do not care about.

[2] In the early 1990s, supercomputers could solve this problem for about $N \sim 10$ electrons without making approximations. Nowadays, in the 2020s, this has improved to only around $N \sim 30$ electrons. The problem is that even though computing power increases exponentially with time (Moore's law), so does the size of the n-electron Hilbert space.

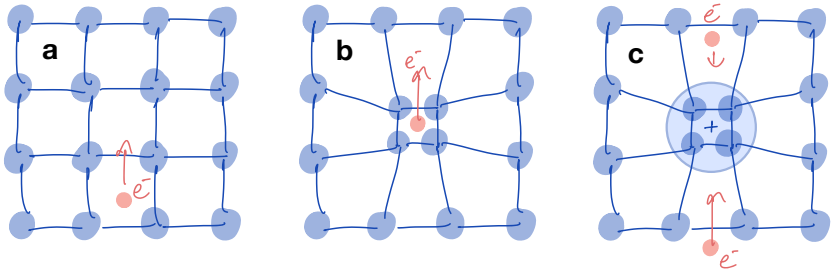

Figure 1: Illustration of the effective attractive interaction between electrons mediated by lattice vibrations. **a** A negatively charged conduction electron (red) passes through a crystalline lattice of positively charged atomic ions (blue). Due to the presence of lower-shell valence electrons (not shown), the overall charge density is neutral. **b** The lattice ions are attracted to the local net negative charge of the conduction electron. The electron moves on quickly, but the ions remain distorted for a little while longer because they are much heavier. This creates a region of net positive charge. **c** A second conduction electron is attracted to this region. At the same time, the original electron is slowed down a little bit as it is drawn back to the positive charge. As a consequence, the two electrons experience a net attraction.

tal lattice around them, creating an accumulation of positive charge that remains long after the electron has moved on. This is because electrons have very low mass compared to atoms, and so the atoms take a much longer time to relax back to their equilibrium state once an electron has passed through. Other electrons then see this accumulation of net positive charge and are attracted to it, creating an overall effective attraction between electrons. For an illustration of this mechanism, see Fig. 1. We should note, however, that a precise derivation of the effective attractive interaction between electrons requires a fully quantum treatment and advanced field theory methods that go beyond the scope of this course.

In this course, we will not delve deeper into deriving the specific form of the attraction, because its details are mostly inessential to the phenomenon of superconductivity: *any* attractive interaction will do the job, a phonon-mediated one is just one example[3]. Usually, electrons in a metal are well approximated by a Hamiltonian of the form

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}} = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma} + \hat{H}_{\text{int}}, \quad \epsilon_p = \frac{|\boldsymbol{p}|^2}{2m^*} - E_{\text{F}}. \tag{3.2}$$

Here, we have left the form of the interaction part of the Hamiltonian $\hat{H}_{\text{int}}$ unspecified for now, and only note that it is attractive rather than repulsive, and that it preserves translational symmetry[4]. In the kinetic part of the Hamiltonian $\hat{H}_{\text{kin}}$, we have assumed the usual non-relativistic energy-momentum dispersion for the electrons, with two modifications: (1) the effective electron mass m^* may differ from the electron mass in vacuum m due to the presence of the crystalline background, and (2) the *Fermi energy* E_{F} makes it energetically favourable to have a finite density of electrons in the metal.[5]

[3] It is, however, the most common example, underlying all so-called "conventional" superconductors.

[4] Later on, we will use that total momentum is a conserved quantity due to the translational symmetry of $\hat{H}$.

[5] Note that without E_F, the lowest energy eigenstate of $\hat{H}_{\text{kin}}$ would be simply the boring fermionic vacuum state $|0\rangle$. This is because all single-electron energies ϵ_p would be non-negative, so that it's best to have no electrons at all.

3.2 Fermi sea

Let us first fully understand the kinetic part of the Hamiltonian $\hat{H}_{\text{kin}}$ before we consider the effect of interactions. The operator $\hat{H}_{\text{kin}}$ is quadratic in the fermion creation and annihilation operators, a

hallmark of a *non-interacting* Hamiltonian: as shown in the section on Fermions, the many-body eigenstates of such an operator are obtained from products over single-electron operators acting on the vacuum. The lowest-energy eigenstate of $\hat{H}_{\text{kin}}$ (the non-interacting *ground state*) $|\text{FS}\rangle$ is obtained when all single-electron states with kinetic energy $|\boldsymbol{p}|^2/2m^* \leq E_{\text{F}}$ are occupied, irrespective of their spin $\sigma = \uparrow, \downarrow$:[6]

$$|\text{FS}\rangle = \prod_{\boldsymbol{p}}^{\epsilon_{\boldsymbol{p}} \leq 0} \prod_{\sigma} c^\dagger_{\boldsymbol{p}\sigma} |0\rangle \,. \tag{3.3}$$

[6] Recall from the Conventions section that in $\prod_{\boldsymbol{p}}^{\epsilon_{\boldsymbol{p}} \leq 0}$, the product ranges over all momenta $\boldsymbol{p}$ for which $\epsilon_{\boldsymbol{p}} \leq 0$ is satisfied.

The state $|\text{FS}\rangle$ is called the *Fermi sea*: you can think of it as an ocean of electrons[7] (which are fermions), and the electrons right at its surface (the *Fermi surface*) have kinetic energy E_{F}. Geometrically, the momenta occupied in the Fermi sea form a ball in momentum space with radius $p_0 = \sqrt{2mE_F}$, bounded by a spherical Fermi surface.[8] The kinetic energy of the Fermi sea is

[7] An ocean in momentum space, admittedly. The analogy is a bit stretched.

$$\hat{H}_{\text{kin}} |\text{FS}\rangle = 2 \sum_{\boldsymbol{p}}^{\epsilon_{\boldsymbol{p}} \leq 0} \epsilon_{\boldsymbol{p}} |\text{FS}\rangle \equiv E_{\text{FS}} |\text{FS}\rangle \,, \tag{3.4}$$

[8] In fact, there are many energetically degenerate (with respect to $\hat{H}_{\text{kin}}$) states that are obtained from $|\text{FS}\rangle$ by removing electrons at the Fermi surface, so we have made a bit of an arbitrary (but harmless) choice in singling out $|\text{FS}\rangle$ as our preferred ground state.

and this is the lowest possible eigenvalue of $\hat{H}_{\text{kin}}$ (recall that all $\epsilon_{\boldsymbol{p}}$ contributing to this sum are *non-positive*).[9] Here, the factor of 2 comes from the spin degeneracy: $\epsilon_{\boldsymbol{p}}$ depends only on electron momentum but not on spin.

Importantly, due to fermionic statistics we have $c^\dagger_{\boldsymbol{p}\sigma} |\text{FS}\rangle = 0$ whenever $\epsilon_{\boldsymbol{p}} \leq 0$. On the other hand, the state $c^\dagger_{\boldsymbol{p}\sigma} |\text{FS}\rangle = 0$ where $\epsilon_{\boldsymbol{p}} > 0$ is well defined and satisfies

$$\hat{H}_{\text{kin}} c^\dagger_{\boldsymbol{p}\sigma} |\text{FS}\rangle = (E_{\text{FS}} + \epsilon_{\boldsymbol{p}}) c^\dagger_{\boldsymbol{p}\sigma} |\text{FS}\rangle \,. \tag{3.5}$$

[9] Please note that $E_{\text{FS}} \neq E_{\text{F}}$. E_{FS} is the extensive energy of the many-body ground state $|\text{FS}\rangle$. E_{F} is the intensive energy of a single electron at the Fermi surface, *i.e.*, the energy of the largest-momentum single-particle states that are occupied in $|\text{FS}\rangle$. I'm sorry for the unfortunate choice of labelling. To make up for it, we will set $E_{\text{FS}} = 0$ shortly, so that it won't bother us much in the future.

Correspondingly, these states sweep out a continuum of $\hat{H}_{\text{kin}}$ eigenstates with energies arbitrarily close to[10], but above, E_{FS}. The Fermi sea $|\text{FS}\rangle$ is said to be *gapless*, as it is not separated from higher-energy states by an energy gap that remains finite in the thermodynamic limit; the absence of such a gap is one of the main characteristics of a metal. In contrast, both insulators and superconductors are characterised by a finite (single-electron) gap above the ground state. As we have found a gapless ground state when considering only $\hat{H}_{\text{kin}}$, this means that we need to take the interaction term $\hat{H}_{\text{int}}$ seriously into account to develop a theory of superconductors: unlike metals, superconductors intrinsically rely on electronic interactions.[11]

[10] The positive energies $\epsilon_{\boldsymbol{p}}$ get arbitrarily close to zero in the thermodynamic limit $L \to \infty$ where the momenta $\boldsymbol{p}$ are spaced infinitely close together.

From now on, we will choose our (many-body) energy axis so that $E_{\text{FS}} \equiv 0$. In this convention, the full many-body spectrum of $\hat{H}_{\text{kin}}$ becomes non-negative.

[11] For insulators, there exists a further, entirely non-interacting mechanism to stabilise an energy gap. This trick relies on having a multi-valued kinetic energy $\epsilon_{\boldsymbol{p}}$, that is, multiple bands of energy exist for any given momentum. Such a gapped *band structure* relies on the specific details of the crystalline lattice of the insulator. It cannot explain the formation of a gap in superconductors, as superconductivity has been observed in a wide variety of crystalline lattices.

3.3 Two-electron states

We now consider the effects of interactions on the Fermi sea. For the Fermi sea state $|\mathrm{FS}\rangle$ to be a good starting point at all for the study of superconductivity, the overall strength of the interactions should be very weak compared to the kinetic energy, and this is in fact the case in the great majority of all materials. To begin with, as a baby problem, we will look only at two electrons that interact above an otherwise calm (non-interacting) Fermi surface. In general, their Hilbert space is spanned by product states of the form

$$|\boldsymbol{p}\boldsymbol{q}\sigma\sigma'\rangle = c^\dagger_{\boldsymbol{p}+\boldsymbol{q}\sigma} c^\dagger_{-\boldsymbol{q}\sigma'} |\mathrm{FS}\rangle\,, \tag{3.6}$$

which have a kinetic energy $\epsilon_{\boldsymbol{p}+\boldsymbol{q}} + \epsilon_{\boldsymbol{q}}$ (recall we had set $E_{\mathrm{FS}} \equiv 0$). The single-electron momenta appearing in these states are chosen to result in a well-defined *total momentum* $\boldsymbol{p}$, which is preserved due to the translational symmetry of the Hamiltonian $\hat{H}$. Correspondingly, $\hat{H}$ may mix between two-electron states with different $\boldsymbol{q}$, but it will always preserve $\boldsymbol{p}$; we can fix $\boldsymbol{p}$ from the outset.

Due to fermionic statistics, $|\boldsymbol{p}\boldsymbol{q}\sigma\sigma'\rangle$ only exists when $\epsilon_{\boldsymbol{p}+\boldsymbol{q}} > 0$ and $\epsilon_{\boldsymbol{q}} > 0$ (otherwise, $|\boldsymbol{p}\boldsymbol{q}\sigma\sigma'\rangle = 0$, which is not a normalisable state). Correspondingly, if it were not for interactions, $|\boldsymbol{p}\boldsymbol{q}\sigma\sigma'\rangle$ would always have an energy that is – at least a bit – larger than the energy of the Fermi sea. We now want to see if we can find a two-particle *bound* state that has a *negative* energy, implying that it has lower energy than *all* non-interacting states[12], on account of the attractive interactions present in $\hat{H}_{\mathrm{int}}$. If such a bound state existed, the Fermi sea would be unstable to pair formation, and could not be the true ground state of the fully interacting system.

To maximise our chance of finding a bound state, we'd first like to minimise the kinetic energy of the electron pair, and therefore set its total momentum to zero: $\boldsymbol{p} = \boldsymbol{0}$.[13] You can convince yourself that $\epsilon_{\boldsymbol{p}+\boldsymbol{q}} + \epsilon_{\boldsymbol{q}}$, when viewed only as a function of $\boldsymbol{p}$, has a minimum at $\boldsymbol{p} = \boldsymbol{0}$. While we're at it, let us also set the total spin of the pair to zero: $\sigma = \uparrow$, $\sigma' = \downarrow$. This choice simplifies the math that follows quite a bit, because it makes the two electrons entering the state $|\boldsymbol{p}\boldsymbol{q}\sigma\sigma'\rangle$ *distinguishable*, which means we don't have to worry about their fermionic statistics too much. Moreover, we expect a net spin-zero (*singlet*) state to have the lowest possible energy given an attractive interaction: since they already differ in their spin, the electrons may then occupy *the same* position in real space, where their attraction is strongest. To summarise, to look for bound states we will work with a basis of two-electron states $|\boldsymbol{q}\rangle$ of the form

$$|\boldsymbol{q}\rangle \equiv |\boldsymbol{0}\,\boldsymbol{q}\uparrow\downarrow\rangle = c^\dagger_{\boldsymbol{q}\uparrow} c^\dagger_{-\boldsymbol{q}\downarrow} |\mathrm{FS}\rangle\,. \tag{3.7}$$

[12] We call all states non-interacting that are obtained from products of fermionic creation and annihilation operators (but not sums of products). That is, all eigenstates of $\hat{H}_{\mathrm{kin}}$ are non-interacting.

[13] We cannot do better than that: you might be tempted to just set all momenta to zero, $\boldsymbol{p} = \boldsymbol{q} = \boldsymbol{0}$, but we are not allowed to do that as only the *total momentum* $\boldsymbol{p}$ is a conserved quantity. The Hamiltonian will mix two-electron states with different *relative* momenta $\boldsymbol{q}$.

3.4 Cooper pairing

To determine the effect of interactions, we express the Hamiltonian $\hat{H}$ in the basis of the two-electron states $|\boldsymbol{q}\rangle$:[14]

$$h_{\boldsymbol{q}\boldsymbol{q}'} \equiv \langle \boldsymbol{q}|\hat{H}|\boldsymbol{q}'\rangle = 2\epsilon_{\boldsymbol{q}}\delta_{\boldsymbol{q}\boldsymbol{q}'} + \langle \boldsymbol{q}|\hat{H}_{\text{int}}|\boldsymbol{q}'\rangle\,, \tag{3.8}$$

where we have used that $\epsilon_{-\boldsymbol{q}} = \epsilon_{\boldsymbol{q}}$. To proceed, we finally have to say a bit more about the form of the attractive interaction Hamiltonian $\hat{H}_{\text{int}}$. The key here is to choose an interaction that is simple enough to allow for a solution, but at the same time complicated enough to capture the essential physics at play. In a seminal 1956 paper, Leon Cooper at the University of Illinois postulated the following form:[15]

$$\langle \boldsymbol{q}|\hat{H}_{\text{int}}|\boldsymbol{q}'\rangle = \begin{cases} -g/V & 0 < \epsilon_{\boldsymbol{q}}, \epsilon_{\boldsymbol{q}'} \leq \omega, \\ 0 & \text{otherwise.} \end{cases} \tag{3.9}$$

Here, $g > 0$ is some positive constant tuning the strength of the interaction, V is the volume of the box in which the electrons live, and ω is a characteristic phonon frequency (the "Debye frequency") that we can assume to be much smaller than the Fermi energy: $\omega \ll E_{\text{F}}$. The minus sign in front of g indicates that the interaction is attractive rather than repulsive: it lowers the energy of a pair of electrons, favouring pair binding. This form of the matrix elements of $\hat{H}_{\text{int}}$ is a dramatic simplification of previous exact calculations. For now, we'll take it for granted and carry on: Clearly, the Hamiltonian matrix $h_{\boldsymbol{q},\boldsymbol{q}'}$ allows for an infinite family of exact eigenvectors $\Psi^{\boldsymbol{p}}_{\boldsymbol{q}}$ of the form[16]

$$\epsilon_{\boldsymbol{p}} > \omega : \Psi^{\boldsymbol{p}}_{\boldsymbol{q}} = \delta_{\boldsymbol{q}\boldsymbol{p}}, \quad \sum_{\boldsymbol{q}'} h_{\boldsymbol{q}\boldsymbol{q}'}\Psi^{\boldsymbol{p}}_{\boldsymbol{q}'} = 2\epsilon_{\boldsymbol{p}}\Psi^{\boldsymbol{p}}_{\boldsymbol{q}}. \tag{3.10}$$

The lowest energy of these eigenvectors is larger than 2ω, which is positive, so they do not contain a bound state. More interestingly, we can think about eigenvectors of the form $\phi_{\boldsymbol{q}} \sim \theta(\omega - \epsilon_{\boldsymbol{q}})$,[17] so that $\phi_{\boldsymbol{q}}$ is only non-zero for $0 < \epsilon_{\boldsymbol{q}} \leq \omega$. These states must satisfy the eigenvalue equation

$$E\phi_{\boldsymbol{q}} = \sum_{\boldsymbol{q}'}^{0<\epsilon_{\boldsymbol{q}'}\leq\omega} h_{\boldsymbol{q}\boldsymbol{q}'}\phi_{\boldsymbol{q}'} = 2\epsilon_{\boldsymbol{q}}\phi_{\boldsymbol{q}} - \frac{g}{V}\sum_{\boldsymbol{q}'}^{0<\epsilon_{\boldsymbol{q}'}\leq\omega} \phi_{\boldsymbol{q}'}. \tag{3.11}$$

We can rearrange this equation as

$$(E - 2\epsilon_{\boldsymbol{q}})\phi_{\boldsymbol{q}} = -\frac{g}{V}\sum_{\boldsymbol{q}'}^{0<\epsilon_{\boldsymbol{q}'}\leq\omega} \phi_{\boldsymbol{q}'}. \tag{3.12}$$

Evidently, the right-hand side of this equation does not depend on $\boldsymbol{q}$.[18] To make sure the left-hand side does not depend on $\boldsymbol{q}$ as well,

[14] Technically, this means we're using the states $|\boldsymbol{q}\rangle$ as a *variational basis*.

[15] Leon N. Cooper. Bound electron pairs in a degenerate fermi gas. *Phys. Rev.*, 104:1189–1190, Nov 1956

[16] This should be read as a family of eigenvectors $\Psi^{\boldsymbol{p}}$, labelled by $\boldsymbol{p}$ where $\epsilon_{\boldsymbol{p}} > \omega$. Each of these vectors have entries $\Psi^{\boldsymbol{p}}_{\boldsymbol{q}}$, where $\boldsymbol{q}$ ranges over all allowed 2-electron states, that is, all momenta satisfying $\epsilon_{\boldsymbol{q}} > 0$.

[17] $\theta(x)$ is the Heaviside step function, which evaluates to $\theta(x) = 1$ for $x \geq 0$ and $\theta(x) = 0$ for $x < 0$.

[18] Note that the variable $\boldsymbol{q}'$ on the right-hand side of the equation is being summed over, so that all possible values of $\boldsymbol{q}'$ enter the expression.

we have to choose $\phi_q = A/(E - 2\epsilon_q)$, where A is some non-zero constant that cancels from both sides of the equation. We obtain

$$1 = -\frac{g}{V} \sum_{q}^{0<\epsilon_q \leq \omega} \frac{1}{E - 2\epsilon_q}, \tag{3.13}$$

where we have replaced the summation label $q' \to q$. To solve this equation, we can go to thermodynamic limit (see the section on Conventions) and replace the sum by an integral:

$$1 = -g \int_0^\omega d\epsilon \, \frac{\rho(\epsilon)}{E - 2\epsilon}. \tag{3.14}$$

Here, $\rho(\epsilon)$ is the density of states defined in Eq. (1.7). To simplify things further, we can assume that $\rho(\epsilon) \approx \rho(0)$ is approximately constant around the Fermi energy $\epsilon = 0$. This will be an okay approximation to make as long as $\omega \ll E_F$. We then find

$$1 = -\rho(0)g \left[-\frac{1}{2} \ln(E - 2\epsilon) \right]_0^\omega = \frac{\rho(0)g}{2} \ln\left(\frac{E - 2\omega}{E} \right). \tag{3.15}$$

Correspondingly, we obtain

$$E = \frac{2\omega}{1 - e^{\frac{2}{\rho(0)g}}} \approx -2\omega \, e^{-\frac{2}{\rho(0)g}}, \tag{3.16}$$

where we have used that the interaction strength g is very small so that $\frac{2}{\rho(0)g} \gg 1$.[19] As a result, even for an *infinitesimally small* attractive interaction, the spectrum of the two-electron Hamiltonian matrix $h_{qq'}$ in Eq. (3.8) has an eigenstate with *negative* energy, corresponding to a bound state of two electrons, a *Cooper pair*.

[19] Note that the density of states $\rho(\epsilon)$ is an *intensive* quantity, meaning that it does not scale with volume and instead converges to a finite value in the thermodynamic limit $L \to \infty$.

A few remarks are in order.

(1) The binding energy approaches zero as $\rho(0) \to 0$. This means that we need a gapless Fermi surface to support superconductivity. There is no Cooper pairing in a gapped insulator where $\rho(0) = 0$ around the Fermi energy.

(2) The binding energy is non-analytic (*i.e.*, does not have a Taylor expansion in terms of positive powers) in the strength of the interaction g. Since perturbation theory around the non-interacting Hamiltonian corresponds to a Taylor expansion g, this implies that Cooper pairing is a *non-perturbative* result that does not show up *at any order in perturbation theory*. This fact has led quite a few physicists astray in the early days of superconductivity!

(3) Recall that we had found a continuum of two-electron states at energies $E > 2\omega$ in Eq. (3.10), as well as a single bound state with *negative* energy. What happened to all the remaining states

of the continuum, *i.e.*, the two-particle states with kinetic energy $0 < E \leq 2\omega$? By a little thought, you can check that these states are still there; in fact they hide in plain sight in Eq. (3.12). See if you can derive their form by setting $E = 2\epsilon_p$ for some specific choice of ϵ_p.

(4) The Cooper pair wavefunction

$$\phi_q = \frac{A}{E - 2\epsilon_q} \approx \frac{1}{\epsilon_q + \omega\, e^{-\frac{2}{\rho(0)g}}} \tag{3.17}$$

decays like $\sim 1/|q|^2$ away from its peak at $\epsilon_q = 0$.[20] Correspondingly, it is large only around the Fermi surface. This fact is reassuring as it means that changing the form of the electron-electron interaction in Eq. (3.9) away from the Fermi surface will not significantly affect Cooper pair formation.

We sketch the 2-electron spectrum of Eq. (3.8) assuming either only the kinetic energy $\hat{H}_{\text{kin}}$ or the full interacting Hamiltonian $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}}$ in Fig. 2. The spectra look almost the same, with the notable exception of a single bound state in the interacting spectrum that is not present in the purely kinetic case.

Since we have found a two-electron bound state with negative energy, the Fermi sea $|\text{FS}\rangle$, which in our conventions has zero energy[21], cannot be the true ground state of the full Hamiltonian $\hat{H}$. What's more, once we established that two electrons can lower their energy by pairing up, who's to say that we can't lower the total energy of the system even further by pairing another two electrons, and another two, and another two, and so on, until no electrons are left?

[20] Recall that we defined ϕ_q to be non-zero only for $\epsilon_q > 0$, so that the singularity at $\epsilon_q = -\omega\, e^{-\frac{2}{\rho(0)g}}$ is avoided.

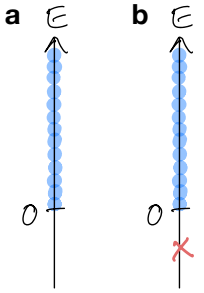

Figure 2: Spectrum of the 2-electron Hamiltonian Eq. (3.8) without and with interactions. **a** Without interactions, $\hat{H}_{\text{int}} = 0$. There are extensively many eigenvalues above $E = 0$ that approximate a continuum in the thermodynamic limit $V \to \infty$. **b** With interactions, where $\hat{H}_{\text{int}} \neq 0$ is given by Eq. (3.9). The continuum of eigenvalues above $E = 0$ remains unaffected, but there is one additional discrete eigenvalue at $E < 0$, corresponding to the Cooper pair bound state. (Technically, the continuum is missing a single state to account for the new bound state at fixed Hilbert space dimension, but this mismatch becomes invisible in the thermodynamic limit.)

[21] You could object that we have not yet considered the effect of $\hat{H}_{\text{int}}$ on the energy of $|\text{FS}\rangle$. However, you can convince yourself that any energy shift of $|\text{FS}\rangle$, effectively changing E_{FS} defined in Eq. (3.4), would also enter in all energy expectation values calculated from the two-electron states $|q\rangle$ defined in Eq. (3.7), and therefore cancels out.

4 Mean field theory

We have seen that the Fermi sea $|\mathrm{FS}\rangle$ is not a good ground state for the Hamiltonian $\hat{H} = \hat{H}_{\mathrm{kin}} + \hat{H}_{\mathrm{int}}$ in Eq. (3.2) as long as $\hat{H}_{\mathrm{int}}$ corresponds to an attractive electron-electron interaction roughly of the form of Eq. (3.9).[1] This is because of the Cooper instability of the Fermi surface that favours the formation of electron-hole pairs. We now have to look for a better ground state than the Fermi sea $|\mathrm{FS}\rangle$.

[1] More elaborate calculations show that the same is true also for more complicated = realistic choices of $\hat{H}_{\mathrm{int}}$, as long as the interaction is attractive around the Fermi surface. See:
Michael Tinkham. *Introduction to superconductivity*, volume 1. Courier Corporation, 2004

Since the Fermi sea contains macroscopically many electrons (more than Avogadro's number $\sim 10^{23}$ in realistic materials, and infinitely many in the thermodynamic limit), forming one or just a few Cooper pairs won't change it enough to invalidate our calculation from the previous section. Hence we can expect that a macroscopic number of Cooper pairs will form (we say that the Cooper pairs *condense*) and the resulting ground state will significantly differ from the Fermi sea. To study this ground state, let us have a look at the full pairing Hamiltonian giving rise to Eq. (3.9)[2]:

$$\hat{H} = \hat{H}_{\mathrm{kin}} + \hat{H}_{\mathrm{int}} = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma} + \sum_{qq'} g_{qq'} c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} c_{-q'\downarrow} c_{q'\uparrow}, \tag{4.1}$$

[2] We will prove in one of the problem sheets that this Hamiltonian results in Eq. (3.9). This model is sometimes called the *reduced BCS Hamiltonian*.

where we have defined

$$g_{qq'} = \begin{cases} -g/V & -\omega \le \epsilon_q, \epsilon_{q'} \le \omega, \\ 0 & \text{otherwise.} \end{cases} \tag{4.2}$$

Note that here we have chosen a symmetric energy window centered around the Fermi surface $\epsilon_q = 0$, while the definition in Eq. (3.9) was manifestly asymmetric. This is not a contradiction, because the variational states $|q\rangle = c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} |\mathrm{FS}\rangle$ vanish for $\epsilon_q < 0$, where $|q\rangle = 0$ holds due to the Pauli principle.

The Hamiltonian in Eq. (4.1) is still quite a bit too complicated to allow us to easily deduce all of its eigenstates and energy eigenvalues[3].

[3] However, it is worth pointing out that an exact (but tedious) solution is in fact possible. In the thermodynamic limit, this solution agrees with the approximation that we'll make, see:
J. Dukelsky, S. Pittel, and G. Sierra. Colloquium: Exactly solvable richardson-gaudin models for many-body quantum systems. *Rev. Mod. Phys.*, 76:643–662, Aug 2004

4.1 Mapping to a spin model

To make progress, let us pretend the kinetic energy is zero and first only try to solve the interacting term on its own:

$$\hat{H}_{\mathrm{int}} = -\frac{g}{V} \sum_{q}^{|\epsilon_q| \le \omega} \sum_{q'}^{|\epsilon_{q'}| \le \omega} c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} c_{-q'\downarrow} c_{q'\uparrow}. \tag{4.3}$$

We can rewrite this Hamiltonian in a more familiar form by introducing the operators[4]

$$\hat{S}^+_q = c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow}, \quad \hat{S}^-_q = c_{-q\downarrow} c_{q\uparrow}, \quad \hat{S}^z_q = \frac{1}{2}\left(c^\dagger_{q\uparrow} c_{q\uparrow} + c^\dagger_{-q\downarrow} c_{-q\downarrow} - 1 \right), \tag{4.4}$$

[4] For now, treat this just as a definition that we make, there is no way to "derive" these equations. Instead we just make this definition and see where it leads us.

which satisfy the commutation relations[5]

$$\left[\hat{S}^+_q, \hat{S}^-_{q'}\right] = \delta_{qq'} 2\hat{S}^z_{q'}, \quad \left[\hat{S}^z_q, \hat{S}^+_{q'}\right] = \delta_{qq'}\hat{S}^+_{q'}, \quad \left[\hat{S}^z_q, \hat{S}^-_{q'}\right] = -\delta_{qq'}\hat{S}^-_{q'}. \tag{4.5}$$

Miraculously, these are *exactly* the same commutation operators as for a system of decoupled quantum spins (one spin for each momentum $\boldsymbol{q}$)[6], where $\hat{S}^z_q$ measures the spin projection on the z-axis, and $\hat{S}^+_q$ and $\hat{S}^-_q$ are spin raising and lowering ladder operators[7]. Moreover, since the interaction Hamiltonian in Eq. (4.3) only ever adds or removes *both* $\uparrow$ and $\downarrow$ electrons at any given momentum $\boldsymbol{q}$, we can safely assume that in the ground state of $\hat{H}_{\text{int}}$, the states $\uparrow$ and $\downarrow$ are either fully occupied or unoccupied at all momenta, so that $\hat{S}^z_q = (n_{q\uparrow} + n_{-q\downarrow} - 1)/2$ can realise eigenvalues[8] $\hat{S}^z_q \in \{\frac{1}{2}, -\frac{1}{2}\}$. As a consequence, the spin operators given in Eq. (4.4) effectively act on a spin-$\frac{1}{2}$ degree of freedom associated with each momentum $\boldsymbol{q}$. We now recall from the theory of quantum mechanical spin[9] that the ladder operators $\hat{S}^+_q$ and $\hat{S}^-_q$ can be written as

$$\hat{S}^+_q = \hat{S}^x_q + \mathrm{i}\hat{S}^y_q, \quad \hat{S}^-_q = \hat{S}^x_q - \mathrm{i}\hat{S}^y_q, \tag{4.6}$$

so that the *Hermitian* operators $\hat{S}^x_q$, $\hat{S}^y_q$, and $\hat{S}^z_q$ satisfy the usual spin algebra

$$\left[\hat{S}^x_q, \hat{S}^y_{q'}\right] = \delta_{qq'}\mathrm{i}\hat{S}^z_{q'}, \quad \left[\hat{S}^y_q, \hat{S}^z_{q'}\right] = \delta_{qq'}\mathrm{i}\hat{S}^x_{q'}, \quad \left[\hat{S}^z_q, \hat{S}^x_{q'}\right] = \delta_{qq'}\mathrm{i}\hat{S}^y_{q'}. \tag{4.7}$$

We also note the following relation:

$$\begin{aligned}\hat{S}^+_q\hat{S}^-_{q'} &= \left(\hat{S}^x_q + \mathrm{i}\hat{S}^y_q\right)\left(\hat{S}^x_{q'} - \mathrm{i}\hat{S}^y_{q'}\right) \\ &= \hat{S}^x_q\hat{S}^x_{q'} - \mathrm{i}\hat{S}^x_q\hat{S}^y_{q'} + \mathrm{i}\hat{S}^y_q\hat{S}^x_{q'} + \hat{S}^y_q\hat{S}^y_{q'},\end{aligned} \tag{4.8}$$

so that using the shorthand $\sum_q^{|\epsilon_q|\leq\omega} \equiv \widetilde{\sum}_q$ for the reduced sums, the interaction Hamiltonian becomes

$$\begin{aligned}\hat{H}_{\text{int}} &= -\frac{g}{V}\widetilde{\sum}_{q,q'}\hat{S}^+_q\hat{S}^-_{q'} = -\frac{g}{V}\widetilde{\sum}_{q,q'}\left(\hat{S}^x_q\hat{S}^x_{q'} + \hat{S}^y_q\hat{S}^y_{q'} - \mathrm{i}\left[\hat{S}^x_q, \hat{S}^y_{q'}\right]\right) \\ &= -\frac{g}{V}\widetilde{\sum}_{q,q'}\left(\hat{S}^x_q\hat{S}^x_{q'} + \hat{S}^y_q\hat{S}^y_{q'}\right) - \frac{g}{V}\widetilde{\sum}_q\hat{S}^z_q.\end{aligned} \tag{4.9}$$

Introducing the extensive *total spin* operators

$$\hat{S}^x \equiv \widetilde{\sum}_q\hat{S}^x_q, \quad \hat{S}^y \equiv \widetilde{\sum}_q\hat{S}^y_q, \quad \hat{S}^z \equiv \widetilde{\sum}_q\hat{S}^z_q, \tag{4.10}$$

the interaction Hamiltonian becomes

$$\hat{H}_{\text{int}} = -\frac{g}{V}\left[(\hat{S}^x)^2 + (\hat{S}^y)^2 + \hat{S}^z\right]. \tag{4.11}$$

We now note that $\hat{S}_{x,y,z}$ are extensive operators defined via sums over a macroscopic number of momentum modes in Eq. (4.10). Since

[5] Check this!

[6] Please do not confuse this "spin" with the actual microscopic spin $\sigma = \uparrow, \downarrow$ of each electron. We only use the term spin here because the commutation relations are the same *as if* $\hat{S}^z_q, \hat{S}^+_q, \hat{S}^-_q$ would really describe a quantum mechanical spin, this is only a mathematical but not a physical analogy.

[7] If it's been a while since you last looked at spin ladder operators, see the documentation on easyspin.org for a helpful cheat sheet.

[8] Recall that $c^\dagger_{q\sigma}c_{q\sigma} = n_{q\sigma}$ is the number operator that has eigenvalue 1 when the electron at momentum $\boldsymbol{q}$ and spin σ is occupied and zero otherwise.

[9] If you do not recall this, you can view the following equation simply as a definition of the operators $\hat{S}^x_q$ and $\hat{S}^y_q$.

the number of momenta in the energy interval $-\omega \leq \epsilon_q \leq \omega$ scales proportionally to the volume V, we expect the relative scaling

$$(\hat{S}^x)^2 \sim \mathcal{O}(V^2), \quad (\hat{S}^y)^2 \sim \mathcal{O}(V^2), \quad \hat{S}^z \sim \mathcal{O}(V). \tag{4.12}$$

It will therefore be safe to neglect the term proportional to $\hat{S}^z$ in the thermodynamic limit $V \to \infty$[10], so that we finally obtain

$$\hat{H}_{\text{int}} \approx -\frac{g}{V}\left[(\hat{S}^x)^2 + (\hat{S}^y)^2\right]. \tag{4.13}$$

[10] Recall that the energy of the full system, as measured by $\hat{H}_{\text{int}}$, should be an extensive quantity that scales $\propto V$.

A remark about symmetry before we go on: Since $\hat{S}^z$ anti-commutes with the other spin operators, $\{\hat{S}^z, \hat{S}^x\} = \{\hat{S}^z, \hat{S}^y\} = 0$, $\hat{H}_{\text{int}}$ has a U(1) rotational symmetry that corresponds to rotations about the z-axis, generated by[11] $\hat{S}^z$: $[\hat{S}^z, \hat{H}_{\text{int}}] = 0$. By writing out $\hat{S}^z$ using Eq. (4.4), we see that this symmetry is nothing but particle number conservation:

$$\begin{aligned}\hat{S}^z &= \frac{1}{2}\widetilde{\sum_q}\left(c^\dagger_{q\uparrow}c_{q\uparrow} + c^\dagger_{-q\downarrow}c_{-q\downarrow} - 1\right) = \frac{1}{2}\widetilde{\sum_q}\left(n_{q\uparrow} + n_{-q\downarrow} - 1\right) \\ &= \frac{1}{2}\widetilde{\sum_{q,\sigma}}\left(n_{q\sigma} - \frac{1}{2}\right) = \frac{1}{2}\left(\tilde{N}_{\text{occ}} - \tilde{N}\right) = \frac{1}{2}\tilde{N}_{\text{occ}} - const.,\end{aligned} \tag{4.14}$$

[11] An arbitrary rotation about the z-axis by an angle ϕ can then be written in terms of the unitary operator $U(\phi) = \exp(i\phi\hat{S}^z)$. The collection of all such operators for different ϕ forms the one-dimensional unitary group U(1).

where $\tilde{N}_{\text{occ}}$ is the total number of electrons that are occupied in the momentum space interval where $-\omega \leq \epsilon_q \leq \omega$ and $\tilde{N}$ is the total number of momenta in the same interval, that is, $\widetilde{\sum}_q 1 = \tilde{N}$. Hence the fact that $[\hat{S}^z, \hat{H}_{\text{int}}] = 0$ commutes can be directly traced back to the fact that $\hat{H}_{\text{int}}$ in Eq. (4.3) preserves overall particle number (every term in the sum creates two electrons and annihilates two electrons) and does not mix between momenta that are respectively outside and inside the interval $-\omega \leq \epsilon_q \leq \omega$.

4.2 Mean field solution

We will now find the ground state of the simplified spin Hamiltonian in Eq. (4.13),

$$\hat{H}_{\text{int}} = -\frac{g}{V}\left[(\hat{S}^x)^2 + (\hat{S}^y)^2\right], \tag{4.15}$$

using two alternative methods: First, in a mean-field approximation, and then by exact solution. While the two methods agree in the thermodynamic limit, their physical interpretation is surprisingly different. This solution will be a helpful stepping stone towards the solution of the full superconductor Hamiltonian in Eq. (4.1).

Mean field theory is a method for finding approximate eigenstates of quantum many-body systems by expanding their Hamiltonian about expectation values (the "mean fields") of certain operators. Mean field theory is universally applicable and renders complicated quantum problems soluble; however, it is fundamentally an approximation that may or may not be valid for a given physical problem.

Sometimes mean field theory gives physically incorrect results, which is why we will compare it to an exact solution later on[12]. We now explain the general strategy for mean field theory and concurrently apply it to the spin model in Eq. (4.15):

1. Expand all operators that appear in the Hamiltonian in terms of their expectation value in the ground state (a complex number), plus their fluctuation away from this mean (an operator), and only keep terms *up to linear order* in the fluctuations.[13]

Application to the spin model

We rewrite the total spin operators as

$$\hat{S}^i = m^i + \left(\hat{S}^i - m^i\right), \quad m^i = \langle \hat{S}^i \rangle \quad (i = x, y). \tag{4.16}$$

Here the expectation value is to be understood with respect to the as of yet undetermined ground state. Plugging into Eq. (4.15), we obtain

$$\hat{H}_{\text{int}} = -\frac{g}{V}\sum_i (\hat{S}^i)^2 \approx -\frac{g}{V}\sum_i \left[(m^i)^2 + 2m^i\left(\hat{S}^i - m^i\right)\right], \tag{4.17}$$

where we have dropped the term that is of second-order in the fluctuations $(\hat{S}^i - m^i)^2$. Dropping all constant terms and only keeping the term that includes the operators $\hat{S}^i$, we end up with a mean-field theory (MFT) Hamiltonian that depends on the set of unknown parameters $\{m^i\}$:

$$\hat{H}_{\text{MFT}}[\{m^i\}] = -\frac{2g}{V}\sum_i m^i \hat{S}^i. \tag{4.18}$$

This Hamiltonian is reminiscent of a Zeeman coupling of the spin vector $\hat{\boldsymbol{S}} = (\hat{S}^x, \hat{S}^y)^{\mathrm{T}}$ to an "external magnetic field" $\boldsymbol{m} = (m^x, m^y)^{\mathrm{T}}$, it favours the alignment of the spin with the mean field. Without loss of generality we can choose this field to point along the positive x-spin direction, so that $m^x > 0$, $m^y = 0$. We then end up with the simplified MFT Hamiltonian

$$\hat{H}_{\text{MFT}}[m^x] = -\frac{2g}{V} m^x \hat{S}^x. \tag{4.19}$$

2. Diagonalise the resulting mean field Hamiltonian to find its ground state.[14]

[12] Using quantum field theory arguments, it can be shown that mean field theory for Hamiltonians with local couplings becomes more and more accurate in higher dimensions; the method usually fails in one or two spatial dimensions but is reliable in three dimensions or higher. The present case of the spin model in Eq. (4.15) formally corresponds to infinite dimensions *in momentum space*: each spin at a given momentum interacts with all others with equal strength, just as if they were all nearest neighbours of one another. We therefore expect mean field theory to be highly accurate.

[13] This results in a mean-field Hamiltonian that is solvable, because the remaining operators are not coupled to each other. At the same time, the Hamiltonian now depends on a new set of parameters, *i.e.*, the presumed ground state expectation values, which we treat as unknown variables for now.

[14] Due to the approximation we have made, this step is now straightforward.

Application to the spin model

The MFT Hamiltonian $\hat{H}_{\text{MFT}}[m^x]$ only depends on the operator $\hat{S}^x$ and so its ground state is an eigenstate of $\hat{S}^x$. Due to the overall minus sign in the Hamiltonian ("ferromagnetic coupling"), to minimise the energy we want the *largest* $\hat{S}^x$ eigenvalue. The best we can do is to built an eigenstate from all the $+\frac{1}{2}$ eigenstates of the spin-$\frac{1}{2}$ operators $\hat{S}^x_q$, so that the largest eigenvalue of the total spin operator $\hat{S}^x = \widetilde{\sum}_q \hat{S}^x_q$ is given by $+\tilde{N}/2$ where $\tilde{N}$ is the total number of momenta in the interval $-\omega \leq \epsilon_q \leq \omega$. Correspondingly, the MFT ground state (GS) is a product state of the form

$$|\text{GS}_{\text{MFT}}\rangle = \widetilde{\otimes}_q |{\uparrow_x}\rangle_q\,, \quad \hat{S}^x_q |{\uparrow_x}\rangle_q = +\frac{1}{2} |{\uparrow_x}\rangle_q\,, \tag{4.20}$$

and it satisfies

$$\hat{H}_{\text{MFT}}[m^x] \, |\text{GS}_{\text{MFT}}\rangle = -\frac{g}{V} m^x \tilde{N} \, |\text{GS}_{\text{MFT}}\rangle\,. \tag{4.21}$$

[Here, $\widetilde{\otimes}_q$ is our shorthand notation to denote the tensor product over all momenta q with $-\omega \leq \epsilon_q \leq \omega$.]

3. Calculate the actual operator expectation values in the ground state and match them with the parameters we had introduced in step (1) to obtain the physical mean field solution.[15]

[15] This matching results in a set of self-consistency equations that must be solved in addition to diagonalising the mean-field Hamiltonian.

Application to the spin model

Since $|\text{GS}_{\text{MFT}}\rangle$ is a product of eigenstates of $\hat{S}^x_q$, it is also an eigenstate of $\hat{S}^x$ and we immediately find

$$\langle \text{GS}_{\text{MFT}}| \, \hat{S}^x \, |\text{GS}_{\text{MFT}}\rangle = \frac{\tilde{N}}{2} \stackrel{!}{=} m^x. \tag{4.22}$$

To calculate the expectation value of $\hat{S}^y$, we note that, in the spin-1/2 basis where $\hat{S}^z_q = \text{diag}(\frac{1}{2}, -\frac{1}{2}) = \sigma_z/2$ is diagonal and σ_i ($i = x, y, z$) are the 2×2 Pauli matrices, we have $|{\uparrow_x}\rangle_q = (1,1)^{\mathrm{T}}/\sqrt{2}$ and $\hat{S}^y_q = \sigma_y/2$ and therefore

$$\langle {\uparrow_x}|_q \, \hat{S}^y_q \, |{\uparrow_x}\rangle_q = \frac{1}{4}(1,1) \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0, \tag{4.23}$$

so that

$$\langle \text{GS}_{\text{MFT}}| \, \hat{S}^y \, |\text{GS}_{\text{MFT}}\rangle = 0 \stackrel{!}{=} m^y, \tag{4.24}$$

confirming the validity of our choice $m^y = 0$. We can then approximate the exact ground state energy using the MFT

solution by calculating the expectation value of $\hat{H}_{\text{int}}$ in the MFT state using Eq. (4.17):

$$E_{\text{MFT}} \equiv \langle \text{GS}_{\text{MFT}} | \hat{H}_{\text{int}} | \text{GS}_{\text{MFT}} \rangle = -\frac{g\tilde{N}^2}{4V}. \tag{4.25}$$

Note that the MFT expectation value of the second-order term $(\hat{S}^x - m^x)^2$, which we had dropped in the second equality of Eq. (4.17), is exactly zero.

4.3 Exact solution

From the basic theory of quantum spin[16], we recall that the full Hilbert space acted upon by the $\hat{S}^i$ operators can be decomposed into states of the form $|s, m_s\rangle$ that satisfy

$$\begin{aligned} (\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}}) |s, m_s\rangle &= s(s+1) |s, m_s\rangle , \\ \hat{S}^z |s, m_s\rangle &= m_s |s, m_s\rangle , \end{aligned} \tag{4.26}$$

where $\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}} = (\hat{S}^x)^2 + (\hat{S}^y)^2 + (\hat{S}^z)^2$. Here,

$$s = 0, \quad 1, \quad 2, \quad \ldots, \quad \frac{\tilde{N}}{2} - 1, \quad \frac{\tilde{N}}{2}$$

is called the total spin quantum number (assuming $\tilde{N}$ is even without loss of generality) and

$$m_s = -s, \quad -s+1, \quad \ldots, \quad s-1, \quad s$$

is the spin projection on the z-axis.[17] Technically, the states $|s, m_s\rangle$ form a basis for the different *irreducible representations* (multiplets) of the rotation group SU(2) that are labelled by their total spin s.[18] Working in such a basis, we note that

$$\begin{aligned} \hat{H}_{\text{int}} &= -\frac{g}{V}\left[(\hat{S}^x)^2 + (\hat{S}^y)^2\right] = -\frac{g}{V}\left[\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}} - (\hat{S}^z)^2\right] \\ &= -\frac{g}{V}\left[s(s+1) - m_s^2\right] = -\frac{g}{V}s(s+1) + \frac{g m_s^2}{V}. \end{aligned} \tag{4.27}$$

The first term is negative and so we would like to maximise its absolute value to minimise the energy, meaning $s = s_{\text{max}} = \frac{\tilde{N}}{2}$ in the ground state. Importantly, in the entire Hilbert space there is only a single multiplet with total spin $s = \frac{\tilde{N}}{2}$, as can be seen from the fact that there is only a single state with spin projection $m_s = \frac{\tilde{N}}{2}$, namely the state where *all* $\hat{S}^z_{\boldsymbol{q}} = \frac{1}{2}$ are pointing up. The second term in Eq. (4.27) is non-negative, and so to minimise the energy we would like to set $m_s = 0$. This means that the *exact* and unique ground state

[16] If you want to revisit this, review "addition of angular momenta" in any quantum mechanics textbook.

[17] In fact, since in general we have that $\sum_{s=0}^{\tilde{N}/2}(2s+1) < 2^{\tilde{N}}$, states with the same total spin s and spin projection m_s can appear *multiple* times in the full $2^{\tilde{N}}$-dimensional Hilbert space.

[18] We don't really need this technical mumbo jumbo here, but maybe it helps you to put things in context.

(GS) of $\hat{H}_{\text{int}}$ is a SU(2) basis state of the form $|s, m_s\rangle$ [Eq. (4.26)] and given by

$$|\text{GS}\rangle = |\frac{\tilde{N}}{2}, 0\rangle\,. \tag{4.28}$$

The ground state energy is obtained from Eq. (4.27) as

$$E_{\text{GS}} = -\frac{g}{V}\frac{\tilde{N}}{2}\left(\frac{\tilde{N}}{2}+1\right) = -\frac{g\tilde{N}^2}{4V} - \frac{g\tilde{N}}{2V}. \tag{4.29}$$

Comparing with the MFT energy from Eq. (4.25), we compare

$$E_{\text{GS}} = E_{\text{MFT}} - \frac{g\tilde{N}}{2V} < E_{\text{MFT}}, \tag{4.30}$$

so that the exact ground state energy is always strictly smaller than the MFT energy. However, in the thermodynamic limit where $\tilde{N} \sim V \to \infty$, the second term in E_{GS} can be neglected so that we find

$$\lim_{V\to\infty} E_{\text{MFT}} = E_{\text{GS}}. \tag{4.31}$$

This implies that our mean field solution works and recovers the correct ground state physics.

4.4 BCS mean-field ansatz

Let us recap what we have learned from applying a mean field approximation to the simple spin model.

- The microscopic Hamiltonian $\hat{H}_{\text{int}} = -\frac{g}{V}[(\hat{S}^x)^2 + (\hat{S}^y)^2]$ of Eq. (4.15) fully preserves spin rotations about the z-axis, which are generated by the operator $\hat{S}^z$: $[\hat{S}^z, \hat{H}_{\text{int}}] = 0$. In the fermionic language, this symmetry corresponds to U(1) charge conservation symmetry [Eq. (4.14)], and fundamentally derives from the fact that each term in the superconductor Hamiltonian in Eq. (4.1) contains an equal number of electron creation and annihilation operators.

- The mean field theory ground state $|\text{GS}_{\text{MFT}}\rangle = \widetilde{\prod}_q |\uparrow_x\rangle_q$ of Eq. (4.20), which approximates the exact ground state energy arbitrarily well in the thermodynamic limit, *breaks* $\hat{S}^z$ spin rotation symmetry – and thereby charge conservation symmetry – because it has all spins oriented in the x-direction. In particular, the expectation value

  $$\langle \text{GS}_{\text{MFT}}|\, \hat{S}^x\, |\text{GS}_{\text{MFT}}\rangle \neq 0 \tag{4.32}$$

  does not vanish, which immediately implies that $\hat{S}^z$ spin rotation symmetry is broken.

- By applying a rotation around the $\hat{S}^z$ axis to $|\mathrm{GS}_{\mathrm{MFT}}\rangle$ about an angle ϕ, we obtain the ϕ-dependent mean field theory states

$$|\mathrm{GS}_{\mathrm{MFT}}(\phi)\rangle \equiv e^{\mathrm{i}\phi\hat{S}^z}\,|\mathrm{GS}_{\mathrm{MFT}}\rangle\,, \tag{4.33}$$

  which are all degenerate in that they have the same energy expectation value:

$$\langle \mathrm{GS}_{\mathrm{MFT}}(\phi)|\hat{H}_{\mathrm{int}}|\mathrm{GS}_{\mathrm{MFT}}(\phi)\rangle = \langle \mathrm{GS}_{\mathrm{MFT}}|\hat{H}_{\mathrm{int}}|\mathrm{GS}_{\mathrm{MFT}}\rangle\,, \tag{4.34}$$

  this follows directly from $[\hat{S}^z, \hat{H}_{\mathrm{int}}] = 0$. We therefore obtain a macroscopic number of energetically degenerate ground states, which all break $\hat{S}^z$ symmetry individually but are mapped to each other under this symmetry. This constitutes a specific example of **spontaneous symmetry breaking**: Even though the underlying Hamiltonian ($\hat{H}_{\mathrm{int}}$) preserves the symmetry, the system may realise a ground state that explicitly breaks it.

Translating back to the fermionic language, we see that the interaction term $\hat{H}_{\mathrm{int}}$ in the Hamiltonian has an approximate (exact in the thermodynamic limit) ground state that **spontaneously breaks U(1) charge conservation symmetry**. Let us now consider the full superconductor Hamiltonian from Eq. (4.1),

$$\hat{H} = \hat{H}_{\mathrm{kin}} + \hat{H}_{\mathrm{int}} = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma} + \sum_{qq'} g_{qq'} c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} c_{-q'\downarrow} c_{q'\uparrow}. \tag{4.35}$$

Solving this Hamiltonian exactly is difficult, but we can still do mean field theory just as before. In particular, note that the kinetic term contains ϵ_p which is very small around the Fermi level where $\epsilon_p = 0$ [recall Eq. (3.2)]. Correspondingly, at least around the Fermi level, we expect that the ground state is similar to $|\mathrm{GS}_{\mathrm{MFT}}\rangle$ in that it spontaneously breaks U(1) charge conservation symmetry. When writing out Eq. (4.32) in the fermionic operators, this spontaneous symmetry breaking manifests itself as follows:

$$\begin{aligned}
&\langle \mathrm{GS}_{\mathrm{MFT}}|\, \hat{S}^x\, |\mathrm{GS}_{\mathrm{MFT}}\rangle \\
&= \widetilde{\sum_q}\, \langle \mathrm{GS}_{\mathrm{MFT}}|\, \hat{S}^x_q\, |\mathrm{GS}_{\mathrm{MFT}}\rangle \\
&= \frac{1}{2}\widetilde{\sum_q}\, \langle \mathrm{GS}_{\mathrm{MFT}}|\, \left(\hat{S}^+_q + \hat{S}^-_q\right) |\mathrm{GS}_{\mathrm{MFT}}\rangle \\
&= \frac{1}{2}\widetilde{\sum_q} \left[\langle \mathrm{GS}_{\mathrm{MFT}}|\, c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow}\, |\mathrm{GS}_{\mathrm{MFT}}\rangle + \langle \mathrm{GS}_{\mathrm{MFT}}|\, c_{-q\downarrow} c_{q\uparrow}\, |\mathrm{GS}_{\mathrm{MFT}}\rangle\right] \\
&\neq 0.
\end{aligned} \tag{4.36}$$

Here we have used Eq. (4.6) in the second line and Eq (4.4) in the third line. Concurrently, we have

$$\begin{aligned}
&\langle \mathrm{GS_{MFT}} | \, \hat{S}^y \, | \mathrm{GS_{MFT}} \rangle \\
&= \widetilde{\sum_q} \langle \mathrm{GS_{MFT}} | \, \hat{S}^y_q \, | \mathrm{GS_{MFT}} \rangle \\
&= \frac{1}{2\mathrm{i}} \widetilde{\sum_q} \langle \mathrm{GS_{MFT}} | \left(\hat{S}^+_q - \hat{S}^-_q \right) | \mathrm{GS_{MFT}} \rangle \\
&= \frac{1}{2\mathrm{i}} \widetilde{\sum_q} \left[\langle \mathrm{GS_{MFT}} | \, c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} \, | \mathrm{GS_{MFT}} \rangle - \langle \mathrm{GS_{MFT}} | \, c_{-q\downarrow} c_{q\uparrow} \, | \mathrm{GS_{MFT}} \rangle \right] \\
&\stackrel{!}{=} 0.
\end{aligned} \tag{4.37}$$

These equations imply that at least some of the expectation values $\langle \mathrm{GS_{MFT}} | \, c_{-q\downarrow} c_{q\uparrow} \, | \mathrm{GS_{MFT}} \rangle \equiv \Phi_q$ are non-zero and real, because $\Phi^*_q = \langle \mathrm{GS_{MFT}} | \, c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} \, | \mathrm{GS_{MFT}} \rangle$. However, recall that we can perform a rotation about the $\hat{S}^z$ axis to any other MFT ground state that is polarised in the spin-xy plane, for instance a state where $\hat{S}^y$ has a non-zero expectation value but $\hat{S}^x$ does not, or any spin orientation in between. Therefore, the most general mean-field theory is obtained by allowing the expectation value Φ_q be a *complex* number, *i.e.*, $\Phi_q \in \mathbb{C}$.[19] In 1957, John Bardeen, Leon Cooper, and Bob Schrieffer (often abbreviated as *BCS*) correspondingly suggested that the actual ground state $|\mathrm{BCS}\rangle$ of the full superconductor Hamiltonian $\hat{H}$ in Eq. (4.35) satisfies[20]

$$\langle \mathrm{BCS} | c_{-q\downarrow} c_{q\uparrow} | \mathrm{BCS} \rangle = \Phi_q \neq 0. \tag{4.38}$$

Here, $\Phi_q \in \mathbb{C}$ is called the *order parameter*[21] and its existence signifies that the state $|\mathrm{BCS}\rangle$ contains an uncertain – but macroscopically large – number of electron pairs: note that for any state with a fixed particle number, the above expectation value vanishes because $c_{-q\downarrow} c_{q\uparrow}$ reduces the number of electrons in the state by 2.[22]

[19] Coincidentally, you can show that the rotation about the $\hat{S}^z$ axis implemented by the operator $\exp(\mathrm{i}\phi\hat{S}^z)$ precisely shifts the phase angle of the complex number Φ_q by ϕ.

[20] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Theory of superconductivity. *Phys. Rev.*, 108:1175–1204, Dec 1957

[21] This name makes contact with statistical mechanics, where an order parameter differentiates between different phases. For instance, in the ferromagnetic phase of a spin model, the order parameter *magnetisation* is non-zero, while it is zero in the paramagnetic phase. Similarly, a normal metal is a phase where the superconducting order parameter vanishes.

[22] In particular, note that $\langle \mathrm{FS} | c_{-q\downarrow} c_{q\uparrow} | \mathrm{FS} \rangle = 0$, since the Fermi sea state as defined in Eq. (3.3) contains a definite number of electrons.

5 BCS theory

Setting the kinetic energy $\hat{H}_{\text{kin}} = 0$ to zero, we have seen that mean field theory yields a ground state that approximates the true ground state of the interaction Hamiltonian $\hat{H}_{\text{int}}$ well in the thermodynamic limit. At the same time, mean field theory is much easier to work out than any exact solution: in particular, in presence of a non-zero kinetic Hamiltonian $\hat{H}_{\text{kin}} \neq 0$, a simple exact solution of the full Hamiltonian $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}}$ is not available anymore, while mean field theory can be straightforwardly applied to *any* model. In this section, we will therefore work out the mean field solution of the full "reduced BCS model" in Eq. (4.1). Of course, unlike in the simple toy model where $\hat{H}_{\text{kin}} = 0$, we do not rigorously know that mean field theory is a good approximation for this model. However, given that $\hat{H}_{\text{kin}} = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma}$ vanishes right around the Fermi surface $\epsilon_p = 0$ where the interaction strength $g_{qq'}$ becomes nonzero, we expect mean field theory to remain a good approximation.

5.1 Bogoliubov-de Gennes Hamiltonian

We now want to find an order parameter Φ_q so that the energy of $|\text{BCS}\rangle$ is minimised. To simplify this problem further, we now make a *mean-field* approximation: inspired by Eq. (4.38), we write

$$c_{-q\downarrow} c_{q\uparrow} = \Phi_q + \left(c_{-q\downarrow} c_{q\uparrow} - \Phi_q\right), \tag{5.1}$$

and then plug this into our expression for $\hat{H}_{\text{int}}$, neglecting terms *quadratic* in the difference $(c_{-q\downarrow} c_{q\uparrow} - \Phi_q)$.[1] Plugging into Eq. (4.35), we obtain

$$\hat{H} = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma} + \sum_{qq'} g_{qq'} \left(\Phi^*_q c_{-q'\downarrow} c_{q'\uparrow} + c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} \Phi_{q'} - \Phi^*_q \Phi_{q'} \right). \tag{5.2}$$

The last term just contributes an overall constant $-\sum_{qq'} g_{qq'} \Phi^*_q \Phi_{q'} \in \mathbb{R}$ to the Hamiltonian and so we can drop it. Up to some further constant shifts[2], we can then reorganise the remaining terms into

$$\begin{aligned} \hat{H} &= \sum_q \begin{pmatrix} c^\dagger_{q\uparrow} & c_{-q\downarrow} \end{pmatrix} \begin{pmatrix} \epsilon_q & \sum_{q'} g_{qq'} \Phi_{q'} \\ \sum_{q'} g_{qq'} \Phi^*_{q'} & -\epsilon_q \end{pmatrix} \begin{pmatrix} c_{q\uparrow} \\ c^\dagger_{-q\downarrow} \end{pmatrix} \\ &\equiv \sum_q \Psi^\dagger_q \mathcal{H}_q \Psi_q, \end{aligned} \tag{5.3}$$

which should be interpreted as a vector-matrix-vector dot product that results in a (operator-valued) scalar. We have used that $\epsilon_q = \epsilon_{-q}$ and $g_{q'q} = g_{qq'}$ in the first line, and in the second line we have introduced the 2-dimensional *Nambu spinor* $\Psi_q = (c_{q\uparrow}, c^\dagger_{-q\downarrow})^{\text{T}}$. We

[1] Physically, this means that we assume that the fluctuations of the operator $c_{-q\downarrow} c_{q\uparrow}$ around its expectation value Φ_q are small at least for the ground state and the other low-energy states.

[2] We will calculate them and derive the full expression for $\hat{H}$ in a problem sheet.

also introduced the 2×2 *Bogoliubov – de Gennes* Hamiltonian $\mathcal{H}_q$; we will simply call it the *BdG* Hamiltonian later on:

$$\mathcal{H}_q = \begin{pmatrix} \epsilon_q & \Delta_q \\ \Delta_q^* & -\epsilon_q \end{pmatrix}, \quad \Delta_q = \sum_{q'} g_{qq'} \Phi_{q'}. \tag{5.4}$$

The parameter Δ_q is also called the *superconducting gap*, we will understand the reason for this name soon. From the definition of $g_{qq'}$ in Eq. (4.2), Δ_q has a very simple q-dependence:

$$\Delta_q = \begin{cases} -g \sum_p^{|\epsilon_p| \leq \omega} \Phi_p / V & -\omega \leq \epsilon_q \leq \omega, \\ 0 & \text{otherwise.} \end{cases} \tag{5.5}$$

Clearly Δ_q is either zero (in the momentum space regions where $|\epsilon_q| > \omega$), or it is a non-zero constant (in the region $|\epsilon_q| \leq \omega$). This means that when we perform a *gauge transformation* on all single-electron states,

$$c_{q\sigma} \to e^{i\alpha} c_{q\sigma}, \quad \alpha \in \mathbb{R}, \tag{5.6}$$

so that according to Eq. (4.38), Δ_q transforms as[3]

$$\Delta_q \to e^{2i\alpha} \Delta_q, \tag{5.7}$$

we can always choose α such that Δ_q is purely real, $\Delta_q \in \mathbb{R}$. **From now on, we will therefore always assume $\Delta_q^* = \Delta_q$ and use this equation to simplify expressions.**

[3] Note that the state $|\text{BCS}\rangle$ also gets multiplied by an overall phase factor under this transformation, but the phase contributed by the bra cancels that of the ket in Eq. (4.38).

5.2 Quasiparticle operators

Importantly, the mean-field approximation has resulted in a Hamiltonian $\hat{H}$ that is bilinear in the Nambu spinors and does not mix between different momenta q. We can therefore solve this many-body Hamiltonian $\hat{H}$ straightforwardly by diagonalising the 2×2 single-particle BdG Hamiltonian $\mathcal{H}_q$. For this, it is helpful to first note a certain symmetry property of $\mathcal{H}_q$ that is called *particle-hole* symmetry: We can see from Eq. (5.4) that $\mathcal{H}_q$ always satisfies[4]

$$\mathcal{H}_q \sigma_y = -\sigma_y \mathcal{H}_q, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{5.8}$$

where σ_y is one of the three Pauli matrices. This symmetry implies that if we find an eigenvector V_q of $\mathcal{H}_q$ satisfying $\mathcal{H}_q V_q = -\lambda_q V_q$, then

$$\mathcal{H}_q \left(\sigma_y V_q\right) = -\sigma_y \mathcal{H}_q V_q = +\sigma_y \lambda_q V_q = +\lambda_q \left(\sigma_y V_q\right), \tag{5.9}$$

meaning that we get a second eigenvector "for free", which reads $W_q = i\sigma_y V_q$[5] and is associated with the eigenvalue $+\lambda_q$.[6] As a conse-

[4] As a technical aside, the general definition of particle-hole symmetry also involves complex conjugation in addition to conjugation by the Pauli matrix σ_y, but this has no effect on the $\mathcal{H}_q$ considered here as it is purely real.

[5] We include the imaginary unit i here out of convention to make $i\sigma_y$ a real matrix: since $\mathcal{H}_q$ is purely real, **we can always choose its eigenvectors to be purely real, and so we should**, because that will make things easier for us in the future.

[6] And thereby, we have happily found all eigenvectors of $\mathcal{H}_q$ since it is only a 2×2 matrix and so only has 2 eigenvectors.

quence, we can always diagonalise the Hermitian BdG Hamiltonian $\mathcal{H}_q$ via the unitary matrix $U_q = (V_q, W_q)$, whose columns are the eigenvectors $V_q = (v_q, u_q)^{\mathrm{T}}$ and $W_q = \mathrm{i}\sigma_y V_q = (u_q, -v_q)^{\mathrm{T}}$:

$$\mathcal{H}_q = U_q^\dagger \Lambda_q U_q, \quad \Lambda_q = \mathrm{diag}(-\lambda_q, \lambda_q), \quad U_q = \begin{pmatrix} v_q & u_q \\ u_q & -v_q \end{pmatrix}. \tag{5.10}$$

In practice, for the BdG Hamiltonian given in Eq. (5.4), we find the explicit expressions[7]

$$\lambda_q = \sqrt{\epsilon_q^2 + \Delta_q^2} \geq 0, \quad \begin{pmatrix} v_q \\ u_q \end{pmatrix} = \begin{pmatrix} \cos\theta_q \\ \sin\theta_q \end{pmatrix}, \quad \theta_q = \arctan\left(\frac{\Delta_q}{\epsilon_q - \lambda_q}\right). \tag{5.11}$$

Notably the eigenvectors are normalised such that $u_q^2 + v_q^2 = 1$, which follows directly from the fact that U_q is unitary: $U_q^\dagger U_q = \mathbb{1}_{2\times 2}$. At the same time, the eigenvectors are real: $u_q, v_q \in \mathbb{R}$, **we will use this to simplify the calculations that follow**. Plugging Eq. (5.10) into Eq. (5.3), we obtain

$$\begin{aligned} \hat{H} &= \sum_q \Psi_q^\dagger U_q^\dagger \Lambda_q U_q \Psi_q \\ &= \sum_q \begin{pmatrix} v_q c_{q\uparrow}^\dagger + u_q c_{-q\downarrow} \\ u_q c_{q\uparrow}^\dagger - v_q c_{-q\downarrow} \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} -\lambda_q & 0 \\ 0 & \lambda_q \end{pmatrix} \begin{pmatrix} v_q c_{q\uparrow} + u_q c_{-q\downarrow}^\dagger \\ u_q c_{q\uparrow} - v_q c_{-q\downarrow}^\dagger \end{pmatrix} \\ &\equiv \sum_q \lambda_q (\gamma_{q\uparrow}^\dagger \gamma_{q\uparrow} + \gamma_{q\downarrow}^\dagger \gamma_{q\downarrow}), \end{aligned} \tag{5.12}$$

where **we have again dropped a constant energy shift**[8] and introduced the *quasiparticle* operators

$$\gamma_{q\downarrow} = v_q c_{q\uparrow}^\dagger + u_q c_{-q\downarrow}, \quad \gamma_{q\uparrow} = u_q c_{q\uparrow} - v_q c_{-q\downarrow}^\dagger. \tag{5.13}$$

Using $u_q^2 + v_q^2 = 1$ and the fact that u_q and v_q are real, it is easy to verify that these operators satisfy the canonical fermionic algebra

$$\begin{aligned} \{\gamma_{q\downarrow}, \gamma_{p\downarrow}^\dagger\} &= \delta_{qp}, & \{\gamma_{q\uparrow}, \gamma_{p\uparrow}^\dagger\} &= \delta_{qp}, \\ \{\gamma_{q\downarrow}, \gamma_{p\downarrow}\} &= 0, & \{\gamma_{q\uparrow}, \gamma_{p\uparrow}\} &= 0, \\ \{\gamma_{q\downarrow}, \gamma_{p\uparrow}\} &= 0, & \{\gamma_{q\downarrow}, \gamma_{p\uparrow}^\dagger\} &= 0. \end{aligned} \tag{5.14}$$

Note in particular the last two equations which are a bit more non-trivial than the other vanishing commutators. These equations mean that the fermionic modes created by $\gamma_{p\uparrow}^\dagger$ and $\gamma_{p\downarrow}^\dagger$ are fully independent from one another.[9]

This is a miraculous result: the superconducting mean-field Hamiltonian

$$\hat{H} = \sum_{p\sigma} \lambda_p \gamma_{p\sigma}^\dagger \gamma_{p\sigma} \tag{5.15}$$

[7] Try to verify this solution for yourself by explicit calculation or using a computer algebra system like *Mathematica*.

[8] In particular, we have rewritten $\gamma_{q\downarrow}\gamma_{q\downarrow}^\dagger = 1 - \gamma_{q\downarrow}^\dagger \gamma_{q\downarrow}$ using the canonical anti-commutation relations from below, Eq. (5.14). Dropping the 1 [which just sums to an overall constant in Eq. (5.12)], this effectively flips the sign of the first eigenvalue $-\lambda_q \gamma_{q\downarrow}\gamma_{q\downarrow}^\dagger \to +\lambda_q \gamma_{q\downarrow}^\dagger \gamma_{q\downarrow}$.

[9] Physically, the $\gamma^\dagger$ operators create Bogoliubov quasiparticles that are superpositions of electrons $c^\dagger$ and holes c. The fact that the BCS mean-field Hamiltonian $\hat{H}$ becomes diagonal in these operators in Eq. (5.12) means that the Bogoliubov quasiparticles are the normal modes of the superconductor.

Mathematically, the Bogoliubov quasiparticles are obtained from electrons and holes by a unitary "rotation" in Fock space. They have a fixed spin but do not have a well-defined charge, similar to the BCS ground state itself.

takes on exactly the same form as the non-interacting Hamiltonian $\hat{H}_{\text{kin}} = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma}$, except that it is "non-interacting" in the *Bogoliubov quasiparticles* γ instead of the electrons c. Moreover, while the single-particle dispersion ϵ_p was gapless[10], the quasiparticle dispersion $\lambda_q = \sqrt{\epsilon_q^2 + \Delta_q^2}$ has a gap of size Δ_q, meaning that Δ_q is the energy of the lowest-lying excitation above the ground state of $\hat{H}$ (more on this later in the section on Quasiparticle excitations). This explains why Δ_q is called the superconducting gap. We have already seen that the gap is intimately related to the superconducting order parameter via $\Delta_q = \sum_{q'} g_{qq'} \Phi_{q'}$, meaning that the transition from a normal metal to a superconductor is always accompanied by a gap opening.

[10] By gapless, we mean that the kinetic energy is minimised by occupying all electronic states up to the Fermi level $\epsilon_p = 0$, and there are further electronic states just above (and infinitesimally close to) $\epsilon_p = 0$. On the other hand, the lowest energy in the Bogoliubov quasiparticle dispersion is $\lambda_q = \Delta_q$, which may not be close to $\lambda_q = 0$ at all.

5.3 BCS ground state

As the γ's are bona fide fermions, the Hamiltonian $\hat{H}$ in Eq. (5.12) simply counts the number of occupied modes created by $\gamma^\dagger_{q\uparrow}$ and $\gamma^\dagger_{q\downarrow}$, multiplies this number by the corresponding energy λ_q, and then sums these contributions over all momenta $\boldsymbol{q}$. Since we have chosen λ_q as the non-negative branch of the square root in Eq. (5.11), the ground state $|\text{BCS}\rangle$ of $\hat{H}$ is simply given by the *vacuum* of the γ-fermions, that is, $\gamma_{q\downarrow} |\text{BCS}\rangle = \gamma_{q\uparrow} |\text{BCS}\rangle = 0$ should hold for all momenta $\boldsymbol{q}$ so that $\hat{H} |\text{BCS}\rangle = 0$. An easy way to ensure this[11] is to define

$$|\text{BCS}\rangle = \frac{1}{\mathcal{N}} \prod_{\boldsymbol{q}} \gamma_{q\uparrow} \gamma_{q\downarrow} |0\rangle \,, \tag{5.16}$$

where $\mathcal{N}$ is a normalisation factor that ensures $\langle \text{BCS} | \text{BCS} \rangle = 1$, and $|0\rangle$ is the usual fermionic vacuum that satisfies $c_{q\sigma} |0\rangle = 0$. Crucially, $|0\rangle$ is the vacuum for the c-fermions (the microscopic electrons), but not for the γ-fermions (the Bogoliubov quasiparticles), meaning that $\gamma_{q\sigma} |0\rangle \neq 0$.[12] Plugging in the explicit expressions for the γ operators from Eq. (5.13), we can expand the ground state as follows:

$$\begin{aligned}
|\text{BCS}\rangle &= \frac{1}{\mathcal{N}} \prod_{\boldsymbol{q}} \left(u_q c_{q\uparrow} - v_q c^\dagger_{-q\downarrow} \right) \left(v_q c^\dagger_{q\uparrow} + u_q c_{-q\downarrow} \right) |0\rangle \\
&= \frac{1}{\mathcal{N}} \prod_{\boldsymbol{q}} \left(u_q c_{q\uparrow} - v_q c^\dagger_{-q\downarrow} \right) v_q c^\dagger_{q\uparrow} |0\rangle \\
&= \frac{1}{\mathcal{N}} \left(\prod_{\boldsymbol{q}} v_q \right) \prod_{\boldsymbol{q}} \left(u_q c_{q\uparrow} c^\dagger_{q\uparrow} - v_q c^\dagger_{-q\downarrow} c^\dagger_{q\uparrow} \right) |0\rangle \\
&= \frac{1}{\mathcal{N}} \prod_{\boldsymbol{q}} \left(u_q + v_q c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} \right) |0\rangle \,.
\end{aligned} \tag{5.17}$$

[11] You can understand how $\hat{H}$ annihilates this state as follows: defining $|\text{BCS}\rangle$ in this way, in every term of the sum that results from writing out $\hat{H} |\text{BCS}\rangle$, there will always appear a factor $\gamma^2_{q\sigma} = 0$ after suitably reordering the γ operators using the anti-commutation relations from Eq. (5.14). Try it!

[12] In fact, instead of $|0\rangle$, we could have also chosen any other reference state $|\Psi\rangle$ that satisfies $\gamma_{q\sigma} |\Psi\rangle \neq 0$ to define $|\text{BCS}'\rangle = \frac{1}{\mathcal{N}'} \prod_{\boldsymbol{q}} \gamma_{q\uparrow} \gamma_{q\downarrow} |\Psi\rangle$. You can show that both these definitions must result in the same state (potentially up to a phase factor), $|\text{BCS}'\rangle = e^{i\phi} |\text{BCS}\rangle$, by using that the simultaneous eigenstates of the occupation number operators $\gamma^\dagger_{q\sigma} \gamma_{q\sigma}$ form an orthonormal basis of the many-body Hilbert space. There is just a single state that has eigenvalue $\gamma^\dagger_{q\sigma} \gamma_{q\sigma} = 0$ for *all* choices of $\boldsymbol{q}$ and σ.

There's a lot going on in this derivation so let's take care to understand each step. (1) First, we have realised that each of the terms

$u_q c_{-q\downarrow}$ can be commuted past all operators to its right until it hits the vacuum and annihilates – the only problematic operator it could interfere with is $c^\dagger_{-q\downarrow}$, but this operator arises just once in the expression to the *left*, not right, of the term in question. Correspondingly we can drop this term in the second line. (2) To go to the third line, we have then pulled out the overall factor $\prod_q v_q$, as any such factor can be absorbed into the normalisation term $\mathcal{N}$ (we have therefore just dropped this factor altogether in line 4, because $\mathcal{N}$ is only implicitly defined anyway). (3) We have then replaced the term $c_{q\uparrow}c^\dagger_{q\uparrow}$ in the third line by $1 - c^\dagger_{q\uparrow}c_{q\uparrow}$ using the canonical anti-commutation relations, however, the operator $c^\dagger_{q\uparrow}c_{q\uparrow}$ can again be commuted past all operators to its right to annihilate the vacuum, leaving us with just 1. In a last step, we have flipped the two creation operators multiplying v_q to get a positive prefactor, which makes the expression look a bit nicer. That's it!

We are now ready to determine the value of the normalisation factor $\mathcal{N}$. For this we calculate

$$\begin{aligned}
\langle \mathrm{BCS}|\mathrm{BCS}\rangle &= \frac{1}{\mathcal{N}^2}\langle 0|\prod_q (u_q + v_q c_{-q\downarrow}c_{q\uparrow})\prod_p (u_p + v_p c^\dagger_{p\uparrow}c^\dagger_{-p\downarrow})\,|0\rangle \\
&= \frac{1}{\mathcal{N}^2}\langle 0|\prod_q (u_q + v_q c_{-q\downarrow}c_{q\uparrow})(u_q + v_q c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow})\,|0\rangle \\
&= \frac{1}{\mathcal{N}^2}\langle 0|\prod_q \left(u_q^2 + v_q^2 c_{-q\downarrow}c_{q\uparrow}c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}\right)|0\rangle \\
&= \frac{1}{\mathcal{N}^2}\langle 0|\prod_q \left(u_q^2 + v_q^2\right)|0\rangle = \frac{1}{\mathcal{N}^2}\times 1 \overset{!}{=} 1,
\end{aligned} \tag{5.18}$$

so that we conclude that our state was already properly normalised after all and we can just set $\mathcal{N} = 1$. Again, let's slowly walk through what happened here: (1) First, we have reordered the terms in the two products over momentum space to obtain a single product. This was possible because the operators $c_{-q\downarrow}c_{q\uparrow}$ and $c^\dagger_{p\uparrow}c^\dagger_{-p\downarrow}$ commute with each other unless $q = p$: for this special case only, we have left the ordering of operators in line 2 exactly as it was in line 1, with $c_{-q\downarrow}c_{q\uparrow}$ appearing to the left of $c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}$. (2) Then, to go to the third line, we have used that the mixed terms in the product vanish: the mixed term $u_q v_q c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}$ can be commuted all the way to the left to annihilate $\langle 0|$, and the mixed term $v_q c_{-q\downarrow}c_{q\uparrow}u_q$ can be commuted all the way to the right to annihilate $|0\rangle$. (3) In the last step, we have noticed that $c_{-q\downarrow}c_{q\uparrow}c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}\,|0\rangle = |0\rangle$ using the canonical anti-commutation relations, and then used that $u_q^2 + v_q^2 = 1$ must hold since the eigenvectors of the BdG Hamiltonian are normalised.

Our final result for the BCS ground state is therefore

$$|\mathrm{BCS}\rangle = \prod_{\boldsymbol{q}} \left(u_{\boldsymbol{q}} + v_{\boldsymbol{q}} c^\dagger_{\boldsymbol{q}\uparrow} c^\dagger_{-\boldsymbol{q}\downarrow} \right) |0\rangle \,. \tag{5.19}$$

A few remarks are in order.

(1) As expected, $|\mathrm{BCS}\rangle$ does not preserve particle number. For every momentum $\boldsymbol{q}$, we have a superposition of a state with zero electrons and a state with an electron pair. This ensures that adding or removing a pair from $|\mathrm{BCS}\rangle$ does not annihilate the state, so that the order parameter defined in Eq. (4.38) is non-zero.

(2) Plotting the expressions for $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ in Eq. (5.11), we observe that $u_{\boldsymbol{q}}$ rises from 0 to 1 as $\epsilon_{\boldsymbol{q}}$ is advanced from $-\omega$ to ω, while $v_{\boldsymbol{q}}$ drops from 1 to 0 in the same interval. (See Fig. 3.) Both functions are approximately of the same size right around the Fermi level $\epsilon_{\boldsymbol{q}} = 0$. This means that the superconductor consists mostly of pairs with momenta around the Fermi surface. For momenta far outside of the Fermi surface, the vacuum state with zero electrons dominates.[13]

(3) The functions $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ vary smoothly with $\boldsymbol{q}$ because they are obtained from a diagonalisation of the smooth BdG Hamiltonian $\mathcal{H}_{\boldsymbol{q}}$. Furthermore, the phase difference between $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ *is the same* for all choices of $\boldsymbol{q}$.[14] This implies that $|\mathrm{BCS}\rangle$ represents a *coherent* collection of electron pairs that all enter with (roughly) the same wavefunction, resembling Bose-Einstein condensation[15]. Coherence is a unique property of the superconducting state, it stabilises macroscopic quantum effects that are visible to the bare eye[16].

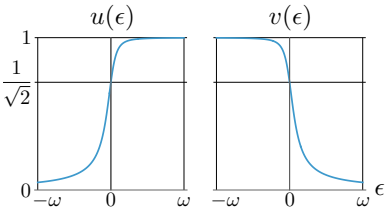

Figure 3: Plotting $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ as a function of energy ϵ between $\epsilon = -\omega$ and $\epsilon = \omega$. For this plot, we have chosen $\Delta_{\boldsymbol{q}} = -0.1\omega$ in the range $-\omega \leq \epsilon_{\boldsymbol{q}} \leq \omega$, and zero outside.

5.4 Self-consistency and gap equation

So far, we have boldly called the ground state of the mean-field Hamiltonian $|\mathrm{BCS}\rangle$, but we still have to make sure that this state actually satisfies the original postulate Eq. (4.38), that is, the expectation value $\langle \mathrm{BCS}| c_{-\boldsymbol{q}\downarrow} c_{\boldsymbol{q}\uparrow} |\mathrm{BCS}\rangle$ should be equal to the order parameter $\Phi_{\boldsymbol{q}}$. Let's calculate this expectation value explicitly:

$$\begin{aligned}
&\langle \mathrm{BCS}| c_{-\boldsymbol{q}\downarrow} c_{\boldsymbol{q}\uparrow} |\mathrm{BCS}\rangle \\
&= \langle 0| \prod_{\boldsymbol{p}} (u_{\boldsymbol{p}} + v_{\boldsymbol{p}} c_{-\boldsymbol{p}\downarrow} c_{\boldsymbol{p}\uparrow}) c_{-\boldsymbol{q}\downarrow} c_{\boldsymbol{q}\uparrow} \prod_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}) |0\rangle \\
&= \langle 0| (u_{\boldsymbol{q}} + v_{\boldsymbol{q}} c_{-\boldsymbol{q}\downarrow} c_{\boldsymbol{q}\uparrow}) c_{-\boldsymbol{q}\downarrow} c_{\boldsymbol{q}\uparrow} (u_{\boldsymbol{q}} + v_{\boldsymbol{q}} c^\dagger_{\boldsymbol{q}\uparrow} c^\dagger_{-\boldsymbol{q}\downarrow}) |0\rangle \\
&= \langle 0| (u_{\boldsymbol{q}} + v_{\boldsymbol{q}} c_{-\boldsymbol{q}\downarrow} c_{\boldsymbol{q}\uparrow}) v_{\boldsymbol{q}} |0\rangle \\
&= \langle 0| u_{\boldsymbol{q}} v_{\boldsymbol{q}} |0\rangle = u_{\boldsymbol{q}} v_{\boldsymbol{q}}.
\end{aligned} \tag{5.20}$$

[13] Note that deep below the Fermi surface, $u_{\boldsymbol{q}} \sim 0$ and $v_{\boldsymbol{q}} \sim 1$, so that for these momenta $|\mathrm{BCS}\rangle$ becomes a simple product state of the same form as the Fermi sea state $|\mathrm{FS}\rangle$ from Eq. (3.3), meaning that there is no pairing either. Pairing only happens around the Fermi surface where $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ are both sizeable.

[14] For the simple model discussed here, this phase difference is always zero because we have chosen $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ to be real. We have seen in Eq. (5.7) that this can be always achieved by a gauge transformation. [If you follow along the calculation below Eq. (5.7), you will see that $\Delta_{\boldsymbol{q}}$ being real implied $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ could be chosen real.] However, it is not possible to gauge away a relative phase *between two regions in space*. This observation leads to the fascinating physics of the *Josephson junction*. Our formalism so far does not cover this possibility, because we have been working in momentum space, which assumes translational invariance so that all regions of space must have the same phase.

[15] Note that Cooper pairs are bosonic in nature because they consist of two fermions – meaning they do not anti-commute with each other. However, to be a bit nitpicky, they are technically not perfect bosons because the operator $c^\dagger_{\boldsymbol{q}\uparrow} c^\dagger_{-\boldsymbol{q}\downarrow}$ does not satisfy the usual bosonic commutation relations. If you're interested in this, look at the literature on the *BCS–BEC crossover*.

[16] An example is the levitation of a magnet above a superconductor, for which you can find some cool videos on YouTube.

In the third line, we have used that the operator $c_{-q\downarrow}c_{q\uparrow}$ only acts nontrivially when $p = k = q$, all other terms in the products over p and k commute past this operator and annihilate because $u_p^2 + v_p^2 = 1$ [this already showed up in the derivation in Eq. (5.18)]. Plugging in the explicit solution from Eq. (5.11), we obtain

$$\langle \mathrm{BCS}|c_{-q\downarrow}c_{q\uparrow}|\mathrm{BCS}\rangle = u_q v_q = -\frac{\Delta_q}{2\sqrt{\Delta_q^2+\epsilon_q^2}} \stackrel{!}{=} \Phi_q. \tag{5.21}$$

Let us now recall that Δ_q has a very simple q-dependence see [Eq. (5.5)]: it is only nonzero in the interval $-\omega \leq \epsilon_q \leq \omega$, where it takes on a q-independent value $\Delta_q \equiv \Delta$.

With this insight, we can convert Eq. (5.21) to an equation involving only Δ by multiplying both sides of the equation by g_{pq} and then summing over q. **Restricting the resulting equation to the interval $-\omega \leq \epsilon_p \leq \omega$**, we obtain

$$\Delta = -\sum_q g_{pq}\frac{\Delta_q}{2\sqrt{\Delta_q^2+\epsilon_q^2}} = \frac{g}{2V}\sum_q^{|\epsilon_q|\leq\omega}\frac{\Delta}{\sqrt{\Delta^2+\epsilon_q^2}}, \tag{5.22}$$

where we have again the definition of g_{pq} in Eq. (4.2). If we manage to find a solution to this condition with a non-vanishing $\Delta \neq 0$, we have successfully constructed a consistent mean-field theory for a condensate of Cooper pairs.[17]

To solve this equation, we cancel Δ from both sides and then replace the last sum over momenta by an integral over energy as explained in the section on Conventions:

$$1 = \frac{g}{2}\int_{-\omega}^{\omega} d\epsilon\, \frac{\rho(\epsilon)}{\sqrt{\Delta^2+\epsilon^2}} \approx \rho(0) g \sinh^{-1}\left(\frac{\omega}{\Delta}\right), \tag{5.23}$$

where in the second line we have assumed that the density of states is essentially constant $\rho(\epsilon) = \rho(0)$ in a window of energy ω around the Fermi level $\epsilon = 0$.[18] We can now finally solve for Δ:

$$\Delta = \frac{\omega}{\sinh\left[1/\rho(0)g\right]} \approx \frac{2\omega}{\exp\left[1/\rho(0)g\right]} = 2\omega e^{-\frac{1}{\rho(0)g}}. \tag{5.24}$$

5.5 Quasiparticle excitations

Let's summarise our results so far. We have expressed the reduced BCS Hamiltonian in the form

$$\hat{H} = \sum_{p\sigma}\lambda_p \gamma_{p\sigma}^\dagger \gamma_{p\sigma}, \qquad \lambda_p \geq 0. \tag{5.25}$$

where the quasiparticle operators $\gamma_{p\sigma}$ satisfy the usual canonical anticommutation relations.[19] Correspondingly, the ground state $|\mathrm{BCS}\rangle$ is

[17] The trivial self-consistent solution where $\Delta = 0$ always exists as well. It just corresponds to the Fermi sea state = a Fermi gas without any pairing. Below the superconducting transition temperature, this solution has a higher overall energy than the superconductor where $\Delta \neq 0$.

[18] For more details, check out Eq. (1.6) as well as the discussion just below Eq. (3.14).

[19] Note that the quasiparticle operator $\gamma_{p\sigma}$, which is defined in Eq. (5.13), does not have a well-defined charge, because it is a superposition of a creation (charge $+1$ in units of electronic charge) and an annihilation operator (charge -1). However, $\gamma_{p\sigma}$ has a well-defined spin $-\sigma$, as it is a superposition of a creation operator with spin $-\sigma$ and an annihilation operator with spin $+\sigma$. Conversely, the quasiparticle creation operator $\gamma_{p\sigma}$ has a spin $+\sigma$ as expected for an operator that adds a particle with definite spin σ.

the *quasiparticle vacuum* defined by $\gamma_{p\sigma}|\text{BCS}\rangle = 0$. This definition led us to the expression

$$|\text{BCS}\rangle = \prod_q \left(u_q + v_q c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow}\right)|0\rangle\,, \tag{5.26}$$

which we used to find the self-consistent value of the mean field order parameter $\Delta_q = \theta(\omega - |\epsilon_q|)\Delta$ with $\Delta = 2\omega e^{-\frac{1}{\rho(0)g}}$, where θ is the Heaviside step function. We would now like to investigate the single-particle excitations above the ground state $|\text{BCS}\rangle$. This is straightforward because the Hamiltonian in Eq. (5.25) is already diagonal in the quasiparticle basis: we can write down an excitation with fixed momentum $\boldsymbol{p}$ and spin σ,

$$|\boldsymbol{p}\sigma\rangle = \gamma^\dagger_{\boldsymbol{p}\sigma}|\text{BCS}\rangle\,, \tag{5.27}$$

and this state is automatically an eigenstate of $\hat{H}$:[20]

$$\hat{H}|\boldsymbol{p}\sigma\rangle = \lambda_{\boldsymbol{p}}|\boldsymbol{p}\sigma\rangle\,. \tag{5.28}$$

Next to the BCS ground state at energy $\hat{H}|\text{BCS}\rangle = 0$, we have therefore found a family of quasiparticle excitations above the ground state with dispersion relation

$$\lambda_p = \sqrt{\epsilon_p^2 + \Delta_p^2} = \sqrt{\left(\frac{|\boldsymbol{p}|^2}{2m} - E_\text{F}\right)^2 + \theta(\omega - |\epsilon_p|)4\omega^2 e^{-\frac{2}{\rho(0)g}}}\,. \tag{5.29}$$

We plot this spectrum in Fig. 4 as a function of the absolute value of momentum p. Importantly, there is a gap compared to the non-interacting dispersion ϵ_p, with an energy difference of exactly Δ at $|\boldsymbol{p}| = \sqrt{2mE_\text{F}}$, the Fermi momentum. This gap represents the minimal energy of any excitation above the BCS ground state.

What do the quasiparticle excitations look like in the electron basis? For this we can calculate for example

$$\begin{aligned}
\gamma^\dagger_{p\uparrow}|\text{BCS}\rangle &= \left(u_p c^\dagger_{p\uparrow} - v_p c_{-p\downarrow}\right)\prod_q \left(u_q + v_q c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}\right)|0\rangle \\
&= \left(u_p c^\dagger_{p\uparrow} - v_p c_{-p\downarrow}\right)\left(u_p + v_p c^\dagger_{p\uparrow}c^\dagger_{-p\downarrow}\right)\prod_{q\neq p}\left(u_q + v_q c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}\right)|0\rangle \\
&= \left(u_p^2 c^\dagger_{p\uparrow} - v_p^2 c_{-p\downarrow}c^\dagger_{p\uparrow}c^\dagger_{-p\downarrow}\right)\prod_{q\neq p}\left(u_q + v_q c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}\right)|0\rangle \\
&= \left(u_p^2 c^\dagger_{p\uparrow} + v_p^2 c^\dagger_{p\uparrow}\right)\prod_{q\neq p}\left(u_q + v_q c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}\right)|0\rangle \\
&= c^\dagger_{p\uparrow}\prod_{q\neq p}\left(u_q + v_q c^\dagger_{q\uparrow}c^\dagger_{-q\downarrow}\right).
\end{aligned} \tag{5.30}$$

Correspondingly, we can interpret the quasiparticle excitation physically in terms of the breaking up of a pair of electrons ($\boldsymbol{p}\uparrow$ and $-\boldsymbol{p}\downarrow$)

[20] Note in particular that $\hat{H}$ does not contain any interactions among the quasiparticles and instead reads like a "kinetic energy" term written in terms of the quasiparticle operators. We have already used up all electronic interactions in constructing the mean field theory and associated quasiparticle operators.

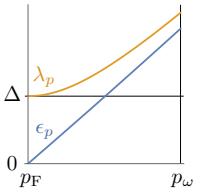

Figure 4: Comparison of the free (ϵ_p) and superconducting (λ_p) dispersion relation in the momentum range $p_\text{F} = \sqrt{2mE_\text{F}}$ to $p_\omega = \sqrt{2m(E_\text{F}+\omega)}$. For this plot, we have chosen $m = 1$, $E_\text{F} = 10$, $\omega = 1$, and $\Delta = 0.5$.

where we keep one electron ($\boldsymbol{p}\ \uparrow$) and discard the other ($-\boldsymbol{p}\ \uparrow$). Since the minimal energy of such an excitation is the gap $\Delta > 0$, the superconducting ground state is stable with respect to all perturbations that have an energy much smaller than this gap. Compare this with the Fermi sea state, which is gapless: as we saw in the section on the Cooper instability, it is exactly this gaplessness (which resulted in a nonzero density of states $\rho(\epsilon)$ in the whole energy range $-\omega \leq \epsilon \leq \omega$) that led to an instability towards the superconducting state.

A Appendix: Mean-field theory as a variational principle

Warning: Things are going to get technical here and this section is entirely optional / not examinable. :)

You might wonder in what sense the mean field approximation we had made in the section on Mean field theory is a good approximation. Recall that in that section we had replaced the original Hamiltonian of the system by an easily diagonalisable mean-field Hamiltonian (the MFT Hamiltonian). Since we also had an exact solution available in the case of the simple spin model [Eq. (4.15)], we were able to compare the MFT solution and the exact solution and showed that the MFT ground state approximates the exact ground state energy arbitrarily well in the thermodynamic limit. However, in the section on the BCS theory and later sections, we treated the full superconductor Hamiltonian Eq. (4.1) with MFT, where an exact solution is not readily available. How much can we trust MFT for such cases where the full Hamiltonian is intractable?

In this appendix, let us be a bit philosophical and look at MFT from a very general perspective. We assume a d-dimensional lattice[1] labelled by coordinates $\boldsymbol{R}$ and consider a general quantum many-body Hamiltonian

$$\begin{aligned} H =& a + \sum_{\boldsymbol{R}\alpha} b_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\alpha} + \sum_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta} \\ &+ \sum_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}''\alpha\beta\gamma} d_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}''\alpha\beta\gamma} O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta} O_{\boldsymbol{R}''\gamma} + \cdots , \end{aligned} \tag{A.1}$$

where the $O_{\boldsymbol{R}\alpha}$ are a collection of few-body operators at lattice position $\boldsymbol{R}$ labeled by the index α and

$$a, \quad b_{\boldsymbol{R}\alpha}, \quad c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta}, \quad d_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}''\alpha\beta\gamma}, \quad \cdots \quad \in \mathbb{C}$$

are a set of model parameters.[2] We assume that the parameters are chosen such that the Hamiltonian is Hermitian, $H = H^\dagger$. Moreover, we choose the operators $O_{\boldsymbol{R}\alpha}$ so that they commute at different lattice points:[3]

$$\left[O_{\boldsymbol{R}\alpha}, O_{\boldsymbol{R}'\beta}\right] \propto \delta_{\boldsymbol{R}\boldsymbol{R}'}. \tag{A.2}$$

This restriction implies that the operators O_α must be bosonic, *i.e.*, they cannot for example be fermionic creation and annihilation operators of the form $c_{\boldsymbol{R}}$, $c^\dagger_{\boldsymbol{R}}$ as these would *anti-commute* at different lattice positions.

MFT now decomposes these operators in terms of their expectation value and fluctuation as follows:

$$O_{\boldsymbol{R}\alpha} = \langle O_{\boldsymbol{R}\alpha} \rangle + (O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha} \rangle). \tag{A.3}$$

[1] This could be a real space lattice or a momentum space lattice or something else entirely; the only thing that's important for our purposes right now is that there are infinitely many lattice points in the thermodynamic limit and that operators at different lattice points commute with each other.

[2] For example, in the case of a spin-1/2 model we could have $O_\alpha = \sigma_\alpha/2$ equal to the 2×2 Pauli matrices, and $\alpha = x, y, z$.

[3] As an example, note that the operators $c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} \equiv O_{q,1}$ and $c_{-q'\downarrow} c_{q'\uparrow} \equiv O_{q',2}$ that appear in the superconductor Hamiltonian in Eq. (4.1) commute when $q \neq q'$.

Here, the average value is taken with respect to the putative MFT ground state that we will determine later. Plugging this expansion into H and keeping only terms linear in the fluctuations $(O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle)$, we obtain a MFT Hamiltonian that depends on the "variables"

$$\langle \boldsymbol{O}\rangle = (\langle O_{\boldsymbol{R}_1,1}\rangle, \langle O_{\boldsymbol{R}_2,1}\rangle, \dots \langle O_{\boldsymbol{R}_N,1}\rangle, \langle O_{\boldsymbol{R}_1,2}\rangle, \dots)^{\mathrm{T}},$$

where $\boldsymbol{R_1} \dots \boldsymbol{R_N}$ is the collection of all N lattice sites and the thermodynamic limit corresponds to $N \to \infty$.[4] The resulting MFT Hamiltonian is then of the general form

$$H_{\mathrm{MFT}}[\langle \boldsymbol{O}\rangle] = A[\langle \boldsymbol{O}\rangle] + \sum_{\boldsymbol{R}\alpha} B[\langle \boldsymbol{O}\rangle]_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\alpha}, \tag{A.4}$$

where $A[\langle \boldsymbol{O}\rangle], B[\langle \boldsymbol{O}\rangle]_{\boldsymbol{R}\alpha} \in \mathbb{C}$ are functions of the variables $\langle \boldsymbol{O}\rangle$ and we have dropped all higher-order terms of the form

$$O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta}, \quad O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta} O_{\boldsymbol{R}''\gamma}, \quad \cdots.$$

To diagonalise the MFT Hamiltonian and find its ground state, we can drop the scalar function $A[\langle \boldsymbol{O}\rangle]$ because it multiplies the identity matrix (it already is diagonal in any basis). We then have to diagonalise the remaining term

$$\sum_{\boldsymbol{R}\alpha} B[\langle \boldsymbol{O}\rangle]_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\alpha}.$$

Crucially, since the operators $O_{\boldsymbol{R}\alpha}$ commute at different lattice positions $\boldsymbol{R}$, all eigenstates $|\Psi\rangle$ of this term – including the ground state – can be written in tensor product form

$$|\Psi\rangle = \prod_{\boldsymbol{R}} |\phi\rangle_{\boldsymbol{R}}, \tag{A.5}$$

where the $|\phi\rangle_{\boldsymbol{R}}$ live in the local Hilbert space at position $\boldsymbol{R}$. This means that they are only acted upon by the operators $O_{\boldsymbol{R}}$ with the same $\boldsymbol{R}$ (all other operators trivially commute past them) and we choose them to satisfy

$$\sum_{\alpha} B[\langle \boldsymbol{O}\rangle]_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\alpha} |\phi\rangle_{\boldsymbol{R}} = E_{\boldsymbol{R}} |\phi\rangle_{\boldsymbol{R}}. \tag{A.6}$$

To confirm that $|\Psi\rangle$ defined in this way is an eigenstate, we compute

$$\begin{aligned}
&\sum_{\boldsymbol{R}\alpha} B[\langle \boldsymbol{O}\rangle]_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\alpha} |\Psi\rangle = \sum_{\boldsymbol{R}\alpha} B[\langle \boldsymbol{O}\rangle]_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\alpha} \prod_{\boldsymbol{R}'} |\phi\rangle_{\boldsymbol{R}'} \\
&= \sum_{\boldsymbol{R}} \left(\prod_{\boldsymbol{R}'\neq\boldsymbol{R}} |\phi\rangle_{\boldsymbol{R}'} \right) \sum_{\alpha} B[\langle \boldsymbol{O}\rangle]_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\alpha} |\phi\rangle_{\boldsymbol{R}} \\
&= \sum_{\boldsymbol{R}} E_{\boldsymbol{R}} \left(\prod_{\boldsymbol{R}'\neq\boldsymbol{R}} |\phi\rangle_{\boldsymbol{R}'} \right) |\phi\rangle_{\boldsymbol{R}} = \left(\sum_{\boldsymbol{R}} E_{\boldsymbol{R}} \right) |\Psi\rangle,
\end{aligned} \tag{A.7}$$

[4] We do not use $N = V$ here because the volume V usually has units while N is a dimensionless number. In the case of a real or momentum space lattice, N will be equal to the volume V up to a dimensionful multiplier.

so that $|\Psi\rangle$ is an eigenstate with eigenvalue $\sum_{\boldsymbol{R}} E_{\boldsymbol{R}}$. For self-consistency, we now need to require

$$\langle O_{\boldsymbol{R}\alpha}\rangle \stackrel{!}{=} \langle\Psi_0|\, O_{\boldsymbol{R}\alpha}\, |\Psi_0\rangle \tag{A.8}$$

where $|\Psi_0\rangle \equiv \prod_{\boldsymbol{R}} |\phi_0\rangle_{\boldsymbol{R}}$ is the ground state that minimises the energy $\sum_{\boldsymbol{R}} E_{\boldsymbol{R}}$. Since $|\Psi_0\rangle$ implicitly depends on the variables $\langle O_{\boldsymbol{R}\alpha}\rangle$, this is a potentially nonlinear equation that relates the $\langle O_{\boldsymbol{R}\alpha}\rangle$ with each other and can in general only be solved numerically.

As soon as self-consistency is achieved, we still need to confirm that our mean-field approximation as a whole is sensible. Recall that we had dropped all higher-order fluctuation terms[5] that to arrive at the MFT Hamiltonian in Eq. (A.4). To see if this is compatible with the MFT solution, let us now calculate the ground state expectation value of the general quadratic fluctuation term:

[5] such as $(O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle)^2$

$$\begin{aligned}
&\langle\Psi_0|\, (O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle)(O_{\boldsymbol{R}'\beta} - \langle O_{\boldsymbol{R}'\beta}\rangle)\, |\Psi_0\rangle \\
&= \langle\Psi_0|\, O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta}\, |\Psi_0\rangle - \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle \\
&= \left(\prod_{\boldsymbol{R}''} \langle\phi_0|_{\boldsymbol{R}''}\right) O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta} \left(\prod_{\boldsymbol{R}'''} |\phi_0\rangle_{\boldsymbol{R}'''}\right) - \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle\,.
\end{aligned} \tag{A.9}$$

We now need to distinguish between the case where (1) $\boldsymbol{R} \neq \boldsymbol{R}'$ and the case (2) $\boldsymbol{R} = \boldsymbol{R}'$.

For case (1), we obtain

$$\begin{aligned}
&= \langle\phi_0|_{\boldsymbol{R}} \langle\phi_0|_{\boldsymbol{R}'} O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta} |\phi_0\rangle_{\boldsymbol{R}'} |\phi_0\rangle_{\boldsymbol{R}} - \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle \\
&= \langle\phi_0|_{\boldsymbol{R}} O_{\boldsymbol{R}\alpha} |\phi_0\rangle_{\boldsymbol{R}} \langle\phi_0|_{\boldsymbol{R}'} O_{\boldsymbol{R}'\beta} |\phi_0\rangle_{\boldsymbol{R}'} - \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle \\
&= \langle\Psi_0|O_{\boldsymbol{R}\alpha}|\Psi_0\rangle \langle\Psi_0|O_{\boldsymbol{R}'\beta}|\Psi_0\rangle - \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle \\
&= 0,
\end{aligned} \tag{A.10}$$

where we have assumed that $|\Psi_0\rangle$ is normalised such that $\langle\phi_0|_{\boldsymbol{R}} |\phi_0\rangle_{\boldsymbol{R}} = 1$ for all choices of $\boldsymbol{R}$. In the last line, we have used that the self-consistency equation (A.8) is fulfilled.

For case (2), $\boldsymbol{R} = \boldsymbol{R}'$, we find

$$= \langle\phi_0|_{\boldsymbol{R}} O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}\beta} |\phi_0\rangle_{\boldsymbol{R}} - \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}\beta}\rangle \equiv \Delta^2_{\boldsymbol{R}\alpha\beta}. \tag{A.11}$$

We cannot simplify this expression further without knowing the precise details of the ground state and so we simply call it $\Delta^2_{\boldsymbol{R}\alpha\beta}$. This is in fact enough to show that it is safe to ignore the fluctuation terms in the full Hamiltonian expectation value: consider for instance the

quadratic part of the full Hamiltonian [Eq. (A.1)],

$$\begin{aligned} H^{(2)} &= \sum_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} O_{\boldsymbol{R}\alpha} O_{\boldsymbol{R}'\beta} = \\ &= \sum_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} \big[\langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle + \langle O_{\boldsymbol{R}\alpha}\rangle \left(O_{\boldsymbol{R}'\beta} - \langle O_{\boldsymbol{R}'\beta}\rangle\right) \\ &\quad + \left(O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle\right) \langle O_{\boldsymbol{R}'\beta}\rangle + (O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle)(O_{\boldsymbol{R}'\beta} - \langle O_{\boldsymbol{R}'\beta}\rangle)\big]. \end{aligned} \tag{A.12}$$

Its expectation value in the MFT ground state becomes

$$\begin{aligned} \langle \Psi_0 | H^{(2)} | \Psi_0 \rangle &= \sum_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} \big[\langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle \\ &\qquad + \langle \Psi_0 | \left(O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle\right)\left(O_{\boldsymbol{R}'\beta} - \langle O_{\boldsymbol{R}'\beta}\rangle\right) | \Psi_0 \rangle \big] \\ &= \sum_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} \big[\langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle + \delta_{\boldsymbol{R}\boldsymbol{R}'} \Delta^2_{\boldsymbol{R}\alpha\beta} \big] \\ &= \underbrace{\sum_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle}_{\sim \mathcal{O}(N^2)} + \underbrace{\sum_{\boldsymbol{R}\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}\alpha\beta} \Delta^2_{\boldsymbol{R}\alpha\beta}}_{\sim \mathcal{O}(N)} \\ &\overset{N\to\infty}{=} \sum_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} c_{\boldsymbol{R}\boldsymbol{R}'\alpha\beta} \langle O_{\boldsymbol{R}\alpha}\rangle \langle O_{\boldsymbol{R}'\beta}\rangle , \end{aligned} \tag{A.13}$$

where N is the number of all lattice sites $\boldsymbol{R}$. Here we have used that the first term is a double sum where most of the terms are non-zero while the second term is only a single sum over the lattice.[6] We note that the last equation in Eq. (A.13) is exactly the same as if we had ignored the fluctuation term from the outset. Along very similar lines, it is now straightforward to show that the expectation values of the fluctuation terms corresponding to cubic and higher interaction terms $H^{(3)}, H^{(4)}, \ldots$ can also be neglected compared to the respective MFT terms.[7]

In conclusion, decomposing the full Hamiltonian of Eq. (A.1) as $H = H_{\text{MFT}} + H_{\text{fluct}}$ where H_{MFT} is the MFT Hamiltonian defined in Eq. (A.4)[8] and H_{fluct} incorporates all fluctuations of the form

$$\begin{aligned} &(O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle)(O_{\boldsymbol{R}'\beta} - \langle O_{\boldsymbol{R}'\beta}\rangle), \\ &(O_{\boldsymbol{R}\alpha} - \langle O_{\boldsymbol{R}\alpha}\rangle)(O_{\boldsymbol{R}'\beta} - \langle O_{\boldsymbol{R}'\beta}\rangle)(O_{\boldsymbol{R}''\gamma} - \langle O_{\boldsymbol{R}''\gamma}\rangle), \quad \cdots , \end{aligned} \tag{A.14}$$

we can show that, in the thermodynamic limit $N \to \infty$,

$$\langle \Psi_0 | H | \Psi_0 \rangle = \langle \Psi_0 | H_{\text{MFT}} | \Psi_0 \rangle = E_{\text{MFT}}, \tag{A.15}$$

where E_{MFT} is the lowest eigenvalue of H_{MFT} assuming the self-consistency equations have been solved. Employing the Rayleigh-Ritz theorem, which states that the expectation value of H in *any* state must be larger equal its exact ground state energy eigenvalue E_{GS}, we

[6] Crucially, this assumes that $\langle O_{\boldsymbol{R}\alpha}\rangle \neq 0$ is non-zero in the thermodynamic limit, meaning that the last equation (and thereby the whole MFT approximation) is not valid when $\langle O_{\boldsymbol{R}\alpha}\rangle = 0$ is the only solution to the self-consistency equation Eq. (A.8).

[7] The basic idea is always that the fluctuation term where $\boldsymbol{R}, \boldsymbol{R}', \boldsymbol{R}'', \ldots$ area all different has zero expectation value in the MFT state, so that only terms of lower order (in N) than the mean field contribution survive.

[8] We have suppressed the dependence on $\langle \boldsymbol{O} \rangle$ for simplicity.

find

$$E_{\mathrm{MFT}} \geq E_{\mathrm{GS}}, \tag{A.16}$$

see Eq. (4.30) for an explicit example of this relation. This implies that MFT is a *variational method*: effectively, we have restricted ourself to a special class of states in Hilbert space [the product states of Eq. (A.5)], and E_{MFT} is the minimal energy expectation value[9] in this variational subspace. Correspondingly, $|\Psi_0\rangle$ is the product state that is closest to the exact ground state of H. Sometimes, there are multiply mean field *ansätze* that we can make, for instance there may be multiple inequivalent choices of the operator basis $O_{\boldsymbol{R}\alpha}$.[10] In this case, Eq. (A.16) guarantees that the ansatz that results in the smallest possible E_{MFT} is one that is closest to the actual solution. This shows why the seemingly innocuous Eq. (A.16) is so important: not only does it prove the intuitive result that the MFT ground state $|\Psi_0\rangle$, and not any other MFT eigenstate $|\Psi\rangle$, is closest to the true ground state of H; it also guarantees that the MFT solution cannot overshoot the true ground state energy and get worse again as we continue to minimise E_{MFT}.

However, unfortunately, we may never achieve $E_{\mathrm{MFT}} = E_{\mathrm{GS}}$ in some cases: Since the exact ground state of H is not necessarily a product state at all, there may always be an offset between E_{MFT} and E_{GS}; meaning MFT would not be a good approximation *even when the self-consistency equations are solved by a non-zero mean field*. Unless we have an exact solution at hand, like in the section on Mean field solution, we can never exclude this case in principle. All we can do is do MFT or make some other approximation and hope for the best.[11]

[9] using the full Hamiltonian H

[10] Take for instance the fermionic Hamiltonian $H = c_1^\dagger c_1 c_2^\dagger c_2 = c_1^\dagger c_2^\dagger c_2 c_1$. We could for example choose to do MFT with the operators $O_1 = c_1^\dagger c_1$, $O_2 = c_2^\dagger c_2$ or the operators $\tilde{O}_1 = c_1^\dagger c_2^\dagger$, $\tilde{O}_2 = c_2 c_1$. The physical predictions from these two choices are not necessarily equivalent, we have to pick the MFT convention that leads to a smaller ground state energy in order to best approximate the true (not MFT) ground state.

[11] As noted before, for the superconductor model Eq. (4.1) that we consider in these notes an exact (but tedious) solution is in fact possible. In the thermodynamic limit, this solution fully agrees with BCS mean field theory and thereby validates it, see:

J. Dukelsky, S. Pittel, and G. Sierra. Colloquium: Exactly solvable richardson-gaudin models for many-body quantum systems. *Rev. Mod. Phys.*, 76:643–662, Aug 2004

Bibliography

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Theory of superconductivity. *Phys. Rev.*, 108:1175–1204, Dec 1957.

[2] Leon N. Cooper. Bound electron pairs in a degenerate fermi gas. *Phys. Rev.*, 104:1189–1190, Nov 1956.

[3] J. Dukelsky, S. Pittel, and G. Sierra. Colloquium: Exactly solvable richardson-gaudin models for many-body quantum systems. *Rev. Mod. Phys.*, 76:643–662, Aug 2004.

[4] Michael Tinkham. *Introduction to superconductivity*, volume 1. Courier Corporation, 2004.