

École polytechnique de Louvain

Computing quantum logic

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Introduction

The Information industry has relied for more than fifty years on Moore's law, which states that the speed of computers (measured by the number of transistors that can be placed on a single chip) roughly doubles every one or two years. However, the fulfilment of that law cannot hold forever [28, 69], leading to the search for new ways of increasing the devices performances.

The always-harder difficulty to stick to Moore's law is principally due to two (quite related) factors, namely that (i) the heat dissipation will become an increasing concern with increasing miniaturisation, and that (ii) such a further miniaturisation of the electronic devices used so far cannot be realised reliably.

The first point is a direct consequence of the Joule effect: when a current flows through a device, it dissipates some heat. The produced heat in itself is not a problem if a single device is considered, however, when a big amount of those devices is considered (today, a chip typically features billions of such devices), the heat extraction problem can become extremely relevant. The second limitation is even more problematic, since it is linked to fundamental limitations: as the dimensions of a device are further decreased, the wave nature of the electron will come into play, leading to tunnel leakage currents. Those leakage currents will generate even more heat by Joule effect, the net effect being a build-up of those two effects.

To overcome those limitations, the micro- and nanoelectronics manufacturers had to come with new ideas to further increase miniaturisation, hence continuing to improve their chips capabilities and try to stick to Moore's law. One of the ideas was to forget about the traditional planar-geometry devices and take advantage of the full three dimensional space. This lead to several new device geometries, such as the 3D FinFET [12, 74], or the gate all-around transistor [27]. However, even if those innovations effectively increase the density of components on a chip, the leakage currents are not suppressed. To get rid of those, something else had to be found.

The solution the Industry came with was quite radical, since the paradigm on which it was previously based was changed: rather than continuing to use electronic devices, which rely solely on the charge of the electron, spintronic devices could be used, which can either combine the charge and the intrinsic spin of an electron, or rely only its spin [71]. Relying on

the spin, the heat generated by Joule effect could be reduced to the physical Shannon – von Neumann – Landauer limit [39]. Moreover, no more leakage currents have to be considered, leading to a minimal computing energy consumption. The concept of spintronic devices is even more interesting, as it can also be used in information storage devices: the manipulation and data storage of information in the electron’s spin could provide new functionalities, such as memory nonvolatility and better computing capabilities [34, 72]. It is at this point that magnetic skyrmions naturally came out: they small size, combined with their long-time stability, made them perfect suitors to traditional CMOS-based electronic and storage devices.

Today, scientists have to tackle more and more involved problems, hence the numerical simulations required to address these issues become more and more demanding. In fact, some problem are even classified as uncomputable with normal computers, such as the factorisation of large numbers, which lies at the heart of the RSA cryptography technique [13]. This picture was broken down by Peter W. Shor in 1994, when he showed that large numbers could easily be factored into a product of prime numbers by a quantum computer, thanks to an algorithm known as the Shor algorithm [59], proving the superiority of quantum computers over classical ones, at least for some applications.

Even if those quantum computers are believed to be a true revolution, they suffer many flaws, the biggest one being that the coherence time of the involved qubits is extremely small, hence a practical large scale application of quantum computers still seems out of reach. This observation lead the scientists all around the World to try to find some tricks to increase the coherence time of the quantum bits required in quantum computers. Different solutions emerged from the work furnished by all the scientists, one of those being to couple magnetic skyrmions to superconductors, as it was shown that in such a case, a so-called Majorana fermion could be hosted in the core of the skyrmion [75]. The key point about those Majorana fermions is that, once entangled, they form topologically protected objects, ensuring a very large coherence time of Majorana-based qubits.

In this work, different aspects linked to skyrmions and superconductors are presented: in the first chapter, some generalities about skyrmions are presented. In particular, some elements allowing to classify the skyrmions, as well as potential applications, are presented. The discussion continues in the second chapter, where some generalities about superconductors are presented. In particular, both the “classical” and “quantum” approaches are briefly discussed, which then allows to introduce more “exotic” superconductors, in which Majorana fermions could be found. The third chapter is concerned with an introduction to the tight-binding formalism, which allows to see how different magnetic textures interact with superconductors. The discussion then ends with a small conclusion and outlook on what remains to be done to gain further insight into the magnetism/superconductor coupling.

Topology in magnetism

The understanding of topological effect in condensed matter, and more specifically in magnetism, has boomed in the recent years. Here, smooth topological textures are considered, which derive their stability from the fact that they cannot be continuously deformed onto one another. An example of such a smooth topological textures is the skyrmion. As opposed to those smooth textures, there exist singular topological point defects, where the magnetisation is forced to vanish in a submanifold. Such defects include Ising domain walls, vortices of easy-plane spins, 3D Bloch points, “hedgehogs”, and monopoles.

In the following, a brief introduction to topology and how it can be used to classify defects is given. From there, the discussion continues with the introduction of some concepts linked to skyrmion dynamics, and the discussion ends with possible technological application of those topological objects.

2.1 A brief synopsis on topological defects

2.1.1 Homotopy

The ubiquity that exists between different magnetic textures in the magnetisation field arises because of their defining mathematical aspects: one configuration can be continuously¹ deformed onto another one if and only if they are topologically equivalent, i.e. they share the same topological invariant. The mathematical theory studying deformations of one function onto another is called homotopy, and has to be used here because the deformation of one magnetic configuration into another one is studied (in this case, the magnetisation field plays the role of generalised function to be used in the homotopy theory).

¹Strictly speaking, the deformations cannot be continuous because a magnetic texture is discontinuous, the discontinuity arising from the discreteness of the underlying lattice. This leads to the fact that a magnetic texture is not stable, but rather metastable. In the following, that difficulty will be neglected.

The concept of homotopy is more easily understood if a mapping f from a n -sphere² into an order parameter space X is considered, i.e. $f : \mathbb{S}^n \rightarrow X$. That general definition will be particularised to the cases where the order parameter X is equal to $X = \mathbb{S}^0$, $\mathbb{S}^1$, and $\mathbb{S}^2$, which correspond to easy-axis, easy-plane, and isotropic spins, respectively. Those particular cases are the most relevant for condensed matter physicists. However, before considering those particular cases, some generalities and nomenclature have to be introduced.

In a first time, if a loop (represented by the mapping f) can be shrunk to a point, it is said to be “null homotopic” or, equivalently, “topologically trivial”. Extending that concept, two mappings f and g are said to be homotopic (i.e. topologically equivalent) if one can be deformed onto the other by a continuous deformation, in which case the notation $f \sim g$ is used. Homotopy being an equivalence relation, the set of loops in X can be subdivided in disjoint homotopy classes. This subdivision extends and generalises the concept of homotopy from simple curves to complete equivalence classes, since the relation $f \sim g$ implies $[f] = [g]$, i.e. two loops are homotopic if the equivalence classes are equivalent. To link with what was previously stated on the classification of magnetic textures, equivalence classes can be classified thanks to a topological invariant, the so-called “winding number” (which signification will become clear later on), “number”, or “index” $w = \deg f$.

In addition to the concept of homotopy and equivalence class, the concept of concatenation can also be considered. A concatenation between mapping f and g generates a new mapping, noted $f \circ g$, and is obtained by first considering f , and subsequently g . It has to be noted that the concatenation of equivalence classes is the same as the equivalence class of the concatenation, i.e. $[f] \circ [g] = [f \circ g]$. With this concatenation operation, the set of homotopy classes gains a group structure and form the homotopy group. The particular mapping $\mathbb{S}^n \rightarrow X$ has to be presented here, since it is of importance in the following. Such a mapping is called the n^{th} homotopy, and is noted $\pi_n(X)$, i.e. $\pi_n(X) : \mathbb{S}^n \rightarrow X$. In the case where $n = 1$, the mapping is called the first homotopy, or fundamental, group.

2.1.2 Winding number

Mutually deformable configurations form equivalence classes. It is now time to discuss the quantity that serves as a definition of those classes. The fingerprint of an equivalence class is its topological charge, named winding number previously. This number is in fact nothing else than the degree of the mapping f , i.e. $w = \deg f$, and configurations with different degrees cannot be continuously deformed onto one another. If the particular case of magnetic textures, the mapping is the magnetisation field $\mathbf{m}$, and if two textures have a different charge, they cannot be deformed onto each other.

In the particular framework of magnetism, a ferromagnetic state is characterised by a 0 winding number, and is said to be topologically trivial. In contrast, a vortex or a skyrmion-like configuration is nontrivial, since they are both characterised by a nonzero topological number.

²The n -sphere $\mathbb{S}^n$ is the surface of the sphere defined in $n + 1$ dimensions.

It has already been stated that the winding number allows to classify equivalence classes of a mapping. Formally, the degree of a mapping $\deg f$ provides a bijection of the homotopy classes into the set of all integers $\mathbb{Z}$, as was shown by Hopf. This bijection is the essence of the classification of the different types of magnetic textures. An interesting result is that the n^{th} homotopy group of the n -sphere $\mathbb{S}^n$ is isomorphic to the group of integers [1, 14], i.e.

$$\pi_n(\mathbb{S}^n) \cong \mathbb{Z} \quad \forall n \geq 1,$$

and the homotopy group is thus Abelian³. Two remarks have to be raised here. The first one is that, for $n < m$, the homotopy groups $\pi_n(\mathbb{S}^m)$ are trivial, i.e. $\pi_n(\mathbb{S}^m) = 0$, which can be easily understood in the particular case $\pi_1(\mathbb{S}^2)$: on a sphere, all loops can be shrunk to a point, hence the homotopy group is trivial. The case where $n > m$ is often nontrivial [1], but not of interest here. A final remark concerns the group $\pi_1(\mathbb{S}^1)$, which can take only two distinct values, i.e. $\pi_0(\mathbb{S}^0) \cong \mathbb{Z}_2$ (as is expected from quantum mechanics, where the spin of an electron can be either up or down, each of those configurations being associated to an unique number).

In order to understand why the degree of a mapping is also called the winding number, a graphical illustration can help. Figure 2.1 shows easy-plane spins arranger on a circle, and the winding number $w_{\mathbb{S}^1}$ corresponds to the mapping $f : \mathbb{S}^1 \rightarrow \mathbb{S}^1$. Different possibilities are shown, corresponding respectively to, from left to right, (a) the uniform state, (b) radial, right-handed, and left-handed vortices, (c) an antivortex, and (d) a double vortex. From the figure, it is easily

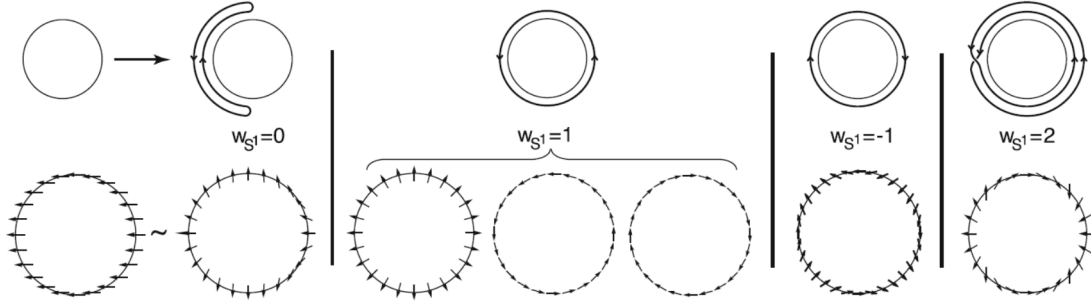


Figure 2.1 – Graphical representation of the winding number, counting how much time an easy-plane spin configuration can be mapped onto a 1-sphere. Different configurations are shown, corresponding to an uniform ferromagnetic state, different types of vortex states, an antivortex state, and a double vortex, from left to right, respectively. Image from [76].

understood that the winding number counts the number of times the target space wraps around the base space. More formally, if the first homotopy group is considered and an arbitrary point $P \in \mathbb{S}^1$ in the image space is considered, the degree of a mapping is obtained by counting the number of times the magnetic textures is mapped onto the point P , i.e. the number of times a point $\mathbf{x}_k$ in the base space is mapped onto P , $\mathbf{m}(\mathbf{x}_k) = P$.

³A group is said to be Abelian when the internal composition rule (the concatenation in this case) is commutative.

In fact the most general and useful form of the winding number is given, in the framework of differential geometry, by the expression [14]

$$\deg f = \frac{\int_M f^* \Omega}{\int_N \Omega}, \quad (2.1)$$

where M and N are the base and target manifolds (which means that a mapping f of the form $f : M \rightarrow N$ is considered), Ω is a differential n -form defined on N , and $f^* \Omega$ denotes its pullback onto M . In magnetism, the case of interest is $M = N = \mathbb{S}^n$, thus Ω is conveniently chosen as a surface volume form with respect to the metric induced from $\mathbb{R}^{n+1}$, i.e. $\Omega = *r \, dr$ [14, 76].

Using the most general formula given in (2.1), different interesting cases can be discussed, including the characterisation of solitary objects, such as solitons and skyrmions. In that case, the target space $\mathbb{S}^2$ can be parametrised by $\mathbf{m} = [m_1, m_2, m_3]$, with the constraint $\|\mathbf{m}\| = 1$, for example, which then leads to [76]

$$w_{\mathbb{S}^2} \equiv \deg f = \frac{1}{4\pi} \int dx_1 dx_2 \mathbf{m} \cdot \left(\frac{\partial \mathbf{m}}{\partial x_1} \times \frac{\partial \mathbf{m}}{\partial x_2} \right).$$

As an illustrative example of the skyrmions resulting from the index, figure 2.2 can be consulted, which shows both skyrmions and an antiskyrmion. Both Bloch and Néel skyrmions correspond

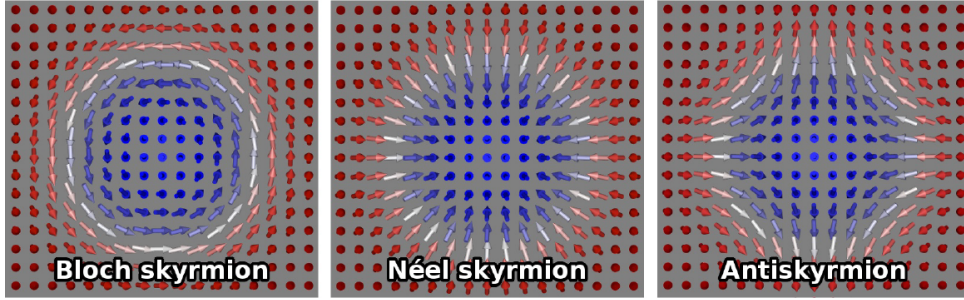


Figure 2.2 – Graphical representation of different skyrmion types. The Bloch and Néel skyrmions both correspond to $w_{\mathbb{S}^2} = 1$, while the antiskyrmion corresponds to $w_{\mathbb{S}^2} = -1$. Image from [15].

to a winding number $w_{\mathbb{S}^2} = 1$, the distinction between those being the rotational direction. The antiskyrmion corresponds to $w_{\mathbb{S}^2} = -1$. The descriptive difference between a skyrmion and an antiskyrmion is the direction of spin rotation: if a straight line across the antiskyrmion core is taken, the magnetisation state looks like a Néel skyrmion, while in other directions it looks like a Bloch skyrmion.

2.2 Skyrmion dynamics

The previous section was focused on the concept of topology, with a particular accent placed on how that concept serves to characterise defects. In this part, it will be shown that topology has

deeper connections to the behaviour of defects such as skyrmions, since their topological charge influence their dynamics. This connection between topology and physical behaviour allows to probe experimentally the previously introduced concepts. This part is divided as follows : first, the equation of motion for a single spin is derived. Building up on that equation, its expression is refined to take damping into account. From there, different supplementary effects are taken into account, such as the interaction between the magnetisation and/or an external magnetic field. The discussion then ends with a presentation of the Thiele equation, which is used to study the time-evolution of magnetic moments.

2.2.1 Pristine spin dynamics

The magnetisation dynamics is intimately linked to that of the spins. In the Heisenberg picture of quantum mechanics, the time evolution of an operator $\hat{O}$ takes the form

$$i\hbar \frac{\partial}{\partial t} \hat{O} = [\hat{O}, \hat{H}], \quad (2.2)$$

where $\hat{H}$ is the Hamiltonian of the system, and $[\hat{O}, \hat{H}] = \hat{O}\hat{H} - \hat{H}\hat{O}$ is the commutator. Here, the concern is to study how a spin interacts with an external magnetic field $\mathbf{B} = \mu_0 \mathbf{H}$, where μ_0 is the free space permeability, and $\mathbf{H}$ is a magnetic field⁴.

It is well known that when an atom is immersed in an uniform magnetic field, each of its fine structure components is divided in a set of equidistant lines, the spacing between those lines being proportional to the strength of the magnetic field [19]. This effect, due to the interaction of the magnetic field with the spin angular momentum of the atom $\hat{\mathbf{S}}$, is known as the Zeeman effect, and the corresponding Hamiltonian takes the form

$$\hat{\mathcal{H}}_{\text{Zeeman}} = -\gamma \hat{\mathbf{S}} \cdot \hat{\mathbf{B}},$$

where γ is known as the gyromagnetic ratio, given by $\gamma = ge/2m = g\mu_B$ (where μ_B is the Bohr magneton), and is the constant of proportionality between the magnetic moment and the angular momentum of an atom. Combining that Hamiltonian with the general expression given in (2.2), the time evolution of the spin operator is given by

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\mathbf{S}} &= i \frac{g\mu_B}{\hbar} [\hat{\mathbf{S}}, \hat{\mathcal{H}}_{\text{Zeeman}}] \\ &= i \frac{g\mu_B}{\hbar} \{ \hat{\mathbf{S}} (\hat{\mathbf{S}} \cdot \hat{\mathbf{B}}) - (\hat{\mathbf{S}} \cdot \hat{\mathbf{B}}) \hat{\mathbf{S}} \}. \end{aligned}$$

Using the commutation relation $[\hat{S}_\alpha, \hat{S}_\beta] = i\hbar \sum_\gamma \epsilon_{\alpha\beta\gamma} \hat{S}_\gamma \ \forall \alpha, \beta, \gamma \in \{x, y, z\}$, where $\epsilon_{\alpha\beta\gamma}$ is the Lévi-Civita tensor defined by

$$\epsilon_{\alpha\beta\gamma} = \begin{cases} +1 & \text{for a cyclic permutation of } (\alpha, \beta, \gamma) \\ -1 & \text{for an acyclic permutation of } (\alpha, \beta, \gamma) \\ 0 & \text{otherwise} \end{cases}$$

⁴A thoughtful discussion between the distinction between $\mathbf{B}$ and $\mathbf{H}$ can be found in the first chapter of [46].

together with an uniform magnetic field pointing along an axis (taken to be the z for facility of computations), the last expression can be rewritten

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\mathbf{S}} &= \gamma\hat{\mathbf{S}} \times \hat{\mathbf{B}} \\ &= -\gamma\hat{\mathbf{B}} \times \hat{\mathbf{S}}\end{aligned}$$

which shows that the spin precesses uniformly around the magnetic field. Going one step further, this relation can be used to study the magnetisation dynamics, since $\mathbf{m}(\mathbf{r}, t) = \langle \hat{\mathbf{S}}(t) \rangle$. Applying the Ehrenfest theorem

$$\frac{\partial}{\partial t} \langle \hat{\mathbf{S}}(t) \rangle = \left\langle \frac{\partial}{\partial t} \hat{\mathbf{S}}(t) \right\rangle + \frac{1}{i\hbar} \langle [\hat{\mathbf{S}}(t), \hat{\mathcal{H}}] \rangle,$$

and considering that the average of the variation of the spin operator is equal to zero, the magnetisation dynamics is dictated by the equation

$$\frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) = -\gamma \mathbf{B}(\mathbf{r}, t) \times \mathbf{m}(\mathbf{r}, t),$$

which shows that, analogously to the spin operator, the magnetisation precesses uniformly around the applied magnetic field.

Even if elegant, the result corresponding to a periodic precession at constant energy of the magnetisation around the applied magnetic field (coming from the fact that the spin degree of freedom is totally decoupled from real space) is physically unacceptable since it lacks some dissipation, originating from the interaction with the crystal lattice or the electronic structure. To take those interactions into account, Landau and Lifshitz introduced in 1935 an additional term in the evolution equation of the magnetisation, leading to the expression

$$\frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) = -\gamma\mu_0 \mathbf{H}(\mathbf{r}, t) \times \mathbf{m}(\mathbf{r}, t) + \gamma\mu_0\lambda [\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t)] \times \mathbf{m}(\mathbf{r}, t).$$

The strength of the damping is given by a positive damping constant λ . Later, Gilbert gave a more satisfactory equation for the magnetisation dynamics, where the damping is proportional to the “speed” of the magnetisation (which is in better agreement with what is known in classical physics, where dissipation is often taken into account by adding a term proportional to a certain power of the speed). The magnetisation dynamics is then governed by the so-called Landau-Lifshitz-Gilbert (LLG) equation, which reads

$$\frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) = -\gamma\mu_0 \mathbf{H}(\mathbf{r}, t) \times \mathbf{m}(\mathbf{r}, t) + \alpha \mathbf{m}(\mathbf{r}, t) \times \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t). \quad (2.3)$$

An alternative form of that last equation is

$$\frac{1 + \alpha^2}{\gamma\mu_0} \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) = -\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t) - \alpha \mathbf{m}(\mathbf{r}, t) \times [\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t)]. \quad (2.4)$$

The equivalence between equation (2.3) and equation (2.4) is given in appendix A. A careful analysis and comparison of those equations with the ones given in the appendix show a small difference: indeed, in appendix A, the magnetic field is an effective one, rather than simply an external one. The signification of such an effective is now discussed.

The effective magnetic field $\mathbf{H}_{\text{eff}}$ takes into account all the magnetic contributions, internal as well as external, and, in the framework of micromagnetics, derives from an energy density, according to the relation

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0 M_s} \nabla_{\mathbf{m}} \mathcal{E}, \quad (2.5)$$

where M_s is the saturation magnetisation, and where $\mathcal{E}$ is the density energy which, once integrated over the whole volume of the sample, gives the energy, which expression reads [14]

$$E = \int_V d^3r \left\{ A \sum_{\nu \in \{x,y,z\}} (\nabla m_\nu)^2 + U(\mathbf{m}) - M_s \mathbf{m} \cdot \mathbf{B} \right\} + E_m. \quad (2.6)$$

In that expression, the first term in the integral represents the exchange energy, the second term represents the anisotropy energy originating from the crystal field, and the last term stands for the Zeeman interaction energy. The constant A represents the strength of the exchange energy, and can be linked to the coupling constant in the Heisenberg Hamiltonian. The last term, E_m , is the dipolar interaction which, in the continuous description offered by the micromagnetic framework, is non local and reads

$$E_m = -\frac{\mu_0}{8\pi} M_0^2 \int_V d^3r \int_V d^3r' \sum_{i,j} \mathbf{m}_i(\mathbf{r}) \mathbf{m}_j(\mathbf{r}') \frac{\partial^2}{\partial r_i \partial r_j} \frac{1}{\|\mathbf{r} - \mathbf{r}'\|}.$$

The LLG equation, equation (2.4), can be further complexioned by incorporating other torque terms. The two most common are the spin-transfer torque (STT) and the spin-orbit torque (SOT), which are needed if the interaction between the magnetic texture and an electrical current is studied. Generally, those effect are taken into account by adding a torque $\mathbf{T}$ to the RHS of equation (2.4). For example, in the case where wants to study STT for an in-plane current, the torque reads [65] $\mathbf{T} = -(\mathbf{u} \cdot \nabla) \mathbf{m} + \beta \mathbf{m} \times (\mathbf{u} \cdot \nabla) \mathbf{m}$, where $\mathbf{u}$ is the drift-velocity of the spin in the direction parallel to the current density vector, and β is a non-adiabatic factor. Incorporating that torque term in the LLG equation leads to an equation that does not derive from an energy anymore.

2.2.2 Stabilisation mechanisms

The previous discussion gave a small summary of different (competing) effects leading to the creation of a skyrmion were introduced. The present subsection aims to refined a bit the different mechanisms which finally lead to the effective creation of a skyrmion.

The Heisenberg exchange

A first term that participates to the creation (and stabilisation) of skyrmions is the Heisenberg exchange interaction, which originates from the overlap of the wavefunction describing the electrons. If a solid is decomposed into “site”, the expression of the Heisenberg exchange interaction is

$$E_{\text{Heis}} = - \sum_{i,j} J_{ij} \mathbf{m}_i \cdot \mathbf{m}_j$$

where the sum runs over the different sites, where the term J_{ij} is the wavefunction overlap integral between sites i and j , and where the minus sign before the sum is a matter of convention. From its expression, it is seen that the exchange interaction is symmetric (with respect to the exchange of sites), and depends only on the relative angle between $\mathbf{m}_i$ and $\mathbf{m}_j$.

The interaction strength decreases rapidly with distance, hence it explains why the Heisenberg interaction is a so-called short-range interaction. The sign of J_{ij} is also important: if $J_{ij} < 0$, a parallel orientation of the magnetisation is favoured, meaning that a ferromagnetic configuration is preferred. On the contrary, if $J_{ij} > 0$, an anti-parallel configuration is preferred, which is known as an antiferromagnetic configuration.

If the discreteness of the lattice on which the magnetic sites are defined somehow “degenerates” into a continuous, the Heisenberg exchange term then takes the form [17]

$$E_{\text{Heis}} = \int d^3r A \{ (\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2 \},$$

which is nothing else than the first term in equation (2.6).

The Dzyaloshinsky-Moriya interaction

The Dzyaloshinsky-Moriya interaction, or DMI, is an antisymmetric and anisotropic exchange interaction, which originates from spin-orbit coupling. It was first predicted by Dzyaloshinsky to explain the “weak” ferromagnetism of some compounds, based on symmetry considerations and spin-orbit coupling [21], and was later extended by Moriya, who considered an interaction through super-exchange, i.e. through an interaction with another atom [50], as schematically shown in figure 2.3. This figure shows that DMI can take place directly in the bulk of a material presenting a large spin-orbit coupling (SOC), or at the interface between a ferromagnetic material and another material, presenting a large SOC.

Keeping the same notation as for the Heisenberg interaction, the expression of DMI takes the form

$$E_{\text{DMI}} = - \sum_{i,j} \mathbf{D}_{ij} \cdot (\mathbf{m}_i \times \mathbf{m}_j),$$

where $\mathbf{D}_{ij}$ is the Dzialonshinskii vector, which expression depends on the symmetry of the lattice on which the DMI takes place. As opposed to the Heisenberg exchange, where a collinear spin configuration is preferred, the DMI tends to have the spins orthogonal to each other, favouring

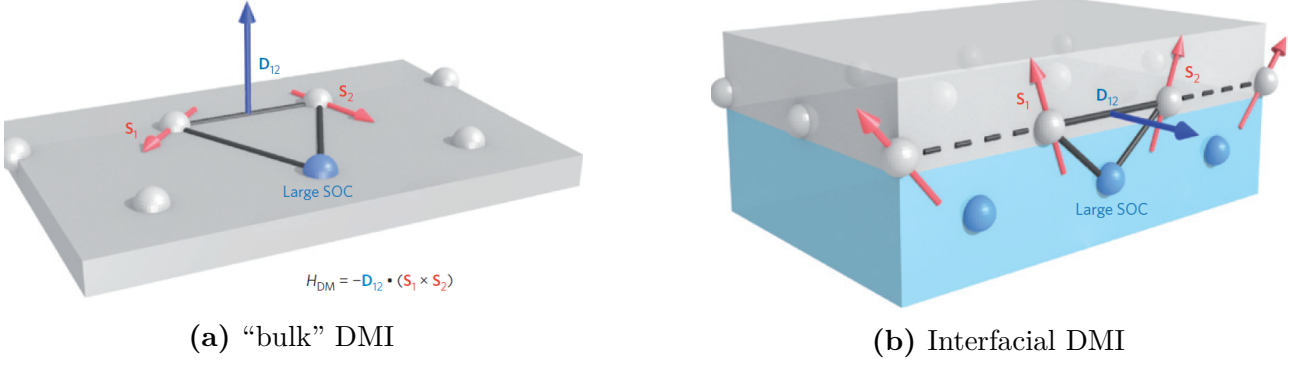


Figure 2.3 – Schematic representation of the DMI taking place between two magnetic moments $\mathbf{S}_1$ and $\mathbf{S}_2$ interacting through a third atom presenting a large spin-orbit coupling. DMI generated by (a) indirect exchange with an atom presenting a large SOC, and (b) the interaction between a ferromagnetic material (in grey) and a material presenting a large SOC (blue). Images from [22].

a noncollinear configuration. Moreover, only a given chirality of the magnetisation is preferred, as in vortices and skyrmions, for example.

The Zeeman interaction

The Zeeman interaction was already introduced. It consists in the interaction between a magnetic moment and an external magnetic field $\mathbf{B} = \mu_0 \mathbf{H}$, where μ_0 is the free-space permeability. The Zeeman interaction reads

$$E_{Zee} = -M_s \sum_i \mathbf{m}_i \cdot \mathbf{B},$$

where M_s is the saturation magnetisation. This interaction tends to align the magnetic moment along the direction of the applied field. The continuous expression of the above expression is given by

$$E_{Zee} = -M_s \int d^3r \mathbf{m} \cdot \mathbf{B},$$

in good agreement with equation (2.6).

Magnetic anisotropy

The last contribution to the total energy comes from the magnetic anisotropy, which can be split into two different contributions: the magnetocrystalline anisotropy, and the dipolar anisotropy.

The magnetocrystalline anisotropy originates from the fact that, in magnetic crystals, some directions are favoured with respect to other ones, obviously leading to anisotropy. The physical origin of such anisotropy is a complex interplay between crystal field (i.e. the interaction

between ions and electrons) and spin-orbit interactions. If a system features only an easy-axis for the magnetisation (a more general treatment is given in [10]), the energy associated to that anisotropy reads

$$E_{\text{ani}} = -K_u \sum_i (\mathbf{m}_i \cdot \mathbf{e}_{\text{ani}})^2,$$

where $\mathbf{e}_{\text{ani}}$ is the unit vector along the easy-axis, and $K_u > 0$ is the strength of the anisotropy. In the continuous limit, the expression becomes

$$E_{\text{ani}} = -K_u \int d^3r (\mathbf{m} \cdot \mathbf{e}_{\text{ani}})^2.$$

The dipolar anisotropy is the interaction between different magnetic moments. It can be understood as follows: each magnetic moment can be decomposed as a magnetic dipole, each of which generates its own field. This means that each magnetic moment feels the different fields originating from the others. The dipolar interaction between two magnetic moments $\mathbf{m}_i$ and $\mathbf{m}_j$ is given by [30]

$$E_{\text{dip}} = \frac{I_{\text{dip}}}{\|\mathbf{r}_{ij}\|^3} \left[\mathbf{m}_i \cdot \mathbf{m}_j - 3 \frac{(\mathbf{m}_i \cdot \mathbf{r}_{ij})(\mathbf{m}_j \cdot \mathbf{r}_{ij})}{\|\mathbf{r}_{ij}\|^2} \right],$$

where I_{dip} is the dipolar interaction strength, and $\mathbf{r}_{ij}$ is the vector between $\mathbf{m}_i$ and $\mathbf{m}_j$.

2.2.3 Evolution equation

The Thiele equation

As previously discussed, the magnetisation dynamics is governed by the LLG equation. However, the cases in which an analytical solution exist are scarce, coming from the integro-differential nature of that equation. Nevertheless, in some cases, simplifying assumptions can be made, and the equation rewritten in a much more simple form. A good example is the Thiele equation, which considers the skyrmions are rigid, underformable, objects.

If the magnetic texture is considered as a rigid body, it means that there exists some magnetisation $\mathbf{m}_0$ that moves in a rigid translation. This means that $\mathbf{m}_0(\mathbf{r})$ depends only on space, and on a time-varying position vector $\mathbf{R}(t)$ such that

$$\mathbf{m}(\mathbf{r}, t) = \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)].$$

Injecting that expression into the time-derivative $\partial_t \mathbf{m}(\mathbf{r}, t)$, it is directly obtained that

$$\frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) = - \sum_{\nu \in \{x, y, z\}} u_\nu \frac{\partial}{\partial r_\nu} \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)],$$

where ν runs over the 3 space coordinates, and $\mathbf{u}$ is the speed of the translation of the magnetisation profile. Considering the case where the effective field $\mathbf{H}_{\text{eff}}$ entering into the LLG

equation derives from an energy density, as illustrated by the relation (2.5), the force acting on the magnetic texture is conservative, and derives from the potential, according to the relation

$$\begin{aligned}\mathbf{F} &= -\nabla_{\mathbf{r}} E = \mu_0 M_s \nabla_{\mathbf{r}} \left\{ \int_V d^3r \mathbf{H}_{\text{eff}}(\mathbf{r}, t) \cdot \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \right\} \\ &= -\mu_0 M_s \int_V d^3r \mathbf{H}_{\text{eff}}(\mathbf{r}, t) \cdot \{\nabla \cdot \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)]\}.\end{aligned}$$

By performing a force equilibrium to get a displacement with constant velocity, the force acting on the structure should compensate all the other forces, namely (i) the external forces $\mathbf{F}_{\text{ext}}$, (ii) the dissipation forces $\mathbf{F}_{\text{dissip}}$, and (iii) all the forces that generate an additional torque $\mathbf{T}$ that do not derive from an energy density, $\mathbf{F}_{\text{gyro}}$. The equilibration of all these forces lead to the relation [76]

$$\begin{aligned}0 = F_{\text{ext},i} + F_{\text{dissip},i} + F_{\text{gyro},i} &= F_i - \frac{\hbar M_s}{\gamma} \int_V d^3r \mathbf{T} \cdot \left(\frac{\partial}{\partial r_i} \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \times \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \right) \\ &\quad - \alpha \frac{\hbar M_s}{\gamma} \sum_j u_j \int_V d^3r \left(\frac{\partial}{\partial r_i} \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \cdot \frac{\partial}{\partial r_j} \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \right) \\ &\quad + \frac{\hbar M_s}{\gamma} \sum_j u_j \int_V d^3r \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \cdot \left(\frac{\partial}{\partial r_i} \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \times \frac{\partial}{\partial r_j} \mathbf{m}_0[\mathbf{r} - \mathbf{R}(t)] \right).\end{aligned}$$

In that quite lengthy expression, the first two terms on the RHS express the external forces that act on the magnetic texture (coming from the translational movement and from the additional torques introduced by the current density), while the third and fourth terms come from the precession of the magnetisation, and from the damping, respectively. It is interesting to note that in the third term, the so-called gyrotropic force, the topological charge serving to characterise the nature of a topological defect (introduced in the first part of the text) appears directly. This shows that the concepts of topology directly impact the dynamical behaviour of the magnetisation texture, as announced in the first section.

2.3 Technological applications

Because of they topological aspect, skyrmions are perfect candidates to be used as memory storage devices. Moreover, the low energy required to move them (as rigid bodies, in accordance with the Thiele equation), make them potential serious contenders to traditional CMOS-based devices. In the following, some of the possible applications of skyrmions will be briefly exposed and discussed.

2.3.1 Memory racetrack

As its name suggests, the racetrack memory is a device comprising an array of magnetic nanowires arranged horizontally or vertically on a silicon substrate. In such a device, information is stored

in columns comprising magnetic domain walls, and modified thanks to individual reading and writing spintronics devices. A schematic view of such a racetrack is given in figure 2.4. The

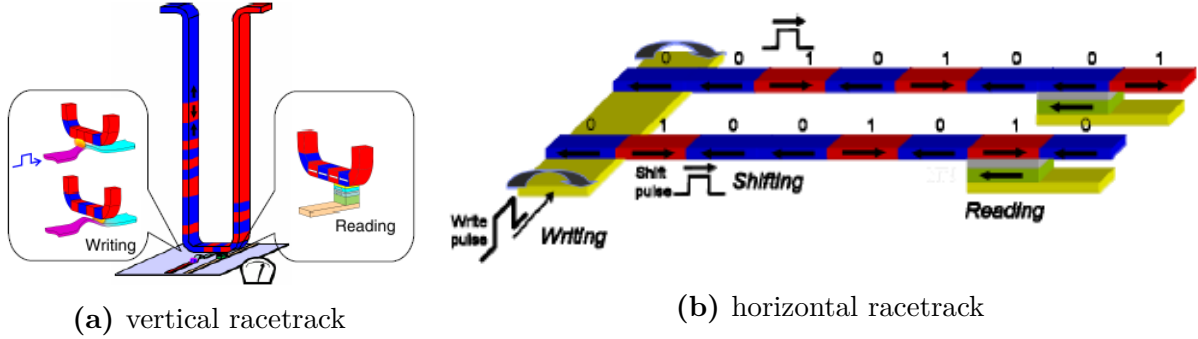


Figure 2.4 – Schematic representation of (a) a vertical racetrack arrangement and (b) a horizontal one. The two schematics show the domain walls that can be manipulated thanks to nanosecond current pulses, and the magnetic tunnel junction needed to read information. Images from [66].

schematic shown on that figure illustrates the fact that information is written (and transported) by nanosecond current pulses, and read by a spintronics device called a magnetic tunnel junction (MTJ). Such a MTJ relies on the giant magnetoresistance (GMR) effect: it consists in two ferromagnetic layers, separated by an ultra thin tunnel barrier. When a given magnetic moment comes in the vicinity of one of the ferromagnetic materials, the resistance of the reading device changes, hence the magnetisation can be deduced from the resistance change of the junction.

From figure 2.4, the interest of skyrmions in such racetrack devices is obvious: indeed, if simple magnetic moments were considered, a high packing density of magnetic moments could create interferences and perturb the magnetic texture. As stated previously, skyrmions are topologically protected, which means that interferences do not come into play anymore. Another advantage of skyrmions over simple domain walls (such as those presented in figure 2.4) is that skyrmions need very low current densities to be moved (of the order of 10^6 A m^{-2}), while domain walls require current densities of the order of 10^{12} A m^{-2} [29]. This illustrates the point that skyrmion-based devices could potentially be operated at much lower current than traditional technologies, meaning that the current consumption could be drastically decreased, with all the advantages it means (longer lifetime of a computer battery, less pollution, etc.).

If skyrmions were truly used in real-life applications, a bunch of technological challenges would first to be dealt with, such as the nucleation, detection, or pinning/depinning along the racetrack. Moreover, temperature and driving current seem to play an important role in the stability of skyrmions: a current bigger than a critical value would increase the “diameter” of the skyrmion, allowing to reach the boundaries of the track, leading to the destruction of the skyrmion and leaving a complex magnetic pattern. On the other hand, temperature plays an important role in the value of the current at which the skyrmion is expelled from the track, i.e. a loss of information. Those considerations have been exposed and discussed in [67].

2.3.2 Magnetic RAM

After having discussed the racetrack memory, another interesting device serving the purpose information storage that can be presented is the magnetic random access memory (MRAM). As the racetrack memory, it is a device based on the principles of spintronics, which as the advantage to preserve stored data, even if the power is turned off, i.e. it is nonvolatile.

The comparison with racetrack memories goes even further: indeed, as in racetrack memories, data is stored in magnetic moments in MRAMs. Such memories hold very promising results, as it was reported that such memories could easily outperform traditional flash memories [49]. Another positive point about such devices is its integration in more traditional semiconductor devices, as was reported by Intel [48].

Nowadays, an amelioration of the MRAM, making use of the spin torque transfer (STT) effect, is also holding great promises. Such a device is called a STT-MRAM. STT relies on the manipulation of magnetic moments in a ferromagnetic element, but without the application of any magnetic field: the magnetic moments are modified by transferring spin angular momentum from a spin-polarised current, a concept first introduced theoretically by Slonczewski [62] and Berger [8], and schematically illustrated in figure 2.5.

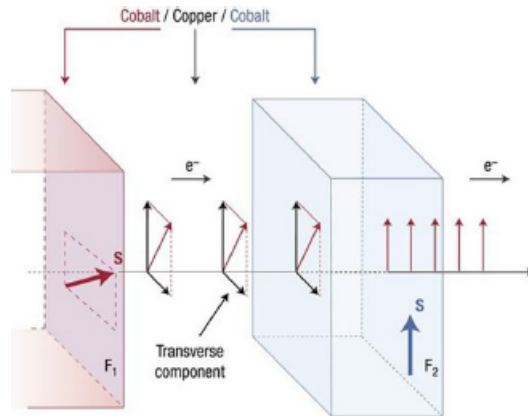


Figure 2.5 – Schematic representation of the spin torque transfer effect. An electrical current is injected in a first ferromagnetic layer F_1 , with a spin polarisation oriented differently than the next ferromagnetic layer F_2 . An electrical current passing through F_1 becomes spin polarised. When it goes through F_2 , the exchange interaction aligns the spin polarisation along the magnetisation direction. Since the interaction is spin conserving, the transverse spin component of the current is transferred to the total spin of F_2 , resulting in a torque. Figure from [23].

From a device point of view, a graphical representation of two different MRAM configurations is given in figure 2.6. It consists in a circuit along which information is carried, and detected by a MTJ element, of which the resistance depends on the magnetic state in its direct vicinity, hence the technological advances in MRAM technologies are closely related to the understanding of magnetism and magnetic textures. By consulting figure 2.6, the advantage of using skyrmions

over more traditional magnetic textures (or spin-polarised currents) is obvious: skyrmions being topologically protected magnetic configurations, (moderated) stray fields cannot perturb their magnetisation state, hence an information is expected to be conveyed much more reliably than what is possible to achieve with other techniques.

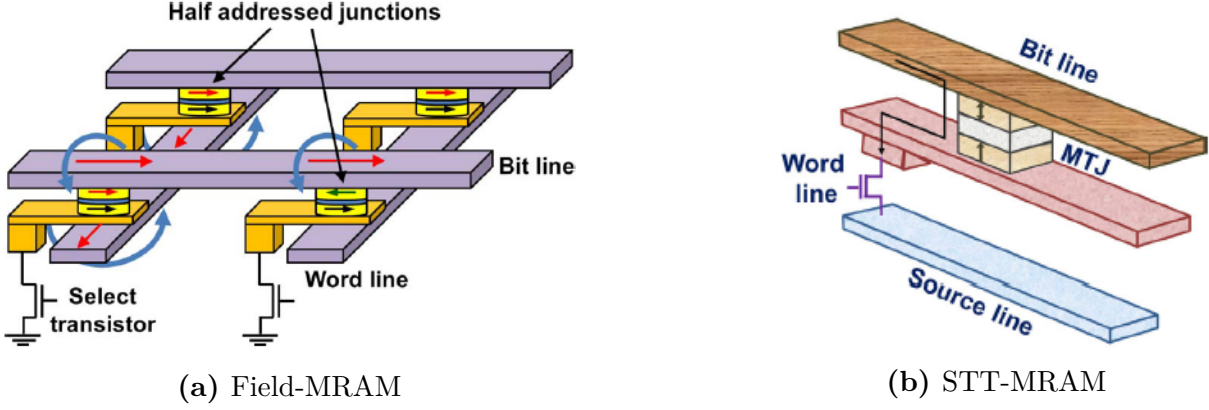


Figure 2.6 – Schematic representation of a (a) field-MRAM, and a (b) STT-MRAM. Both pictures show that a MRAM features a MTJ, which resistance is linked to the magnetisation state of the information to be read. The big difference between the two configurations lies in the way in which information is written. Images from [3] and [11], respectively.

A careful inspection of figures 2.6a and 2.6b shows that the STT-MRAM configuration does not rely on in-plane magnetic anisotropy, but rather on a perpendicular one, allowing to decrease drastically the dimensions of the device, hence increasing drastically the memory density [11]. The point with magnetic anisotropy is that it can be modified by external means [32], which can be of great interest in skyrmion-based transistors, for example.

2.3.3 Skyrmion-based transistors

Instead of a traditional transistor-like architecture, where charge carriers are transported through a channel as a function of an applied voltage (i.e. the gate voltage), a device in which the information is stored and transported in skyrmions, which are controlled by an external gate, can be imagined, as schematically illustrated in figure 2.7.

The working principle is as follows: first, a skyrmion is created by a MTJ (which serves the role of source) or spin valve, and is then dragged away by a spin-polarised current, where it is finally detected at the drain by a change in the tunnel magnetoresistance (TMR) of the read head. Even if the working principle is quite simple and similar to that of a classical transistor, there are some difficulties lying in the nature of the skyrmion itself: for instance, there exist some pinning forces, which make that a skyrmion-based transistor is normally in OFF state [31]. Fortunately, those pinning forces can be overcome if the driving polarised current, as well as the gate voltage, are chosen wisely [32, 81].

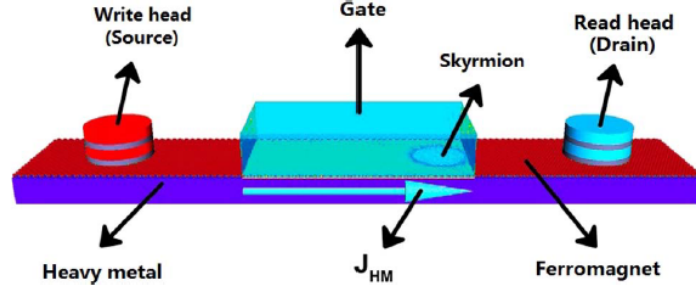


Figure 2.7 – Schematic representation of a skyrmion-based transistor. The skyrmion is first created by a write head (which plays the role of source), and is dragged to the drain by a spin-polarised current. Image from [31].

The control of the anisotropy by an external magnetic field is linked to charge accumulation at the interface between the different materials composing the skyrmion-based transistor, leading to a modification of the occupation of the surface states, hence a modification of the net anisotropy [53]. Another, more macroscopic, way to understand the effect of an electric field is that it creates an effective potential barrier (opposing or favouring) for the skyrmion.

Superconductivity

The history of superconductivity dates back to 1911, when H. Kamerlingh-Onnes experimentally reported that below a given temperature, the electrical resistance of a mercury sample became so small that it could not be experimentally measured [68]. This vanishingly small electrical resistance under a given temperature (called the critical temperature T_C) was called superconductivity, and the term remained attached to a zero resistance up to 1933, where the Meissner effect was explained by the London brothers [44]. From that time, superconductivity became associated to the mixed effect of vanishingly small electrical resistance and (almost) perfect diamagnetism.

To explain the superconductivity phenomenon, theories, such as the Ginzburg-Landau theory or the BCS theory have been developed. Those theories led to accurate description of a certain superconductors, but failed to describe some others, highlighting the fact that some other, more subtle mechanisms, were playing an important role in these materials.

3.1 Classical considerations

3.1.1 Infinite conductivity and London equations

An electrical resistance going down to zero can be understood as a conductivity going up to infinity. In order to gain insights into the physical meaning of an infinite conductivity, a thought experiment can be made: imagine a metallic ring, through which a magnet passes, creating an electromotive force (hence a current) opposing the flux variation, in agreement with Faraday's law. A cartoon picture of such a situation is given in figure 3.1. If the metal were in the normal state, as soon as the magnet stops moving, the current would decay according to the resistance and self-inductance of the ring. On the contrary, if the metal were in the superconducting state, the current would flow for an arbitrarily long time, since there would be no dissipation. A permanent current is now flowing in the ring, which was experimentally verified in [43].

If the conductivity of the material goes to infinity, the constitutive relation $\mathbf{J} = \sigma \mathbf{E}$ (with $\mathbf{J}$, σ , and $\mathbf{E}$ the current density, conductivity, and electric field, respectively) cannot be used

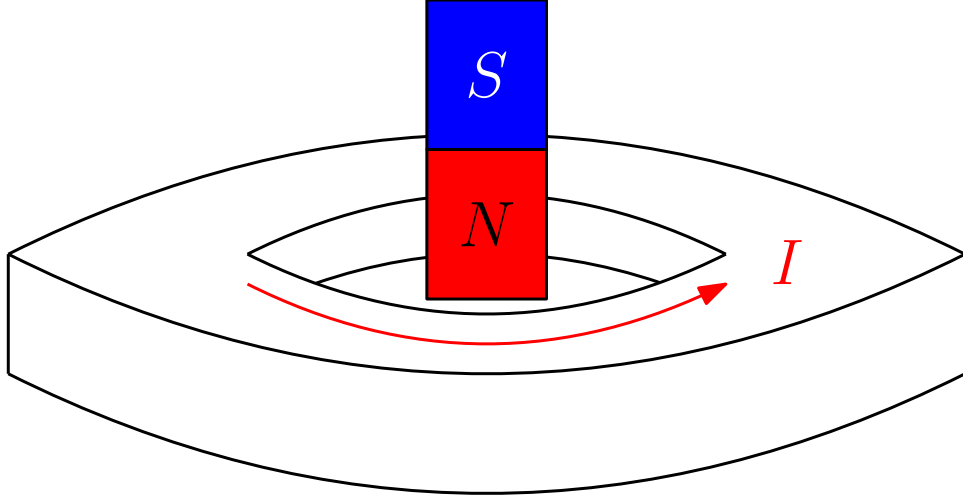


Figure 3.1 – Cartoon picture of a thought experiment, where a magnet is slid in and out of a metallic ring, allowing a current to flow. If the ring were perfectly conducting (i.e. presenting a zero electrical resistance), the current would flow for an arbitrary long time. On the contrary, in the case of a normal metal, the current would decay with time, according to the resistive and inductive characteristics of the setup.

anymore. Moreover, if there is no resistance, there would be no heat dissipation by Joule effect, but what about the inductive effects ? To get an idea, the Drude model in the frequency domain can be used, which leads to a frequency-dependent conductivity, i.e. $\sigma = \sigma(\omega)$. In frequency space, the constitutive relation linking the current density to the electric field takes the form

$$\bar{\mathbf{J}} = \sigma(\omega) \bar{\mathbf{E}},$$

where the bar over the symbol expresses the fact that phasors are used. In that expression, the frequency dependence of the conductivity on frequency takes the form

$$\sigma(\omega) = \frac{nq^2\tau_{\text{tr}}}{m} \frac{1}{1 + j\omega\tau_{\text{tr}}},$$

where m , q , and n are the electron mass, charge, and density, respectively, and where τ_{tr} is the transit time of electrons, i.e. the average time between two collision events. The conductivity being a complex quantity indicates that there is still, somehow, a resistive and inductive part in the material, which act as parasitics if a perfect dissipationless setup is wanted.

To get rid of those parasitics, the London brothers introduced the idea of “super electrons”, i.e. electrons having an infinite transit time (meaning they never undergo collisions). With that hypothesis, the conductivity of the system can be rewritten under the form

$$\sigma^*(\omega) = \frac{1}{j\omega\Lambda^*},$$

with $\Lambda = \frac{m^*}{n^*(q^*)^2}$, the $\star$ indicating that the quantities are those linked to the “super electrons”. This new expression of the conductivity highlights that the behaviour of the system is now purely inductive. The first London equation can be derived, which reads [44]

$$\mathbf{E} = \frac{\partial}{\partial t}(\Lambda^* \mathbf{J}). \quad (3.1)$$

From experimental considerations, it was observed that a superconductor cooled down under T_C exhibit perfect diamagnetism whatever the experimental conditions¹. Therefore, the usual constitutive relation $\mathbf{B} = \mu \mathbf{H}$ with $\mu \rightarrow 0$ cannot be applied anymore, and a new one is required. To get that new equation, the relations

$$\nabla \times \mathbf{H} = \mathbf{J} \quad \text{and} \quad \nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t},$$

combined with equation (3.1), leads to the equation

$$\left(\frac{1}{\lambda^2} - \nabla^2 \right) \frac{\partial}{\partial t} \mathbf{H} = \mathbf{0},$$

where $\lambda = \sqrt{\frac{\Lambda^*}{\mu_0}}$ is the London penetration depth, i.e. the characteristic length over which the field decays in a superconductor, hence the length over which the superconductor does not act as a perfect diamagnetic material. Going once again to the frequency space, and considering the assumption

$$\left(\frac{1}{\lambda^2} - \nabla^2 \right) \mathbf{B} = \mathbf{0} \quad \forall \omega,$$

the second London equation can be found, which expression reads [44]

$$\nabla \times \frac{\partial}{\partial t}(\Lambda^* \mathbf{J}) = -\frac{\partial}{\partial t} \mathbf{B}.$$

3.1.2 Two-fluid model

In the previous discussion, the fact that superconductivity is a thermodynamic phenomenon² was neglected. It was explained that the transport properties of a superconductor were due to two *different* types of charge carriers: “normal” electrons in a normal material, and “super” electrons in a superconductor. Such a segregation between “different types” of electrons allowed to explain the fact that a magnetic field penetrates a superconductor only in a thin region,

¹This is to be contrasted with a perfect conductor, which exhibits perfect diamagnetism only in zero cooled field experiments, i.e. in experiments where the sample is first cooled down to a temperature $T < T_C$, and then exposed to a magnetic field.

²Superconductivity originates from a phase transition between the normal state and the superconducting state, the transition being possible upon cooling the system.

and everything seemed to be fine. Now, if the superconducting state is regarded as a phase transition, the question to know where the “normal” electrons go at the transition arises.

To answer that question, it can be enlightening to first analyse an experience conducted by F. London, which showed that temperature dependence of the penetration depth reads [45]

$$\lambda(T) = \frac{\lambda_0}{\sqrt{1 - \left(\frac{T}{T_C}\right)^4}} \quad \text{for } T < T_C,$$

where λ_0 is the penetration depth at 0 K. This relation shows that, even if superconductivity is a phase transition, the penetration depth does not directly jump to λ_0 below T_C . Since the penetration depth is linked to physical quantities such as the charge carrier density, and that it depends on temperature, at least one of the quantities used in the definition of λ should depend on temperature. The most reasonable guess is to assume that it is the superelectron density which depends on temperature, which dependence is then given by the relation

$$n^*(T) = n_0^* \left[1 - \left(\frac{T}{T_C}\right)^4 \right] \quad \text{for } T < T_C,$$

showing a *monotonically* decrease with temperature (up to T_C , where $n^*(T_C) = 0$), hence the transition between normal and super electrons does not happen abruptly, but rather continuously.

To resume the situation: for temperature above T_C , the material behaves like a normal metal, the transport properties being due to normal electrons. At absolute zero, all the electrons become superelectrons. The question is, in between, what happens? The answer is: as the total amount of charges in the material is conserved, and because the density of superelectrons is a continuous function, the transport properties in the range $0 < T < T_C$ are due to a mix of both normal and super electrons. This is exactly what is meant by two-fluid model. Consequently, the total current density flowing in a material can be written under the form

$$\mathbf{J}_{\text{tot}} = \mathbf{J}_n + \mathbf{J}_{\text{sup}},$$

where $\mathbf{J}_n$ and $\mathbf{J}_{\text{sup}}$ refer to the current densities due to normal and super electrons, respectively. This two-component current density can be used with the London equations, as in [54]. From there, a new constitutive relation for the current density can be derived, which reads

$$\mathbf{J} = \left[\frac{\tilde{\sigma}_0(T)}{1 + j\omega\tau_{\text{tr}}} + \frac{1}{j\omega\mu_0\lambda^2(T)} \right] \mathbf{E}, \quad \text{where } \tilde{\sigma}_0(T) = \frac{n_{\text{tot}}q^2\tau_{\text{tr}}}{m} \left(\frac{T}{T_C}\right)^4 \quad \text{for } T < T_C.$$

For completeness, the second London equation takes the form

$$\nabla \times [\Lambda^*(T)\mathbf{J}_{\text{sup}}] = -\mathbf{B},$$

where the temperature dependence of Λ is given by [54]

$$\Lambda(T) = \frac{m}{n_{\text{tot}}q^2} \frac{1}{1 - (T/T_C)^4} \quad \text{for } T < T_C.$$

The point about separating the total current density into a normal and superconducting part is to show that the Meissner effect is due only to the superelectrons, not the normal ones.

3.1.3 Superconductivity and magnetism

So far, it was stated that a superconductor is characterised by a zero resistance and almost perfect diamagnetism under a critical temperature T_C , and that superconductivity is a phase transition. This is true for some superconductors, but not for others: those for which the previous statements hold are known under the name type-I superconductors, and are well described in the framework of the BCS (see later) theory. On the contrary, the Meissner effect should but nuanced for other type of superconductors, known as type-II superconductors.

It was previously stated that superconductivity can be regarded as a temperature-dependent phase transition. This statement stays true, but should be nuanced: a superconducting system stays in that state under a given temperature *and applied magnetic field*. The phase diagrams of type-I and type-II superconductors are given in figure 3.2. As can be seen on that figure, the

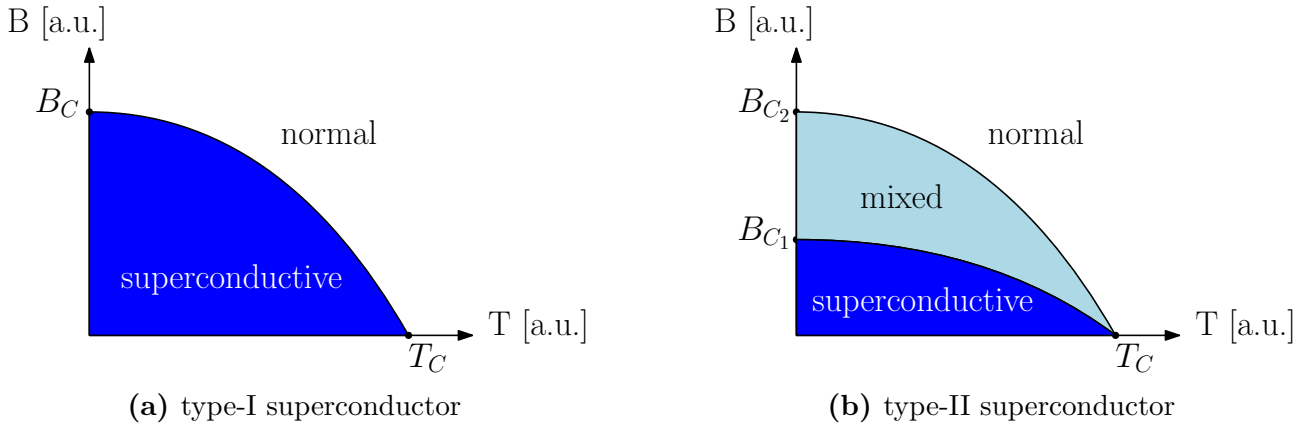


Figure 3.2 – Phase diagram of type-I and type-II superconductors.

fundamental difference between the two types of superconductors is the existence of a mixed state, in which the superconductor is still a very good diamagnet, except on certain locations, where the magnetic field penetrates the material under the form of vortex-like “tubes”, organised in an Abrikosov lattice.

Whatever the type of superconductor considered (be it type-I or type-II), magnetic fields are detrimental. For the type-I superconductors, it can be explained quite easily: it is generally admitted that superconductivity is due to electrons pairing up (so-called Cooper pairs, see later). When one such Cooper pair is immersed into a magnetic field, one of the electrons will align its spin on the magnetic field (due to the Zeeman interaction), while the other will align in an antiparallel fashion (to respect the Pauli principle). This stays true up to the point where the magnetic field is so intense that the Zeeman energy becomes greater than the pairing energy, breaking the “link” between the electrons. Unfortunately, no satisfactory explanation for the destruction of superconductivity can be found for type-II superconductors.

3.1.4 Ginzburg-Landau theory

Another theory that was used to explain the superconducting properties of certain materials when cooled down below their T_C is due to V. Ginzburg and L. Landau. This theory relies on the idea that the superconducting properties originates from a phase transition between a normal state and a superconducting one, and is a phenomenological theory.

In the framework of the description of a superconductor as a phase transition, the electrons “condensing” in the superconducting state are described by a (complex) order parameter, modelling the symmetry of the system. For example, in the case of a ferromagnet, the order parameter is the magnetisation $\mathbf{m}$. The appropriate thermodynamic potential can then be written as a certain function of that order parameter, hence it can be written under the form

$$F = F(\Delta, T),$$

where Δ and T are the order parameter, and the temperature T . The definition of F is very general, and can a lot of different quantities, such as a free energy, a free enthalpy, or something else depending on which quantities are given (pressure, volume, etc.). From there, the system described by F is said to be in equilibrium when F is minimum. The point is that the exact expression of the thermodynamic potential is generally not known, which lead to the idea of Landau of expanding the F in power series of Δ , with the expansion having to take the symmetries of the system into account.

In the case of a superconductor, the order parameter Ginzburg and Landau chose was the amplitude of the superconducting wavefunction, i.e. the density of superelectrons n^* . The series expansion they came up with was

$$F = \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \mathcal{O}(|\psi|^6).$$

In the case of superconductors, $\beta > 0$, meaning that the expression of F is bounded from below [16]. Two cases have to be discussed, namely

- the case in which $\alpha \geq 0$, for which F has a minimum located at $\psi = 0$. In such a case, the density n^* is null, hence the system is a normal metal.
- The second case occurs for $\alpha < 0$, in which case F has a set of minima with the same amplitude, but arbitrary phase. It is easily found that the solutions to the equation $\partial_{|\psi|} F = 0$ are either $|\psi| = 0$ (which then corresponds to a maximum in F), or $|\psi| = \sqrt{-\alpha/\beta}$.

A graphical representation of the general shape of F is given in figure 3.3. The case $\alpha < 0$ is often called the “Mexican hat”, which can be visualised if the graph is rotated around the vertical axis to find F as a function of the complex ψ .

By definition, the order parameter becomes equal to 0 at T_C , hence it could be enlightening to expand the coefficients α and β as functions of T around T_C , leading to

$$\begin{aligned}\alpha &\cong \alpha'(T - T_C), \quad \alpha' > 0, \\ \beta &\cong \text{const.}\end{aligned}$$

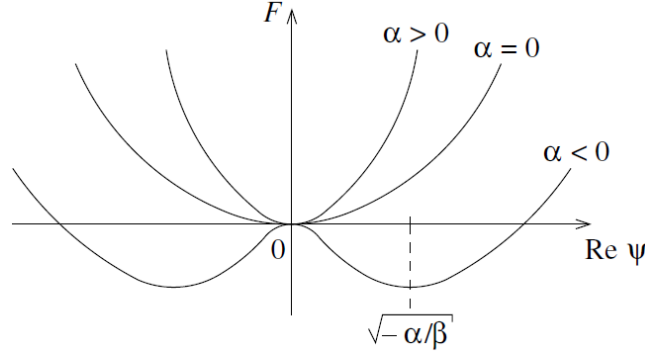


Figure 3.3 – Graphical representation of the thermodynamic potential F as a function of the real part of the order parameter. Image from [16].

which allows to rewrite the order parameter under the form $|\psi| \cong \sqrt{\frac{-\alpha'(T-T_C)}{\beta}}$. A system having such an order parameter will always minimise the free energy, hence will always be achieved experimentally. The point is: in an experiment, only one outcome is possible, hence there is still a degree of freedom in the expression of ψ , which comes from its phase: indeed, the order parameter can always be written under the form $\psi = |\psi|e^{i\phi}$. Such a freedom on the phase shows that the solution is not invariant under phase rotation, hence it is said to break spontaneously the $U(1)$ symmetry.

The previous discussion does not include space variations of the order parameter. To include it, Ginzburg and Landau incorporated an additional term in the power development of the free energy to include terms involving gradients. Moreover, in the case of superconductors, the magnetic field contribution has to be taken into account as well. These considerations lead to a new expression, known under the name *Ginzburg-Landau functional*, which is given by [16]

$$F[\psi, \mathbf{A}] \cong \int d^3r \left[\alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right)^2 \psi + \frac{\|\mathbf{B}\|^2}{8\pi} \right].$$

To get that expression, different assumption have been made. The first one, which is the most fundamental, is to consider that $\psi(\mathbf{r})$ plays the role of wavefunction of the superconductor, which justifies the replacement $\nabla\psi \rightarrow \frac{\hbar}{i}\nabla - q\mathbf{A}$, with c the speed of light. This rewriting basically states that the modification of the wavefunction of the superconductor is due to the its kinetic energy, and the action of an external magnetic field, described by a vector potential $\mathbf{A}$. The other hypothesis is that the electric field does not contribute to the functional, which can be understood since in a normal conductor at equilibrium, the electric field vanishes.

Now, the functional depends both on ψ and $\mathbf{A}$. Minimising the expression with respect to ψ leads to the equation

$$\frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right)^2 \psi + \alpha\psi + \beta|\psi|^2\psi = 0.$$

To see what the minimisation condition looks like when the vector potential is considered, it can be rewritten under the form $\mathbf{A}(\mathbf{r}) = \mathbf{A}_0(\mathbf{r}) + \mathbf{a}(\mathbf{r})$, which then leads to

$$F[\psi, \mathbf{A}_0 + \mathbf{a}] = F[\psi, \mathbf{A}_0] + \int d^3r \left\{ -\frac{q}{2m^\star} \left[\left(\frac{\hbar}{i} \nabla \psi \right)^* \psi + \psi^* \frac{\hbar}{i} \nabla \psi \right] \cdot \mathbf{a} \right\} \\ + \int d^3r \left\{ \frac{q^2}{m^\star} |\psi|^2 \mathbf{A}_0 \cdot \mathbf{a} + [\nabla \times \mathbf{B}_0] \cdot \mathbf{a} \right\} + \mathcal{O}(a^2),$$

where Gauss theorem, as well as the relation $\nabla \times \mathbf{A}_0 = \mathbf{B}_0$, were used. At equilibrium, only the first term should remain, which leads to the equation

$$-i \frac{q\hbar}{2m^\star} [(\nabla \psi^*)\psi - \psi^* \nabla \psi] + \frac{q^2}{m^\star} |\psi|^2 \mathbf{B}_0 + \nabla \times \mathbf{B}_0 = \mathbf{0},$$

which allows to express the (super)current density thanks to Ampère's law. It takes the form

$$\mathbf{j} = \nabla \times \mathbf{B} = i \frac{q\hbar}{2m^\star} [(\nabla \psi^*)\psi - \psi^* \nabla \psi] - \frac{q^2}{m^\star} |\psi|^2 \mathbf{A}.$$

If the variations of ψ are negligible, i.e. if the gradients are equal to 0, the current density can be rewritten under the form

$$\mathbf{j} = -\frac{q^2 |\psi|^2}{m^\star} \mathbf{A},$$

which should be equal to the London supercurrent. Furthermore, a new expression of the penetration depth λ can be expressed as a function of the wavefunction, i.e. $\lambda = \lambda(|\psi|^2)$. In the end, two lengths can be used to characterise the superconductor: the penetration depth λ , and the length over which the superconducting wavefunction varies, ξ . By taking their dimensionless ratio (roughly temperature independent), a distinction between type-1 and type-2 superconductors can be made: $\kappa = \lambda/\xi < 1/\sqrt{2} \Rightarrow$ type-1. Otherwise, the superconductor is type-2.

3.2 Quantum considerations

The roots of superconductivity lies at the electron-phonon interaction [25], which allows to pair electrons up and create so-called Cooper pairs. Such a pair of electrons behaves as bosons, meaning they can populate macroscopically a given state. In the following, the quantum theory behind the standard and generalised BCS theories will be presented.

3.2.1 Standard BCS theory

Simple contact interaction

To take electron-phonon interactions into account in the Hamiltonian describing a superconductor, different refinement levels can be considered. In this subsection, a structureless contact interaction

will be considered, which leads to the Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + g \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ q}} \hat{c}_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger \hat{c}_{\mathbf{k}'-\mathbf{q}\downarrow}^\dagger \hat{c}_{\mathbf{k}'\uparrow}^\dagger \hat{c}_{\mathbf{k}\downarrow}, \quad (3.2)$$

where the first term corresponds to the kinetic energy of the electrons, and the second term to their interaction. In (3.2), $\xi_{\mathbf{k}}$ is the energy of the electrons measured relative to the chemical potential, i.e. $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, $\hat{c}_{\mathbf{k}\sigma}^\dagger$ ($\hat{c}_{\mathbf{k}\sigma}$) creates (annihilates) an electron in state $|\mathbf{k}\sigma\rangle$, and g models the two-body interaction between the electrons forming the pairs. This corresponds to an attractive contact interaction $U(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}')$, with $g < 0$, such that $V_{\mathbf{k}\mathbf{k}'} = V(\mathbf{q} = \mathbf{k} - \mathbf{k}') = \int d\mathbf{r} U(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} = g$ [60].

Considering only the scattering processes leading to a null momentum of the pair, i.e. scattering between elements of the basis $\{|\mathbf{k}\uparrow\rangle \otimes |-\mathbf{k}\downarrow\rangle\}$, the Hamiltonian (3.2) takes the form

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + g \sum_{\mathbf{k}, \mathbf{k}'} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow}. \quad (3.3)$$

In 1957, Bardeen, Cooper, and Schrieffer proposed that the ground state of that last Hamiltonian was made of a superposition of electrons and holes [6], i.e. of the form

$$|\Phi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \right) |0\rangle, \quad (3.4)$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are coefficients representing the probability that a pair $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty or occupied, respectively, and are submitted to the condition $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$. The precise expression of these coefficients will be derived later on. Coming back to the Hamiltonian (3.3), the interaction term can be somewhat simplified if a mean-field approach, i.e. an approach in which fluctuations are neglected, is considered. By defining

$$\hat{b}_{\mathbf{k}}^\dagger = \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger, \quad \hat{b}_{\mathbf{k}'} = \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow}, \quad \text{and} \quad \Delta = -g \sum_{\mathbf{k}'} \langle \hat{b}_{\mathbf{k}'} \rangle = -g \sum_{\mathbf{k}'} \langle \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \rangle,$$

and using the substitution

$$\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} = \langle \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \rangle \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} + \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \langle \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \rangle - \langle \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \rangle \langle \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \rangle,$$

the mean-field Hamiltonian takes the form

$$\hat{H}^{\text{MF}} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left[\Delta \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger + \Delta^* \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} - \Delta \langle \hat{b}_{\mathbf{k}}^\dagger \rangle \right], \quad (3.5)$$

which is bilinear in the creation and annihilation operators. In order to treat that Hamiltonian, the so-called Bogoliubov-de Gennes (BdG) transformation can be used, which redefines the creation and annihilation operators as superposition of electron-like and hole-like excitations. Such a transformation reads

$$\begin{cases} \hat{c}_{\mathbf{k}\uparrow} &= u_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}\downarrow}^\dagger, \\ \hat{c}_{-\mathbf{k}\downarrow}^\dagger &= -v_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}\downarrow} + u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}\uparrow}^\dagger. \end{cases} \quad (3.6)$$

By imposing the transformation to be canonical, i.e. enforcing it to obey the same anti-commutation properties than those of fermionic creation and annihilation operators, the condition $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ comes out spontaneously. By plugging the new expression for the creation and annihilation operators into the expression (3.3), an expression for the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ can be obtained, and reads

$$\begin{cases} |u_{\mathbf{k}}|^2 &= \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \\ |v_{\mathbf{k}}|^2 &= \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \end{cases} \quad \text{where} \quad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}.$$

Using the BdG transform (3.6) in the expression of the mean-field Hamiltonian (3.5), it acquires a diagonal form given by

$$\hat{H}^{\text{MF}} = \sum_{\mathbf{k}, \sigma} E_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}\sigma}^\dagger \hat{\gamma}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \left[\xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta \langle \hat{b}_{\mathbf{k}}^\dagger \rangle \right].$$

A last quantity has to be determined, namely the gap Δ . To find its expression, the BdG transformation is injected in the definition of the gap, which leads to the equality

$$\Delta = -g \sum_{\mathbf{k}'} \langle \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \rangle = -g \sum_{\mathbf{k}'} u_{\mathbf{k}'}^* v_{\mathbf{k}'} \langle 1 - \hat{\gamma}_{\mathbf{k}'\uparrow}^\dagger \hat{\gamma}_{\mathbf{k}'\uparrow} - \hat{\gamma}_{\mathbf{k}'\downarrow}^\dagger \hat{\gamma}_{\mathbf{k}'\downarrow} \rangle.$$

To go further, the definition of the Fermi-Dirac distribution

$$\langle \hat{\gamma}_{\mathbf{k}\sigma}^\dagger \hat{\gamma}_{\mathbf{k}\sigma} \rangle = f(E_{\mathbf{k}}) = \frac{1}{1 + \exp(\beta E_{\mathbf{k}})},$$

with $\beta = \frac{1}{k_{\text{B}} T}$ is used, where k_{B} is the Boltzmann constant, and T the temperature. The gap equation then reads

$$\Delta = -g \sum_{\mathbf{k}} u_{\mathbf{k}}^* v_{\mathbf{k}} [1 - 2f(E_{\mathbf{k}})] = -g \sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right),$$

for which 2 solutions exist, namely the trivial solution $\Delta = 0$, which corresponds to a classical metal, and the non-trivial solution $\Delta \neq 0$. In the later case, the gap equality can be rewritten under the form

$$-\frac{1}{g} = \int_0^{\hbar\omega_c} d\xi N(\xi) \frac{\tanh\left(\frac{1}{2}\beta\sqrt{\xi^2 + \Delta^2}\right)}{\sqrt{\xi^2 + \Delta^2}},$$

where $N(\xi)$ is the density of state (DOS), which can be approximated by its value near the Fermi energy, since only the electrons near that energy contribute to transport [4], and where the cutoff energy $\hbar\omega_c$ was introduced because of the divergence of the integrand. The gap equation is an implicit equation, which has to be solved numerically. However, some particular values can be derived. First, its value at zero kelvin. In that case, the above integral can be computed, and gives

$$\Delta(T = 0) = 2\hbar\omega_c \exp\left(-\frac{1}{gN(0)}\right).$$

The critical temperature T_C , i.e. the temperature at which the gap becomes 0, can also be derived. Its expression is given by

$$\begin{aligned}\Delta(T = T_c) = 0 \Rightarrow E_{\mathbf{k}} = \xi_{\mathbf{k}} \Rightarrow -\frac{1}{gN(0)} &= \int_0^{\hbar\omega_c/k_B T} dx \frac{\tanh(x)}{x}, \quad x = \frac{1}{2} \frac{\xi}{k_B T} \\ &= \ln(A\beta\hbar\omega_c), \quad A = \frac{2\gamma}{\pi} \approx 1.13,\end{aligned}$$

where γ is the Euler constant. Solving that equation for β allows to finally find

$$k_B T_c = 1.13 \hbar \omega_c \exp\left(-\frac{1}{gN(0)}\right).$$

As a last remark, it should be emphasised that an alternative approach to solve the Hamiltonian (3.5) is often used in literature (see [9] for example). It consists in introducing a four-component spinor

$$\Psi_{\mathbf{k}} = \begin{bmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}_{\mathbf{k}\downarrow} \\ \hat{c}_{-\mathbf{k}\uparrow}^\dagger \\ \hat{c}_{-\mathbf{k}\downarrow}^\dagger \end{bmatrix},$$

in term of which the Hamiltonian can be rewritten under the form

$$\hat{H} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \hat{H}^{\text{BdG}}(\mathbf{k}) \Psi_{\mathbf{k}} + \text{constant},$$

where the part $\hat{H}^{\text{BdG}}(\mathbf{k})$ is the BdG form of the Hamiltonian, which takes the explicit form

$$\hat{H}^{\text{BdG}}(\mathbf{k}) = \frac{1}{2} \begin{bmatrix} \xi_{\mathbf{k}} & 0 & 0 & \Delta \\ 0 & \xi_{\mathbf{k}} & -\Delta & 0 \\ 0 & -\Delta^* & -\xi_{-\mathbf{k}} & 0 \\ \Delta^* & 0 & 0 & -\xi_{-\mathbf{k}} \end{bmatrix},$$

which can be decomposed as [9]

$$\hat{H}^{\text{BdG}} = \xi_{\mathbf{k}} \hat{\tau}_z \otimes \mathbb{I}_{2 \times 2} - \text{Re}\{\Delta\} \hat{\tau}_y \otimes \hat{\sigma}_y - \text{Im}\{\Delta\} \hat{\tau}_x \otimes \hat{\sigma}_y,$$

where the $\hat{\tau}'s$ are the Pauli matrices in particle-hole space, the $\hat{\sigma}'s$ are the spins, and $\mathbb{I}_{2 \times 2}$ is the 2×2 identity matrix. Because the different matrices making up the Hamiltonian are anticommuting, the energy spectrum can be easily found, because $(\hat{H}^{\text{BdG}})^2 = (\xi_{\mathbf{k}}^2 + |\Delta|^2) \mathbb{I}_{4 \times 4}$ [9]. This means that the energy spectrum is made of two doubly degenerated bands, with energies $E_{\pm} = \pm \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$, as shown in figure 3.4.

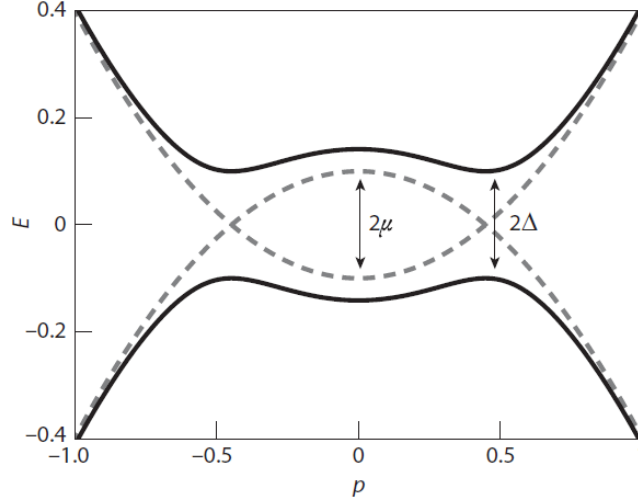


Figure 3.4 – Dispersion relation for a conventional s -wave superconductor (the conversion between momentum and wavevector is trivial). The dotted line correspond to a gapless situation, and the solid line to a superconductor in which the chemical potential μ has the same value as the gap, i.e. $\mu = |\Delta|$. Image from [9].

More precise interaction

In the previous discussion, neither the charge, nor the spin of the electrons were considered in the interaction potential. If charge is taken into account, the coupling to the lattice becomes important, since it leads to charge screening effects. The scattering matrix elements between electrons with momenta $\mathbf{k}$ and $\mathbf{k}'$ is given by a Coulomb-like potential, where the dielectric constants depends on the momenta [60]. The expression of such a potential is given by

$$V_{\mathbf{k}\mathbf{k}'} = \frac{4\pi e^2}{\|\mathbf{q}\|^2 \epsilon(\mathbf{q}, \omega)}, \quad (3.7)$$

where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$, and the dielectric constant $\epsilon(\mathbf{q}, \omega)$ takes dynamic charge screening into account. The expression appearing in (3.7) can be simplified if the electronic and phonon contribution can be decoupled, which is possible for example if the electronic effects are considered to be instantaneous, i.e. frequency-independent. This leads to the definition of an effective interaction taking the form

$$V_{\mathbf{k}\mathbf{k}'}^{\text{eff}} = \underbrace{\frac{4\pi e^2}{\|\mathbf{q}\|^2 + \|\mathbf{k}_{\text{TF}}\|^2}}_{\text{electronic contrib.}} + \underbrace{\frac{4\pi e^2}{\|\mathbf{q}\|^2 + \|\mathbf{k}_{\text{TF}}\|^2} \frac{\omega_q^2}{\omega^2 - \omega_q^2}}_{\text{phonon contrib.}},$$

where $\mathbf{k}_{\text{TF}}$ is the length over which the screening takes place, $\hbar\omega = \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}$, and where ω_q is the phonon dispersion spectrum. It is directly seen that $\omega^2 > \omega_q^2$ leads to repulsive interactions, while $\omega^2 < \omega_q^2$ leads to attractive interactions.

Both contribution are short ranged [60], which justifies the assumption made in the previous subsection, where the interaction was considered to be a contact interaction. Even if the previous discussion allows to get an intuitive picture of the electron-phonon interaction, its lack of quantitative results and expression is a weakness. This means that a more formal treatment is needed, which can be found in [5], where different approximations are made, namely that (i) the anisotropy effects are neglected, (ii) the electrons interact only with longitudinal phonons, (iii) the interactions depends only on the difference between wave vectors, and (iv) only the valence electrons, which are treated as free electrons, are important. The total Hamiltonian then takes the form

$$\hat{H} = \sum_i \frac{\hat{\mathbf{p}}^2}{2m_e} + \sum_{i,I} V(\mathbf{r}_i - \mathbf{R}_I) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\|\mathbf{r}_i - \mathbf{r}_j\|} + \hat{H}_{\text{ion}},$$

where the first term is the kinetic energy of the electrons, the second term is electron-ion interaction, the third term is the electron Coulomb interaction, and the last term is the ionic energy, which features the kinetic and potential energies of the ions. This expression can be further simplified by considering that the ionic part $\hat{H}_{\text{ion}}$ only features a component linked to longitudinal phonons. The total Hamiltonian thus features the kinetic energy of the electrons, they electrostatic interaction with phonons as well as with other electrons, and the phonon energy. A final simplification, in which the electrostatic interactions are neglected, leads to the final expression of the Hamiltonian [26]

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \hat{a}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}} + i \sum_{\substack{\mathbf{k}, \mathbf{q} \\ \sigma}} D_{\mathbf{q}} \hat{c}_{\mathbf{k}+\mathbf{q}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} (\hat{a}_{\mathbf{q}} - \hat{a}_{-\mathbf{q}}^\dagger), \quad (3.8)$$

where $\hat{a}_{\mathbf{q}}^\dagger$ ($\hat{a}_{\mathbf{q}}$) creates (destroys) a phonon with momentum $\mathbf{q}$. To book progress with the Hamiltonian, the electron-phonon interaction can be discarded perturbatively, leading to an effective Hamiltonian which depends solely on fermionic operators. To do so, the Hamiltonian appearing in (3.8) is split as a major contribution $\hat{H}_0$, and a small perturbation $\hat{H}'$, which allows to reexpress the Hamiltonian under the form $\hat{H} = \hat{H}_0 + \lambda \hat{H}'$. Performing a canonical transformation allows to rewrite

$$\begin{aligned} \hat{\tilde{H}} &= e^{-\hat{S}} \hat{H} e^{\hat{S}} = \hat{H} + [\hat{H}, \hat{S}] + \frac{1}{2} [[\hat{H}, \hat{S}], \hat{S}] + \dots \\ &= \hat{H}_0 + \lambda \hat{H}' + [\hat{H}_0 + \lambda \hat{H}', \hat{S}] + \frac{1}{2} [[\hat{H}_0 + \lambda \hat{H}', \hat{S}], \hat{S}] + \dots \\ &= \hat{H}_0 + \lambda \hat{H}' + \underbrace{[\hat{H}_0, \hat{S}]}_{\star} + \lambda [\hat{H}', \hat{S}] + \dots \end{aligned}$$

In the last expression, we want the expression marked by a star to be equal to zero. To do so, the equation $[\hat{H}_0, \hat{S}] + \lambda \hat{H}' = 0$ is solved in the basis of the eigenstates of $\hat{H}_0$, which leads to

$$\langle \phi_n | \hat{S} | \phi_m \rangle = \lambda \frac{\langle \phi_n | \hat{H}' | \phi_m \rangle}{\epsilon_m - \epsilon_n}, \quad \text{where} \quad \hat{H}_0 | \phi_n \rangle = \epsilon_n | \phi_n \rangle.$$

By considering only one phonon processes, the matrix elements of the interaction can be computed, and are given by

$$\begin{aligned}\langle 1_q | \hat{S} | 0 \rangle &= iD \sum_{\mathbf{k}, q} \frac{\langle 1_q | \hat{c}_{\mathbf{k}+q\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} (\hat{a}_q - \hat{a}_{-q}^\dagger) | 0 \rangle}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+q} - \omega_q} \quad \text{and} \quad \langle 0 | \hat{S} | 1_q \rangle = iD \sum_{\mathbf{k}', q} \frac{\langle 0 | \hat{c}_{\mathbf{k}'+q\sigma}^\dagger \hat{c}_{\mathbf{k}'\sigma} (\hat{a}_q - \hat{a}_{-q}^\dagger) | 1_q \rangle}{\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}'+q} - \omega_q} \\ &= iD \sum_{\mathbf{k}, \sigma} \frac{\hat{c}_{\mathbf{k}+q\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+q} - \omega_q} \quad \quad \quad = iD \sum_{\mathbf{k}', \sigma} \frac{\hat{c}_{\mathbf{k}'+q\sigma}^\dagger \hat{c}_{\mathbf{k}'\sigma}}{\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}'+q} - \omega_q}.\end{aligned}$$

Moreover, if there are no phonons in the ground state of the system, the matrix element corresponding to $[\hat{H}', \hat{S}]$ is given by

$$\begin{aligned}\langle 0 | [\hat{H}', \hat{S}] | 0 \rangle &= \langle 0 | \hat{H}' \hat{S} | 0 \rangle - \langle 0 | \hat{S} \hat{H}' | 0 \rangle \\ &= \sum_q \left[\langle 0 | \hat{H}' | 1_q \rangle \langle 1_q | \hat{S} | 0 \rangle - \langle 0 | \hat{S} | 1_q \rangle \langle 1_q | \hat{H}' | 0 \rangle \right] \\ &= \frac{D^2}{2} \sum_{\mathbf{k}, \mathbf{k}', q} \hat{c}_{\mathbf{k}'+q}^\dagger \hat{c}_{\mathbf{k}'\sigma} \hat{c}_{\mathbf{k}-q}^\dagger \hat{c}_{\mathbf{k}\sigma} \left(\frac{1}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-q} - \omega_q} - \frac{1}{\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}'+q} + \omega_q} \right)\end{aligned}$$

which allows finally to write the interacting part as [5]

$$\hat{\hat{H}} = D^2 \sum_{\mathbf{k}, \mathbf{k}', q} \frac{\omega_q}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-q})^2 - \omega_q^2} \hat{c}_{\mathbf{k}'-q}^\dagger \hat{c}_{\mathbf{k}-q}^\dagger \hat{c}_{\mathbf{k}} \hat{c}_{\mathbf{k}'},$$

which shows that the interaction is attractive if the difference in energy is smaller than the phonon energy. This last point, namely that the interactions are attractive if the energy difference is smaller than the phonon energy, is not specific to the electron-phonon interaction, but is a general feature of systems (quantum or not) interacting with harmonic oscillators³ [40].

3.2.2 Generalised BCS theory

The previous model can be generalised if an extended form of the interaction between pairs of electrons is considered. Here, the case of a pair with null total momentum is still considered, but the scattering due to the spins is taken into account. This leads to an Hamiltonian of the form [60]

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} V_{\mathbf{k}, \mathbf{k}'}^{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \hat{c}_{\mathbf{k}\sigma_1}^\dagger \hat{c}_{-\mathbf{k}\sigma_2}^\dagger \hat{c}_{-\mathbf{k}'\sigma_3} \hat{c}_{\mathbf{k}'\sigma_4}, \quad (3.9)$$

where the scattering element

$$V_{\mathbf{k}, \mathbf{k}'}^{\sigma_1 \sigma_2 \sigma_3 \sigma_4} = \langle -\mathbf{k}\sigma_1; \mathbf{k}\sigma_2 | \hat{V} | -\mathbf{k}'\sigma_3; \mathbf{k}'\sigma_4 \rangle$$

³As a first approximation, phonons can be treated as decoupled harmonic oscillators.

obeys to fermionic commutations rules, which imposes the conditions

$$V_{\mathbf{k},\mathbf{k}'}^{\sigma_1\sigma_2\sigma_3\sigma_4} = -V_{-\mathbf{k},\mathbf{k}'}^{\sigma_2\sigma_1\sigma_3\sigma_4} = -V_{\mathbf{k},-\mathbf{k}'}^{\sigma_1\sigma_2\sigma_4\sigma_3} = V_{-\mathbf{k},-\mathbf{k}'}^{\sigma_2\sigma_1\sigma_4\sigma_3}.$$

Those relations basically mirror the fact that the wavefunction of electrons is antisymmetric, hence a permutation of two electrons comes with a sign flip. To deal with such a Hamiltonian, a mean-field approach is once more used. Defining

$$\hat{b}_{\mathbf{k}}^{\sigma\sigma'} = \langle \hat{c}_{-\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma'} \rangle, \quad \Delta_{\mathbf{k}}^{\sigma\sigma'} = - \sum_{\substack{\mathbf{k}' \\ \sigma_3, \sigma_4}} V_{\mathbf{k},\mathbf{k}'}^{\sigma\sigma'\sigma_3\sigma_4} \hat{b}_{\mathbf{k}}^{\sigma_3\sigma_4}, \quad \text{and} \quad (\Delta_{\mathbf{k}}^{\sigma\sigma'})^* = - \sum_{\substack{\mathbf{k}' \\ \sigma_3, \sigma_4}} V_{\mathbf{k}',\mathbf{k}}^{\sigma_1\sigma_2\sigma'\sigma} (\hat{b}_{\mathbf{k}}^{\sigma_2\sigma_3})^*,$$

the mean-field Hamiltonian takes the form

$$\hat{H}^{\text{MF}} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} - \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}' \\ \sigma_1, \sigma_2}} \left[\Delta_{\mathbf{k}}^{\sigma_1\sigma_2} \hat{c}_{\mathbf{k}\sigma_1}^\dagger \hat{c}_{-\mathbf{k}\sigma_2}^\dagger + (\Delta_{\mathbf{k}}^{\sigma_1\sigma_2})^* \hat{c}_{\mathbf{k}\sigma_1} \hat{c}_{-\mathbf{k}\sigma_2} \right] + \hat{K} + \text{small terms},$$

where $\hat{K} = -\frac{1}{2} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} V_{\mathbf{k},\mathbf{k}'}^{\sigma_1\sigma_2\sigma_3\sigma_4} \langle \hat{c}_{\mathbf{k}\sigma_1}^\dagger \hat{c}_{-\mathbf{k}\sigma_2}^\dagger \rangle \langle \hat{c}_{-\mathbf{k}'\sigma_3} \hat{c}_{\mathbf{k}'\sigma_4} \rangle$. The gap parameter is no longer a scalar, but a 2×2 matrix, which can be written under the form

$$\hat{\Delta}_{\mathbf{k}} = \begin{bmatrix} \Delta_{\mathbf{k}}^{\uparrow\uparrow} & \Delta_{\mathbf{k}}^{\uparrow\downarrow} \\ \Delta_{\mathbf{k}}^{\downarrow\uparrow} & \Delta_{\mathbf{k}}^{\downarrow\downarrow} \end{bmatrix}.$$

If spin-orbit coupling is neglected, the momentum and spin degrees of freedom can be decoupled, which allows to rewrite the gap as a product of an orbital and of a spin part, i.e.

$$\Delta_{\mathbf{k}}^{\sigma_1\sigma_2} = \chi_{\sigma_1\sigma_2} \Delta(\mathbf{k}).$$

The parity of the orbital part and the spin configuration are linked to the antisymmetry condition of the fermionic wavefunctions, which imposes

$$\begin{aligned} \text{(even parity)} \quad \Delta(\mathbf{k}) &= \Delta(-\mathbf{k}) \iff \chi_{\sigma_1\sigma_2} = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) & \text{spin singlet} \\ \text{(odd parity)} \quad \Delta(\mathbf{k}) &= -\Delta(-\mathbf{k}) \iff \chi_{\sigma_1\sigma_2} = \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{cases} & \text{spin triplet} \end{aligned}$$

Those conditions impose that the gap function follows

$$\Delta_{\mathbf{k}}^{\sigma_1\sigma_2} = -\Delta_{-\mathbf{k}}^{\sigma_2\sigma_1} = \begin{cases} \Delta_{-\mathbf{k}}^{\sigma_1\sigma_2} = -\Delta_{\mathbf{k}}^{\sigma_2\sigma_1} & \text{even} \\ -\Delta_{-\mathbf{k}}^{\sigma_1\sigma_2} = \Delta_{\mathbf{k}}^{\sigma_2\sigma_1} & \text{odd} \end{cases}$$

From those considerations, it is obvious that the matrix representing the gap function has to be parametrised. In short, its expression can be written under the form

$$\Delta_{\mathbf{k}}^{\sigma_1\sigma_2} = i[\Delta_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}] \hat{\sigma}_y, \quad (3.10)$$

where $\Delta_0(\mathbf{k})$ encodes the spin singlet state, and $\mathbf{d}(\mathbf{k})$ encodes the spin triplet and $\hat{\boldsymbol{\sigma}}$ is the vector of Pauli matrices.

3.3 Topological superconductors and Majorana Fermions

The quest in unconventional superconductors have been double along the years: (i) explaining the microscopic mechanisms producing the unconventional pairing of electrons, and (ii) trying to observe and explain new (quasi)particle phenomena. Since only the part concerned with the new quasiparticles is of direct interest for technological applications (such as the use of Majorana fermions to realise solid-state qubits), only this subject will be exposed in the following. Moreover, as Majorana fermions are their own antiparticle (as will be shown later), it is quite natural to search for them in superconductors, since the Bogoliubov quasiparticles are described as a superposition of electrons and holes, according to the relation (3.4).

3.3.1 p -wave superconductors in 1D

The simplest topological superconductors which can be dealt with are those described by a mean-field BdG Hamiltonian, made from spinless fermions in lower dimension (1D and 2D). The simplest model of 1D spinless p -wave superconductor is due to Kitaev [35], in which Majorana zero-modes appear in a simple way. If a discrete 1D lattice is considered, the minimum Hamiltonian (which breaks time-reversal symmetry because the electrons are not spin degenerate) describing that system is [2]

$$\hat{H} = -\mu \sum_x \hat{c}_x^\dagger \hat{c}_x - \frac{1}{2} \left(t \hat{c}_x^\dagger \hat{c}_{x+1} + \Delta e^{i\phi} \hat{c}_x \hat{c}_{x+1} + \text{h.c.} \right), \quad (3.11)$$

where t represents the chance that a particle “hops” from one point to another in the system, $\Delta \geq 0$ is the p -wave pairing amplitude, ϕ is a superconducting phase, and h.c. stands for hermitian conjugate. To get a better insight into the behaviour of the system, the Hamiltonian can be expressed in reciprocal space by performing a Fourier transform. Introducing the two-component spinor $\Psi_{\mathbf{k}}^\dagger = \begin{bmatrix} \hat{c}_{\mathbf{k}}^\dagger & \hat{c}_{-\mathbf{k}} \end{bmatrix}$, the problem can be rewritten under the form

$$\hat{H} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \hat{H}(\mathbf{k}) \Psi_{\mathbf{k}}, \quad \text{with} \quad \hat{H}(\mathbf{k}) = \begin{bmatrix} \xi_{\mathbf{k}} & \tilde{\Delta}_{\mathbf{k}}^* \\ \tilde{\Delta}_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{bmatrix}, \quad (3.12)$$

where the kinetic energy $\xi_{\mathbf{k}}$ takes the form $\xi_{\mathbf{k}} = -\mu - t \cos k$, and where $\tilde{\Delta}_{\mathbf{k}} = -i\Delta e^{i\phi} \sin k$ is the Fourier transform of the pairing potential. As can be seen, the pairing potential is an odd function of the wavevector, as expected: indeed, in the case of a p -wave pairing (i.e. spin triplet state), there is a symmetry in the spin configuration. The Pauli principle imposing an antisymmetric behaviour of the wavefunction, the odd character has to come from the pairing potential. Using a BdG transformation, the Hamiltonian can be written under a diagonal form (up to a constant)

$$\hat{H} = \sum_{\mathbf{k}} E_{\text{bulk}}(\mathbf{k}) \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}},$$

where

$$\hat{a}_{\mathbf{k}} = u_{\mathbf{k}}\hat{c}_{\mathbf{k}} + v_{\mathbf{k}}\hat{c}_{\mathbf{k}}^{\dagger}, \quad \text{with} \quad \begin{cases} u_{\mathbf{k}} &= \frac{\tilde{\Delta}}{|\tilde{\Delta}|} \frac{\sqrt{E_{\text{bulk}} + \epsilon}}{\sqrt{2E_{\text{bulk}}}} \\ v_{\mathbf{k}} &= \left(\frac{E_{\text{bulk}} - \epsilon}{\tilde{\Delta}}\right) u_{\mathbf{k}} \end{cases} \quad \text{and} \quad E_{\text{bulk}} = \sqrt{\xi_{\mathbf{k}}^2 + |\tilde{\Delta}_{\mathbf{k}}|^2}.$$

The BdG Hamiltonian in (3.12) is particle-hole symmetric, in the sense that for each solution with an energy ϵ , there exist a solution with an energy $-\epsilon$. In Kitaev's work [35], the creation and annihilation operators are rewritten as a linear combination of new creation and annihilation operators, leading to the expressions

$$\hat{c}_i = \frac{e^{-i\phi/2}}{2}(\hat{\gamma}_{i,A} + i\hat{\gamma}_{i,B}) \quad \text{and} \quad \hat{c}_i^{\dagger} = \frac{e^{i\phi/2}}{2}(\hat{\gamma}_{i,A} - i\hat{\gamma}_{i,B})$$

where the new operators are the Majorana operators at site i . Using the standard anticommutation rules for fermionic operators, it is found that the new operators satisfy

$$\{\hat{\gamma}_{i,A}, \hat{\gamma}_{j,B}\} = 2\delta_{ij}\delta_{AB}, \quad \hat{\gamma}_{i,A} = \hat{\gamma}_{i,A}^{\dagger}, \quad \text{and} \quad \hat{\gamma}_{i,A}^2 = \left(\hat{\gamma}_{i,A}^{\dagger}\right)^2,$$

which shows that a Majorana fermion is its own antifermion (because the creation and annihilation operators are equal), and the last relation indicates that Majorana fermions are not submitted to Pauli's principle. In fact, it is even difficult to think of occupation of a Majorana mode, since a Majorana fermion is its own anti-particle. If we try to define a number operator, the result will always be 1, i.e. $\hat{n}_i^{\text{MF}} = \hat{\gamma}_{i,A}^{\dagger}\hat{\gamma}_{i,A} = 1$.

With the definition of the Majorana operators, the Hamiltonian in (3.11) can be rewritten under the form [2]

$$\hat{H} = -\frac{\mu}{2} \sum_x (1 + i\hat{\gamma}_{x,B}\hat{\gamma}_{x,A}) - \frac{i}{4} \sum_x [(\Delta + t)\hat{\gamma}_{x,B}\hat{\gamma}_{x+1,A} + (\Delta - t)\hat{\gamma}_{x,A}\hat{\gamma}_{x+1,B}].$$

It is often the case that the parameters μ , Δ and t induce complex couplings between the Majorana modes; however, the picture can be simplified in two cases.

First simplifying case

The first simplifying case occurs for $\mu \neq 0$ and $\Delta = t = 0$. In that case, the Hamiltonian of the system takes the form (discarding the constant term, which only introduces a shift in the energies)

$$\hat{H} = -i\frac{\mu}{2} \sum_x \hat{\gamma}_{x,B}\hat{\gamma}_{x,A}.$$

That expression shows that there is a coupling only between Majorana modes $\hat{\gamma}_{x,A}$ and $\hat{\gamma}_{x,B}$ at the same site, as schematically shown in figure 3.5.

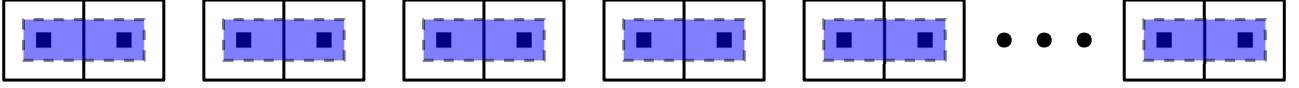


Figure 3.5 – Schematic representation of pairs of Majorana modes in the case $\mu \neq 0$, $\Delta = t = 0$. As can be seen, no modes are unpaired.

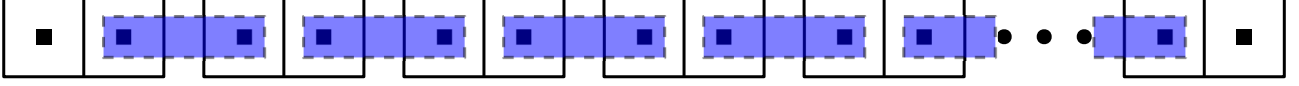


Figure 3.6 – Schematic representation of pairs of Majorana modes in the case $\mu = 0$, $\Delta = t \neq 0$. As can be seen, Majorana modes on adjacent sites are coupled, leading to two unpaired modes at the edges of the system.

Second simplifying case

The second simplifying case corresponds to the case $\mu = 0$, $\Delta = t \neq 0$. In that case, the Hamiltonian of the system takes the form

$$\hat{H} = -i\frac{t}{2} \sum_x \hat{\gamma}_{x,B} \hat{\gamma}_{x+1,A},$$

which couples Majorana modes at adjacent sites, as illustrated in figure 3.6. An interesting point is that the two edge modes are unpaired, which is very interesting: those two unpaired modes could be combined together to form an ordinary (even if highly nonlocal) fermion.

The nonlocal fermion can be written as $\hat{f} = \frac{1}{2}(\hat{\gamma}_1 + i\hat{\gamma}_2)$, and costs zero energy since the operators appearing in the definition of $\hat{f}$ are absent from the Hamiltonian. Moreover, it induces a two-fold degeneracy of the ground state: if $|0\rangle$ is a ground state satisfying $\hat{f}|0\rangle = 0$, then the condition $|1\rangle = \hat{f}^\dagger|0\rangle$ has to be a ground state as well. This nonlocal pairing can give a physical intuition about the stability of the new pair: as the Majorana modes are located “far” apart from each other, a local perturbation of one of the modes cannot destroy the pairing, meaning that it is somehow protected or, to make a link with the previously introduced vocabulary, they are somehow topologically protected from destruction.

3.3.2 p -wave superconductors in 2D: the $p_x + ip_y$ case

The discussion on topological p -wave superconductor can be considered in two dimensions. The best example of topological superconductor is then the chiral $p_x + ip_y$ superconductor, which exhibit Majorana modes in vortices (rather than on edge states, as was the case in 1D). In order to be able to have a very clear picture of the situation, a lattice model of the superconductor

will be considered, which is described by the Hamiltonian [9]

$$\begin{aligned} \hat{H} = \sum_{m,n} \{ & -t(\hat{c}_{m+1,n}^\dagger \hat{c}_{m,n} + \text{h.c.}) - t(\hat{c}_{m,n+1}^\dagger \hat{c}_{m,n} + \text{h.c.}) - (\mu - 4t)\hat{c}_{m,n}^\dagger \hat{c}_{m,n} \} \\ & + \sum_{m,n} \{ (\Delta \hat{c}_{m+1,n}^\dagger \hat{c}_{m,n}^\dagger + \Delta^* \hat{c}_{m,n} \hat{c}_{m+1,n}) + (i\Delta \hat{c}_{m,n+1}^\dagger \hat{c}_{m,n}^\dagger - i\Delta^* \hat{c}_{m,n} \hat{c}_{m+1,n}) \}. \end{aligned} \quad (3.13)$$

For simplicity, the lattice constant a has been set equal to unity. As can be seen in the previous Hamiltonian, the coupling is not onsite, hence the pairing term will have a momentum dependence. Using a BdG transformation and using a two-component spinor of the form $\Psi_{\mathbf{k}} = [\hat{c}_{\mathbf{k}} \quad \hat{c}_{-\mathbf{k}}^\dagger]$, the Hamiltonian expressed in reciprocal space can be written under

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \begin{bmatrix} \xi_{\mathbf{k}} & 2i\Delta(\sin k_x + i \sin k_y) \\ -2i\Delta^*(\sin k_x + i \sin k_y) & -\xi_{\mathbf{k}} \end{bmatrix} \Psi_{\mathbf{k}}.$$

From the 1D case, it can be expected that the Hamiltonian appearing in (3.13) has different behaviours depending on the relative values of Δ , t , and μ . To see those different phases, a gauge transformation of the form $\hat{c}_{\mathbf{k}} \rightarrow e^{i\theta/2} \hat{c}_{\mathbf{k}}$, with $\Delta = |\Delta|e^{i\theta}$ can be made, which allows to rewrite the Hamiltonian under the form

$$\hat{H} = (2 - \mu - \cos k_x - \cos k_y)\tau_z - 2|\Delta| \sin k_x \tau_y - 2|\Delta| \sin k_y \tau_x.$$

If $|\Delta| \neq 0$, the Hamiltonian has several gapped superconducting phases, separated by gapless critical points [9]. To see this, a chemical potential varying in space can be considered on a disc of radius R , which definition is

$$\mu(r) = \begin{cases} \mu < 0, & \text{for } r < R \\ \mu > 0, & \text{for } r < R \end{cases}$$

for which it is known that a single branch of Majorana modes is located on the circumference of the disc at $r = R$ [9], which looks odd since, due to particle-hole symmetry in superconductors, a solution to a BdG Hamiltonian with energy ϵ should have a corresponding solution with energy $-\epsilon$, hence at 0 energy there should be 2 (degenerated) solutions. This apparent inconsistency is lifted if by the fact that in $\mathbb{R}^2$, any closed interface cannot host Majorana zero modes [64]. This can be seen by considering the transformation

$$\hat{\gamma}_{\mathbf{k}}^\dagger = e^{i\theta/2} u(\mathbf{k}) \hat{c}_{\mathbf{k}}^\dagger + e^{-i\theta/2} v(\mathbf{k}) \hat{c}_{\mathbf{k}},$$

where θ is the phase of the order parameter. It is directly seen from that relation that when the order parameter is rotated by 2π , $\hat{\gamma}_{\mathbf{k}}^\dagger$ transforms into $-\hat{\gamma}_{\mathbf{k}}^\dagger$, indicating *antiperiodic* boundary conditions for the quasiparticle wavefunction. The trick to have Majorana zero mode on the boundary of the disk is to shift from antiperiodic boundary condition to a periodic one. This

change in boundary condition can be realised by applying an external magnetic field to the disk, because it will give a Aharonov-Bohm π -phase to the edge fermionic states [9, 64].

In a superconductor, a π -flux (i.e. a quantum of flux $h/2e$) causes a 2π winding of the order parameter and creates a vortex. The application of an external magnetic field also leads to the creation of Majorana zero modes, hence it is expected to have trapped Majorana modes in the vortices of spinless 2D p -wave superconductors. Thus, if two vortices are considered, the boundary condition will again swap from periodic to antiperiodic, destroying edge states, but “vortex-core” states will be preserved, leaving a system with two Majorana zero modes. This means that in a superconductor with $2N$ well-separated vortices, the ground state in thermodynamic equilibrium will have a degeneracy of 2^N [52]. To get a clear picture of that statement, two vortices can first be considered, which give a degeneracy of 2 (coming from the combination of the Majorana states, which combine into a single fermionic state, which can be either occupied or not). Extending that reasoning, $2N$ Majorana modes form N fermionic states (giving a degeneracy of 2^N), which can be broken up into the subspace of 2^{N-1} states with even/odd fermion parity [9]. The statistics of those vortices, hence the Majorana modes, will now be discussed, as it is of direct importance for quantum computations applications [51].

3.3.3 Vortices statistics and Majorana fermions braiding

Since vortices in topological superconductors can host Majorana fermions, they exhibit non-Abelian statistics, which could be used to make reliable solid-state qubits [41, 51, 57, 63]. The idea behind non-Abelian (exchange) statistics can be understood simply if a group of three particles is considered. If the particles 1 and 2 are first exchanged, followed by the exchange of particle 2 and 3, or if particles 2 and 3 are first exchanged, followed by the exchange of 1 and 2, the final outcome will be different, as shown in figure 3.7.



Figure 3.7 – Graphical representation of a non-Abelian exchange between three particles.

The graphical representation given in figure 3.7 is, as stated, an example. In the physical systems of concern in this work, the particles are undistinguishable, hence there is no numbering of the different components. Moreover, the non-Abelian statistics which applies to the vortices in chiral superconductors is intimately linked to their two-dimensional nature: in one and three dimensions, particles are either bosons or fermions, not anyons. This finding comes from the fact that in 1D and 3D, when two particles are adiabatically exchanged twice, the process is equivalent to take one particle around an other adiabatically. In three dimensions, such a winding of one particle around the other is topologically equivalent to a process in which none of the particles have moved, the wavefunction corresponding to the system should be left unchanged by such an “interchange”. The only possibility for the wavefunction is the gain a $\pm$ sign, which corresponds to the exchange of two bosons (+ sign) or fermions (- sign). In the case of two-dimensional configurations, the situation is quite different [73]: when a particle loops around another one in 2D, the trajectory of that encircling particle cannot be deformed to a point without going through the other particle, which means that when two particles are interchanged in a clockwise manner, their trajectory implies a nontrivial winding, giving the possibility to the system of being in another configuration than it was in the beginning. This topological difference between 2D and 3D system was highlighted some time ago [42, 70]. A graphical representation of the exchange of Majorana fermions hosted by vortices in a 2D chiral $p_x + ip_y$ superconductor is given in figure 3.8.

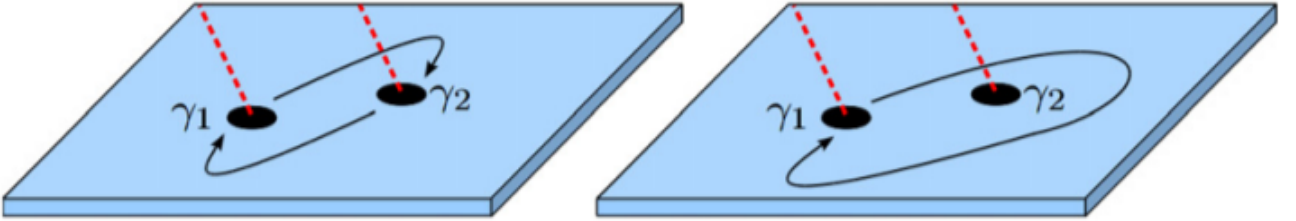


Figure 3.8 – Graphical representation of the particular exchange mechanism between particles in a two-dimensional space. The dashed lines represent the limit through which a phase jump is measured. In the left picture, vortex 1 necessarily crosses the line, while if it is wound around vortex 2, both vortices cross the line. Image from [41].

In that picture, two vortices are represented, which host Majorana fermions described by the operators $\hat{\gamma}_1$ and $\hat{\gamma}_2$. Each of these vortices is associated with a 2π winding of the superconducting phase. This phase is chosen to be single-valued everywhere, except at the location of the dashed red line in figure 3.8. The result of the clockwise vortices exchange is

$$\hat{\gamma}_1 \rightarrow -\hat{\gamma}_2, \quad \text{and} \quad \hat{\gamma}_2 \rightarrow +\hat{\gamma}_1,$$

which can be described by the braiding operator $\hat{B}_{12}$ such that $\hat{\gamma}_i \rightarrow \hat{B}_{12}\hat{\gamma}_i\hat{B}_{12}^\dagger$, which expression is given by [41]

$$\hat{B}_{12} = \frac{1}{\sqrt{2}}(1 + \hat{\gamma}_1\hat{\gamma}_2).$$

If an anti-clockwise exchange was instead considered, the result of the exchange would have been $\hat{\gamma}_1 \rightarrow \hat{\gamma}_2$ and $\hat{\gamma}_2 \rightarrow -\hat{\gamma}_1$, hence the braiding operator would have had the form $\hat{B}_{12} = (1 - \hat{\gamma}_1 \hat{\gamma}_2)/\sqrt{2}$. Moreover, if the “cutting lines” in figure 3.8 had been chosen differently, the expression of the operators could have been different, but it does not matter as long as a convention is chosen and stuck to.

In the case where one vortex is swung around another one and brought back to its original position, the situation is different but topologically equivalent to two successive exchanges. The associated braiding operator is then given by $\hat{B}_{12}^2 = \hat{\gamma}_1 \hat{\gamma}_2$, which leads to the transformation

$$\begin{aligned}\hat{\gamma}_1 &\rightarrow (\hat{\gamma}_1 \hat{\gamma}_2) \hat{\gamma}_1 (\hat{\gamma}_1 \hat{\gamma}_2)^\dagger = -\hat{\gamma}_1, \\ \hat{\gamma}_2 &\rightarrow (\hat{\gamma}_1 \hat{\gamma}_2) \hat{\gamma}_2 (\hat{\gamma}_1 \hat{\gamma}_2)^\dagger = -\hat{\gamma}_2,\end{aligned}$$

which shows that bringing one vortex around another one, and back to its original location introduces a “-” sign into each Majorana operator. A graphical representation of that situation is sketched in the right part of figure 3.8, where it is clear that each vortex crosses the cutting line, hence each get a phase shift of π .

Coupling between magnetism and superconductivity

In the previous chapter, it was stated that magnetism and superconductivity were not really compatible, since magnetism as the tendency to destroy the Cooper pairs making up the superconductor. It was also stated that topological quantum computing applications could be realised thanks to the Majorana fermions hosted in the vortices of 2D chiral p -wave superconductors. In 2016, it was shown by G. Yang *et al.* [75] that skyrmions with an even azimuthal winding number can bind a zero-mode Majorana fermion in their core. To check the parameter range in which a coupling between a superconductor and a skyrmion can effectively host a Majorana fermion, a tight-binding code can be used.

4.1 Motivation

Basically, the job of every condensed-matter physicist is to find the eigenvalues and eigenvectors of the Hamiltonian

$$\hat{\mathcal{H}}_{\text{tot}} = \hat{\mathcal{T}}_e + \hat{\mathcal{T}}_N + \hat{\mathcal{V}}_{ee} + \hat{\mathcal{V}}_{eN} + \hat{\mathcal{V}}_{NN}, \quad (4.1)$$

where the terms represents, from left to right, the kinetic energy of the electrons and ions, the electron-electron, electron-ion, and ion-ion interactions. The expression of these terms read

$$\begin{aligned} \hat{\mathcal{T}}_e &= -\frac{\hbar^2}{2m_e} \sum_{i=1}^{n_e} \nabla_{\mathbf{r}_i}^2, & \hat{\mathcal{V}}_{ee} &= \frac{e^2}{8\pi\epsilon_0} \sum_{i=1}^{n_e} \sum_{i'=1}^{n_e} \frac{1}{\|\mathbf{r}_i - \mathbf{r}_{i'}\|}, \\ \hat{\mathcal{T}}_N &= -\sum_{I=1}^{N_I} \frac{\hbar^2}{2m_I} \nabla_{\mathbf{R}_I}^2, & \hat{\mathcal{V}}_{eN} &= -\frac{e^2}{8\pi\epsilon_0} \sum_{i=1}^{n_e} \sum_{I=1}^{N_I} \frac{Z_I}{\|\mathbf{r}_i - \mathbf{R}_I\|}, \\ & & \hat{\mathcal{V}}_{NN} &= \frac{e^2}{8\pi\epsilon_0} \sum_{I=1}^{N_I} \sum_{I'=1}^{N_I} \frac{Z_I Z_{I'}}{\|\mathbf{R}_I - \mathbf{R}_{I'}\|}. \end{aligned}$$

In those expressions, the sums over small letters (i for instance) indicate sums over electrons (which have a position given by $\mathbf{r}_i$), while sums over capital letters (I for instance), indicate sums over ions (which have a position given by $\mathbf{R}_I$). n_e , N_I , Z_I , e , and ϵ_0 represent the total number of electrons, the total number of ions, their atomic number, the fundamental electric charge, and the vacuum permittivity, respectively.

Obviously, finding the eigenvalues and corresponding eigenvectors for the total Hamiltonian (4.1) is extremely difficult, hence simplifications have to be introduced. The first one is the so-called Born-Oppenheimer (BO) approximation, originating from the big mass difference between electrons and ions, which is valid if phonons are not important. If the BO approximation can be applied, the ionic positions $\mathbf{R}_I$ are supposed fixed, and enter as simple parameters in the electronic Hamiltonian

$$\hat{\mathcal{H}}_e = \hat{\mathcal{T}}_e + \hat{\mathcal{V}}_{ee} + \hat{\mathcal{V}}_{eN}.$$

Finding the eigenvalues and corresponding eigenvectors that electronic Hamiltonian is possible thanks to techniques such as DFT calculations, which lie at the basis of most *ab-initio* codes, such as ABINIT.

DFT calculations lead to incredibly accurate results since very few assumptions are made. The drawback of those methods is that, even if satisfactory results are found, they are very time- and resource-demanding. To get rid of that difficulty, artefacts exist, such as the parametrised tight-binding method, in which only a few parameters are required (generally provided by DFT computations) to run computations leading to qualitative results. This motivates its use in atomistic simulations.

4.2 Tight-binding

4.2.1 General formalism

The idea of a tight-binding (TB) description of a problem is to describe the wavefunction of the system as a combination of localised function, usually chosen to be atomic orbitals or Wannier functions. The total energy contained in the system is described by the Hamiltonian $\hat{\mathcal{H}}_{\text{tot}}$, given in (4.1). The one-electron Hamiltonian is the sum of a kinetic energy $\hat{\mathcal{T}}$ and of atomic potentials $\hat{\mathcal{V}}_{n,i}^{\text{atomic}}$. Its expression reads

$$\hat{\mathcal{H}} = \hat{\mathcal{T}} + \sum_{n,i} \hat{\mathcal{V}}_{n,i}^{\text{atomic}}. \quad (4.2)$$

In the TB formalism using atomic orbitals, the total wavefunction of the system is given by

$$|\Psi\rangle = \sum_{n,i,\lambda} c_{ni\lambda} |n, i, \lambda\rangle, \quad (4.3)$$

where n indicates the n^{th} unit cell, given by a Bravais vector $\mathbf{r}_n$, where i indicates the i^{th} atom in the unit cell n , located at position $\boldsymbol{\tau}_i$, and where λ is the orbital of that atom. A schematic representation of the system is given in figure 4.1.

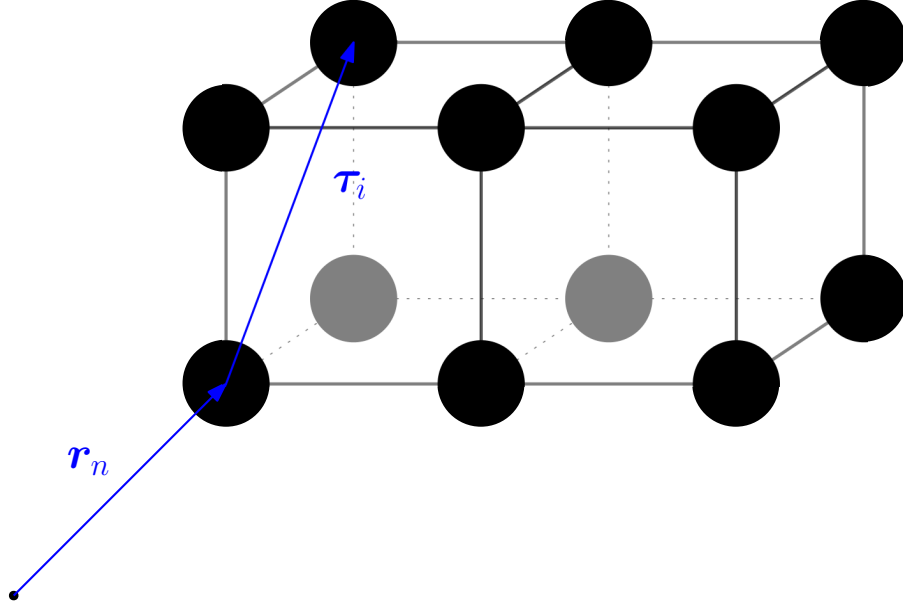


Figure 4.1 – Schematic representation of the system composed of unit cells (marked by a Bravais vector $\mathbf{r}_n$), and atoms in it (marked by a vector $\mathbf{\tau}_i$).

The matrix representation of the one-electron Hamiltonian (4.2) in the basis on which the wavefunction (4.3) is developed is given by the expression

$$\begin{aligned}
 [\mathbf{H}]_{n,i,\lambda}^{m,j,\mu} &= \langle m, j, \mu | \hat{\mathcal{H}} | n, i, \lambda \rangle = \langle m, j, \mu | \hat{\mathcal{T}} + \sum_{p,k} \hat{\mathcal{V}}_{p,k} | n, i, \lambda \rangle \\
 &= \epsilon_{n,i} [\mathbf{S}]_{m,j,\mu}^{n,i,\lambda} + \langle m, j, \mu | \sum_{p \neq n} \hat{\mathcal{V}}_{p,i} | n, i, \lambda \rangle + \langle m, j, \mu | \sum_{k \neq i} \hat{\mathcal{V}}_{n,k} | n, i, \lambda \rangle \\
 &\quad + \langle m, j, \mu | \sum_{\substack{p \neq n \\ k \neq i}} \hat{\mathcal{V}}_{p,k} | n, i, \lambda \rangle,
 \end{aligned} \tag{4.4}$$

where $\epsilon_{n,i}$ is the atomic energy for an electron in the i^{th} atom in the n^{th} unit cell, $[\mathbf{S}]_{m,j,\mu}^{n,i,\lambda} = \langle m, j, \mu | n, i, \lambda \rangle$ the overlap matrix, and where the three last terms correspond to the potential matrix. With those definitions, the Schrödinger equation for the complete system can be solved,

which reads

$$\begin{aligned}
\hat{\mathcal{H}}|\Psi\rangle = E|\Psi\rangle &\Rightarrow \langle\Psi|\hat{\mathcal{H}}|\Psi\rangle = E\langle\Psi|\Psi\rangle \\
&\Leftrightarrow \sum_{\substack{n,i,\lambda \\ n',i',\lambda'}} c_{n',i',\lambda'}^* c_{n,i,\lambda} \langle n',i',\lambda'|\hat{\mathcal{H}}|n,i,\lambda\rangle = E \sum_{\substack{n,i,\lambda \\ n',i',\lambda'}} c_{n',i',\lambda'}^* c_{n,i,\lambda} \langle n',i',\lambda'|n,i,\lambda\rangle \\
&\Leftrightarrow \sum_{\substack{n,i,\lambda \\ n',i',\lambda'}} c_{n',i',\lambda'}^* c_{n,i,\lambda} [\mathbf{H}]_{n',i',\lambda'}^{n,i,\lambda} = E \sum_{\substack{n,i,\lambda \\ n',i',\lambda'}} c_{n',i',\lambda'}^* c_{n,i,\lambda} [\mathbf{S}]_{n',i',\lambda'}^{n,i,\lambda}.
\end{aligned}$$

This last expression can be rewritten in a matrix form as

$$\mathbf{c}^* \cdot [\mathbf{H}] \cdot \mathbf{c} = E \mathbf{c}^* \cdot [\mathbf{S}] \cdot \mathbf{c},$$

where $\mathbf{c}$ is the vector containing all the $c_{n,i,\lambda}$ coefficients appearing in (4.3). This last expression shows that the tight-binding formalism can be written under the form

$$[\mathbf{H}] \cdot \mathbf{c} = E \cdot [\mathbf{S}] \cdot \mathbf{c}.$$

An equivalent relation in reciprocal space can be obtained thanks to Bloch's theorem, by the application of which the basis functions take the form

$$|\Psi_{i,\lambda}(\mathbf{k})\rangle = \frac{1}{\sqrt{N}} \sum_n e^{i\mathbf{k}\cdot(\mathbf{r}_n+\boldsymbol{\tau}_i)} |n,i,\lambda\rangle,$$

where N is the number of unit cells considered in the system. The wavefunction describing the system can then be rewritten under the form

$$|\Psi(\mathbf{k})\rangle = \sum_{i,\lambda} c_{i,\lambda}^{(\alpha)}(\mathbf{k}) |\Psi_{i,\lambda}(\mathbf{k})\rangle = \frac{1}{\sqrt{N}} \sum_{n,i,\lambda} c_{i,\lambda}^{(\alpha)}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_n+\boldsymbol{\tau}_i)} |n,i,\lambda\rangle, \quad (4.5)$$

where the coefficients in (4.3) and (4.5) are linked through the relation $c_{ni\lambda} = \frac{1}{\sqrt{N}} c_{i,\lambda}^{(\alpha)}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_n+\boldsymbol{\tau}_i)}$. Applying the same developments as previously, it can be shown that the final equation to solve has the form [7]

$$[\mathbf{H}(\mathbf{k})] \cdot \mathbf{c}^{(\alpha)}(\mathbf{k}) = \epsilon_\alpha(\mathbf{k}) [\mathbf{S}(\mathbf{k})] \cdot \mathbf{c}^{(\alpha)}(\mathbf{k}),$$

where $\epsilon_\alpha(\mathbf{k})$ is the so-called bandstructure of the crystal.

The expression of the Hamiltonian matrix elements, $[\mathbf{H}]_{n,i,\lambda}^{m,j,\mu}$, have to be determined. These elements can be split into different components, namely (i) on-site elements, or diagonal matrix elements, where both unit cell and atomic positions are equal, and (ii) off-site, or off-diagonal matrix elements, where either or both unit cells and atomic positions are different.

On-site elements are elements of type $[\mathbf{H}]_{n,i,\lambda}^{n,i,\mu}$, take the form

$$\begin{aligned}
[\mathbf{H}]_{n,i,\lambda}^{n,i,\mu} &= \langle n, i, \mu | \hat{\mathcal{H}} | n, i, \lambda \rangle \\
&= \langle n, i, \mu | \hat{\mathcal{T}} + \hat{\mathcal{V}}_{n,i} | n, i, \lambda \rangle + \langle n, i, \mu | \sum_{p \neq n} \hat{\mathcal{V}}_{p,i} + \sum_{k \neq i} \hat{\mathcal{V}}_{n,k} + \sum_{\substack{p \neq n \\ k \neq i}} \hat{\mathcal{V}}_{p,k} | n, i, \lambda \rangle \\
&= \epsilon_{n,i}^{\text{atomic}} \delta_{\mu,\lambda} + \underbrace{\sum_{p \neq n} \langle n, i, \mu | \hat{\mathcal{V}}_{p,i} | n, i, \lambda \rangle + \sum_{k \neq i} \langle n, i, \mu | \hat{\mathcal{V}}_{n,k} | n, i, \lambda \rangle + \sum_{\substack{p \neq n \\ k \neq i}} \langle n, i, \mu | \hat{\mathcal{V}}_{p,k} | n, i, \lambda \rangle}_{\text{crystal field}},
\end{aligned} \tag{4.6}$$

where $\delta_{\mu,\lambda}$ is the Kronecker index, indicating that orbitals of a same atom are orthogonal.

Off-site elements are elements of type $[\mathbf{H}]_{n,i,\lambda}^{m,j,\mu}$, and their general expression was given in (4.4). For such elements, only the potential terms will be developed, since the overlap can be found in Slater-Koster tables [61]. Removing the overlap part, the off-diagonal components of the Hamiltonian read

$$\begin{aligned}
[\mathbf{H}]_{m,j,\mu}^{n,i,\lambda} &= \sum_{p \neq n} \langle m, j, \mu | \hat{\mathcal{V}}_{p,i} | n, i, \lambda \rangle + \sum_{k \neq i} \langle m, j, \mu | \hat{\mathcal{V}}_{n,k} | n, i, \lambda \rangle + \sum_{\substack{p \neq n \\ k \neq i}} \langle m, j, \mu | \hat{\mathcal{V}}_{p,k} | n, i, \lambda \rangle \\
&= \langle m, j, \mu | \hat{\mathcal{V}}_{m,i} | n, i, \lambda \rangle + \langle m, j, \mu | \hat{\mathcal{V}}_{n,j} | n, i, \lambda \rangle + \sum_{\substack{k \neq i \\ k \neq j}} \langle m, j, \mu | \hat{\mathcal{V}}_{n,k} | n, i, \lambda \rangle \\
&\quad + \sum_{\substack{p \neq n \\ p \neq m}} \langle m, j, \mu | \hat{\mathcal{V}}_{p,i} | n, i, \lambda \rangle + \sum_{\substack{p \neq n \\ k \neq i}} \langle m, j, \mu | \hat{\mathcal{V}}_{p,k} | n, i, \lambda \rangle \\
&= \langle m, j, \mu | \hat{\mathcal{V}}_{m,i} | n, i, \lambda \rangle + \langle m, j, \mu | \hat{\mathcal{V}}_{n,j} | n, i, \lambda \rangle + \langle m, j, \mu | \hat{\mathcal{V}}_{m,j} | n, i, \lambda \rangle \\
&\quad + \sum_{\substack{p \neq n \\ p \neq m}} \langle m, j, \mu | \hat{\mathcal{V}}_{p,i} | n, i, \lambda \rangle + \sum_{\substack{k \neq i \\ k \neq j}} \langle m, j, \mu | \hat{\mathcal{V}}_{n,k} | n, i, \lambda \rangle + \sum_{\substack{p \neq n, \\ k \neq i, \\ p \neq m, \\ k \neq j}} \langle m, j, \mu | \hat{\mathcal{V}}_{p,k} | n, i, \lambda \rangle
\end{aligned} \tag{4.7}$$

In the last expression, the first three terms are two-centre integrals, since the centre of the potential lies at the same location as one of the basis functions, while the last three terms are three-centre integrals, for obvious reasons.

Such relations can be derived in a similar way in reciprocal space. The biggest difference with the real space representation is the appearance of a phase factor, due to the definition of the Bloch waves. In a similar way to what was done in real space, the matrix elements for the Hamiltonian and for the overlap matrices can be defined, and their expression read

$$\begin{aligned}
[\mathbf{H}(\mathbf{k})]_{j,\mu}^{i,\lambda} &= \langle \Psi_{j,\mu}(\mathbf{k}) | \hat{\mathcal{H}} | \Psi_{i,\lambda}(\mathbf{k}) \rangle & \text{and} & \quad [\mathbf{S}(\mathbf{k})]_{j,\mu}^{i,\lambda} = \langle \Psi_{j,\mu}(\mathbf{k}) | \Psi_{i,\lambda}(\mathbf{k}) \rangle \\
&= \sum_{n,n'} e^{i\mathbf{k} \cdot (\mathbf{r}_n - \mathbf{r}_{n'} + \boldsymbol{\tau}_i - \boldsymbol{\tau}_j)} \langle n', j, \mu | \hat{\mathcal{H}} | n, i, \lambda \rangle, & & = \sum_{n,n'} e^{i\mathbf{k} \cdot (\mathbf{r}_n - \mathbf{r}_{n'} + \boldsymbol{\tau}_i - \boldsymbol{\tau}_j)} \langle n', j, \mu | n, i, \lambda \rangle.
\end{aligned}$$

Again, the matrix representation of the Hamiltonian will consist in diagonal and off-diagonal terms, which read

$$[\mathbf{H}(\mathbf{k})]_{i,\mu}^{i,\lambda} = \langle \Psi_{i,\mu}(\mathbf{k}) | \hat{\mathcal{H}} | \Psi_{i,\lambda}(\mathbf{k}) \rangle \quad \text{and,} \quad [\mathbf{H}(\mathbf{k})]_{j,\mu}^{i,\lambda} = \langle \Psi_{j,\mu}(\mathbf{k}) | \hat{\mathcal{H}} | \Psi_{i,\lambda}(\mathbf{k}) \rangle$$

respectively. The first ones, the diagonal terms, correspond to on-site energies, while the second ones, the off-diagonal terms, correspond to hopping energies. From those different definitions, different quantities can be computed. An example of one such quantity is the dispersion relation, given

$$\begin{aligned} \hat{\mathcal{H}} |\Psi(\mathbf{k})\rangle &= E(\mathbf{k}) |\Psi(\mathbf{k})\rangle \quad \Rightarrow \quad \langle \Psi(\mathbf{k}) | \hat{\mathcal{H}} | \Psi(\mathbf{k}) \rangle = E(\mathbf{k}) \langle \Psi(\mathbf{k}) | \Psi(\mathbf{k}) \rangle \\ &\Leftrightarrow E(\mathbf{k}) = \frac{\langle \Psi(\mathbf{k}) | \hat{\mathcal{H}} | \Psi(\mathbf{k}) \rangle}{\langle \Psi(\mathbf{k}) | \Psi(\mathbf{k}) \rangle}. \end{aligned}$$

4.2.2 Some simplifications

The previous definitions, even if very general, are cumbersome and difficult to use. It is therefore necessary to somehow simplify their expressions. First of all, a very common approach in solving a problem governed by matrices of the form (4.6) and (4.7) is to consider only nearest neighbour (NN) interactions. Moreover, without loss of generality, a crystal with one atom per unit cell can be considered. Consequently, the second index in the kets can be discarded, i.e. go from $|n, i, \mu\rangle$ to $|n, \mu\rangle$ (for example).

If only on-site energies are kept, if the so-called two-centre approximation (which consists in ignoring all three-centre integrals) is made, and by further neglecting the crystal field, the remaining Hamiltonian gets a relatively easy form, featuring only on-site energies, and hopping terms [24]. Its expression can be written under the form

$$\hat{\mathcal{H}} = \sum_{i,\alpha} (\epsilon_{i\alpha} - \mu_i) \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} - \sum_{\substack{i,j \\ \alpha,\beta}} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\beta}, \quad (4.8)$$

where μ_i is the chemical potential of atom i , and $t_{ij}^{\alpha\beta}$ is the hopping parameter between orbital α of atom i and orbital β of atom j . In that expression, the spin of the electrons can also be taken into account, leading to a model in which magnetism can be taken into account. A detailed transition between the general Hamiltonian (4.4) and the simplified one (4.8) can be found in [47], where spin is taken into account.

4.3 Some electronic properties

4.3.1 The Fermi and band energies

The first (very important) quantity that can be computed is the Fermi energy, which determines the total number of electrons in the system. By definition, if $\epsilon_{\mathbf{k},n}$ represents the energy at $\mathbf{k}$ for

the n^{th} level, and if N represents the total number of electrons in the system, the Fermi energy ϵ_F is defined as

$$N = \sum_{n,\mathbf{k}} f(\epsilon_{\mathbf{k},n}, \epsilon_F),$$

where $f(\epsilon_{\mathbf{k},n}, \epsilon_F)$ is the Fermi-Dirac distribution. From there, the total energy of a band can be computed according to the relation

$$E_{\text{band}} = \sum_{n,\mathbf{k}} \epsilon_{\mathbf{k},n} f(\epsilon_{\mathbf{k},n}, \epsilon_F).$$

Those band energies can be put on the same diagram as a function of the wave vector $\mathbf{k}$, leading to what is known as band diagrams. The bandstructure of the most common crystallographic structures (shown with their first Brillouin zone (1BZ) representation in figure 4.2) are given in figure 4.3. In that figure, the first row correspond to a SC crystal in 1D, 2D, and 3D, respectively, while the second row corresponds to a BCC, FCC, and HCP crystal, respectively. Moreover, in the case of a SC configuration, a comparison between a numerical computation of the band diagram and analytical results is given.

4.3.2 The density of states

The density of states (DOS) indicates the repartition of the electrons across the different energy levels. By definition, its expression reads

$$D(\epsilon) = \sum_{n,\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k},n}).$$

More than the total DOS, a partial one can be defined [55]. For instance, the partial DOS of the j^{th} atom in the basis in the orbital μ is given by the expression

$$D_{j\mu}(\epsilon) = \sum_{n,\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k},n}) \langle \Psi_{nj\mu}(\mathbf{k}) | [\mathbf{S}] | \Psi_{nj\mu}(\mathbf{k}) \rangle.$$

4.3.3 Charges

The charge of the j^{th} atom in the μ^{th} orbital can be computed according to

$$n_{j,\mu}^{\text{Müll}} = 2 \sum_{n,\mathbf{k}} f(\epsilon_{\mathbf{k},n}, \epsilon_F) \langle \Psi_{nj\mu}(\mathbf{k}) | [\mathbf{S}] | \Psi_{nj\mu}(\mathbf{k}) \rangle,$$

where the factor 2 arises because of spin degeneracy in this case. obviously, these partial charges have to fulfil the charge-conservation condition, i.e.

$$N = \sum_{j,\mu} n_{j,\mu}^{\text{Müll}}.$$

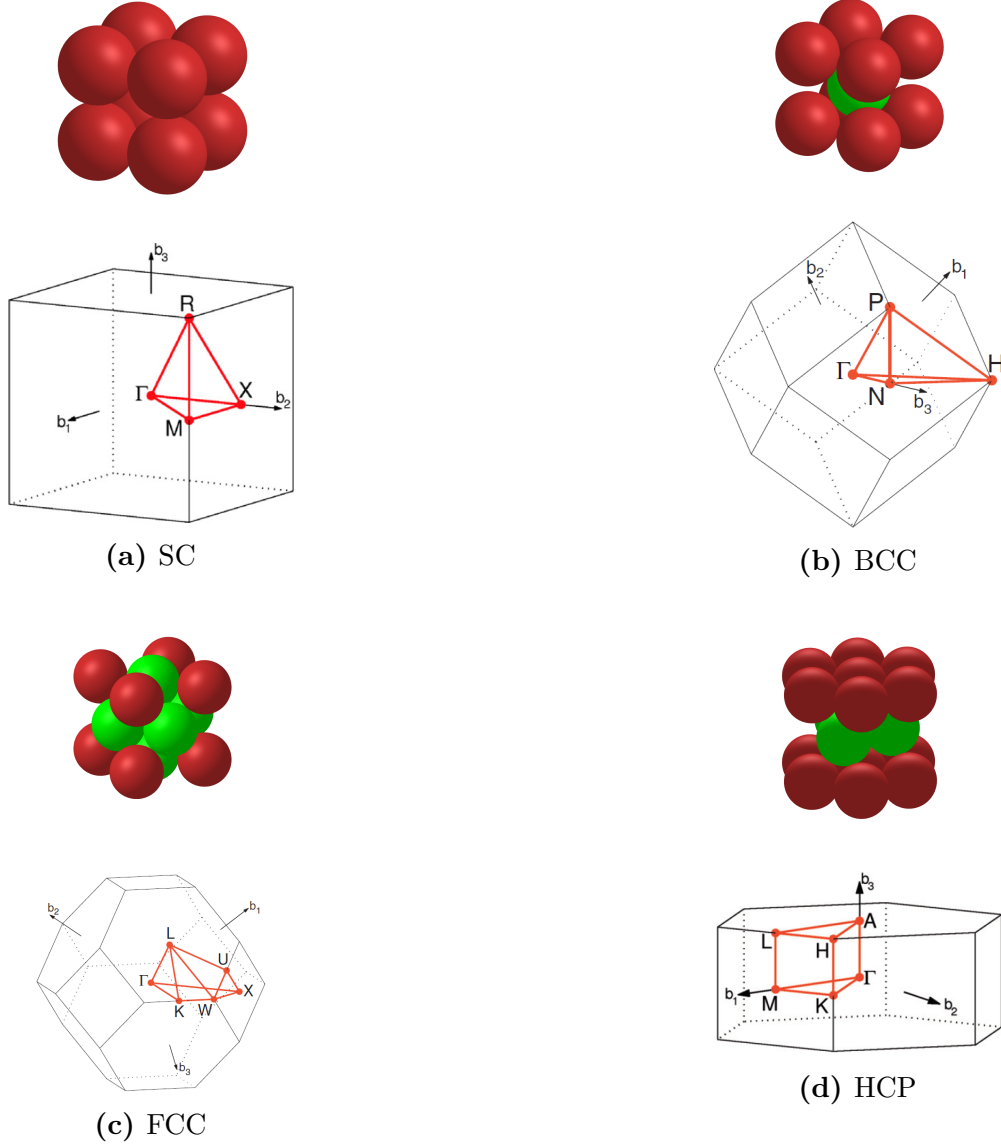


Figure 4.2 – Schematic representation of the most common crystallographic configurations (upper row), and the corresponding 1BZ representation (lower row). SC stands for simple cubic, BCC for body-centered cubic, FCC for face-centered cubic, and HCP for hexagonal close-packed. The 1BZ images are from [58].

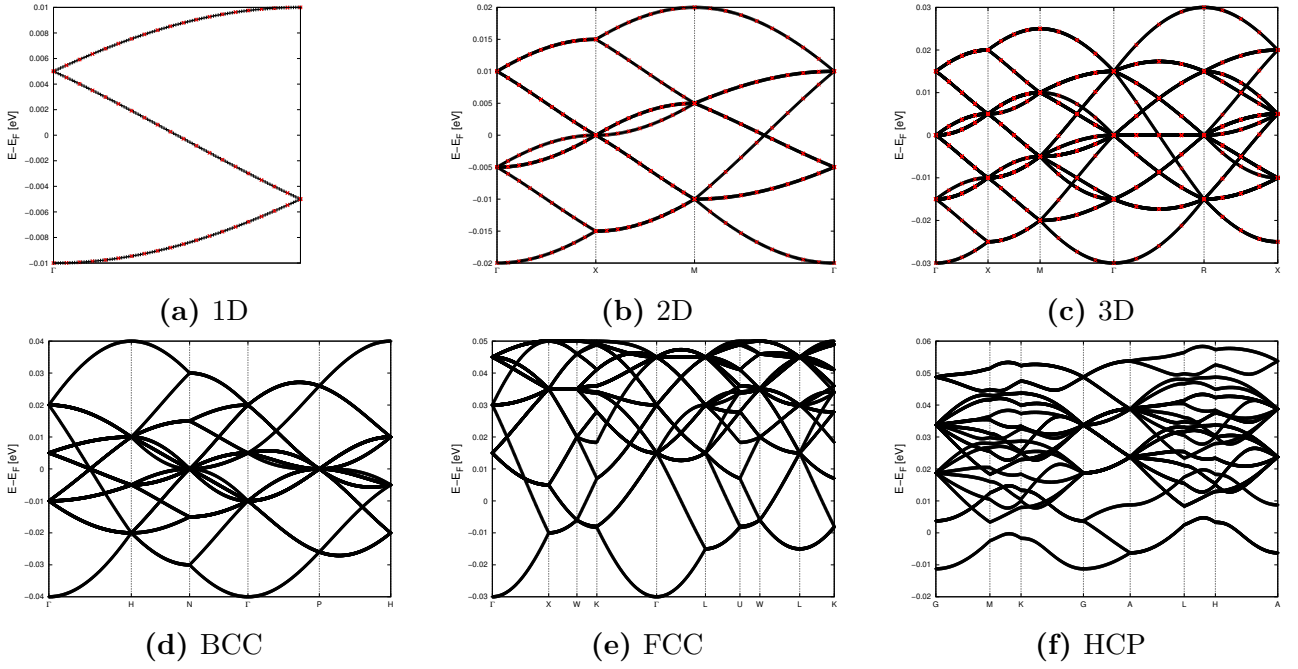


Figure 4.3 – Bandstructure of a SC crystal (top row, in 1D, 2D, and 3D, from left to right), and of a BCC, FCC, and HCP (second row, from left to right) crystal. In the case of a SC arrangement, a comparison between numerical result (black) and analytic results (in red) are given, showing a very good agreement. The computations were carried out with $N_{\text{cell}} = 3$ in 1D, $N_{\text{cell}} = 3 \times 3$ in 2D, and $N_{\text{cell}} = 3 \times 3 \times 3$ in 3D.

4.4 Magnetism and superconductivity: the interplay

In traditional theories, magnetism is due to localised electrons, while superconductivity is linked to delocalised electrons forming Cooper pairs, hence the two concepts are not compatible at first sight. However, a model in which these two types of electrons coexist can be imagined. If the localised electrons are *d*-type and the delocalised ones *s*-type, the model is called *s-d* model and, in its simplest form, is represented by a lattice Kondo Hamiltonian of the form [20, 33, 77, 78, 79, 80]

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + J_{sd} \sum_j \mathbf{m}_j \cdot \hat{c}_{j\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{j\beta}. \quad (4.9)$$

In that expression, the localised electrons are modelled by a classical magnetic moment $\mathbf{m}$, while the delocalised ones are modelled through the vector of Pauli matrices $\boldsymbol{\sigma}$. A graphical representation of the model is given in figure 4.4, where the *s*-electrons are represented as a kind of “gas” spanning the whole system, while the *d*-electrons are located at the lattice sites.

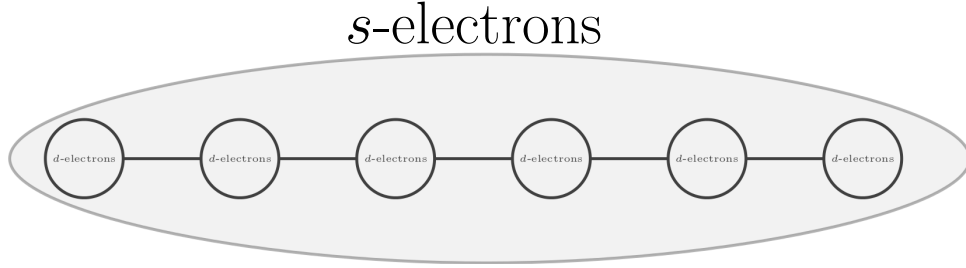


Figure 4.4 – Graphical representation of a model in which localised *d*-electrons are coupled to delocalised *s*-electrons (modelled as a “gas” spanning the whole system).

In order to be fully able to model the interplay between magnetism and superconductivity, the model has, however, to be complexioned a little: first, a TB version of superconductors Hamiltonian has to be found. From there, it has to be added to the Hamiltonian describing different magnetisation textures (such as spin spirals, merons, skyrmions, etc.). Once the Hamiltonian of the coupled system has been derived, only then can some of the properties listed previously (band energies and density of states, for example) be computed.

4.4.1 TB treatment of superconductivity

The general expression for the BCS Hamiltonian was given in (3.9). It featured an onsite term, and an electron-phonon term, both expressed in reciprocal space. The particularity of this work is that the BCS Hamiltonian, usually expressed in reciprocal space, will be treated in direct space. To make the transition possible, the different creation and annihilation operators have to be brought back into real space, by Fourier-transforming them. The expressions of the operators

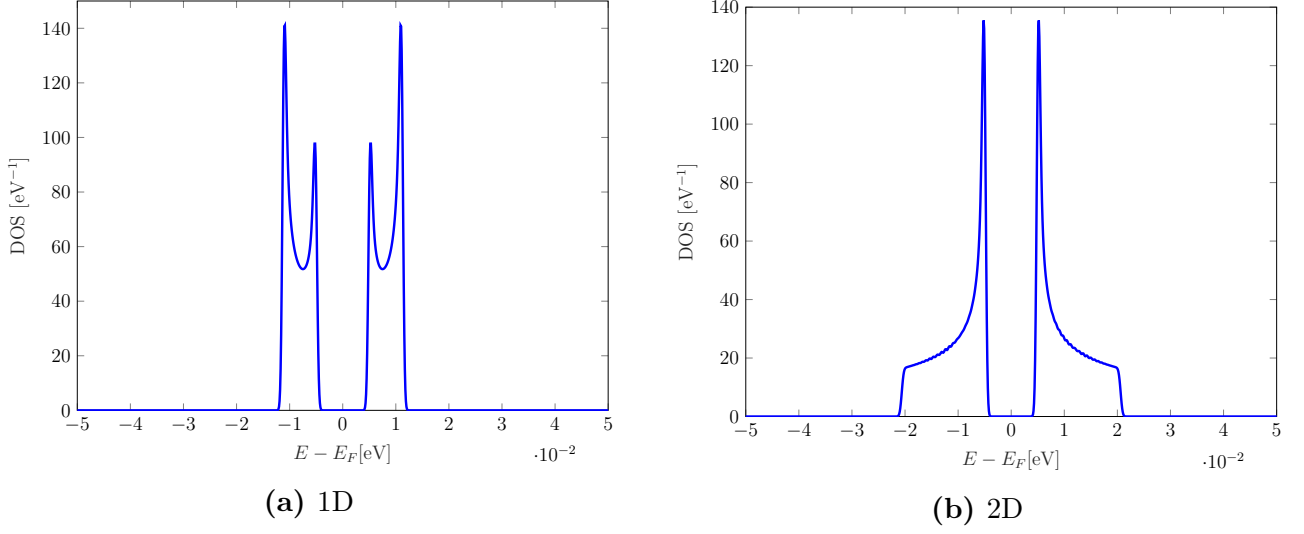


Figure 4.5 – Density of states of a SC superconductor in one and two dimensions

are given by

$$\begin{aligned}
 \hat{c}_{\mathbf{k}\sigma} &= \frac{1}{\sqrt{N}} \sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j} \hat{c}_{j\sigma} \quad \text{and} \quad \hat{c}_{\mathbf{k}\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \hat{c}_{j\sigma}^\dagger \\
 \Rightarrow \hat{c}_{j\sigma} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} \hat{c}_{\mathbf{k}\sigma} \quad \Rightarrow \hat{c}_{j\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_j} \hat{c}_{\mathbf{k}\sigma}^\dagger.
 \end{aligned} \tag{4.10}$$

where the subscript j indicates that the j^{th} site is considered, and where N is the number of lattice points in the system. A real-space mean-field version of the mean-field reciprocal-space BCS Hamiltonian can then be derived, which expression reads [82]

$$\hat{\mathcal{H}} = \sum_{\substack{i,j \\ \sigma,\sigma'}} \hat{c}_{i\sigma}^\dagger \hat{h}_{i\sigma,j\sigma'} \hat{c}_{j\sigma'} + \sum_{i,j} \left[\Delta_{ij} \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger + \Delta_{ij}^* \hat{c}_{j\downarrow} \hat{c}_{i\uparrow} \right] + E_{\text{const}},$$

where $\hat{h}_{i\sigma,j\sigma'}$ is a general enough operator allowing to take non-local and spin-flip effects into account, and where E_{const} is a constant, whose precise expression is irrelevant.

Based on that real-space mean-field Hamiltonian, the density of states can be computed, for example. The case for a SC crystal in 1D and 2D is shown in figure 4.5, and the gap is clearly visible. Even if the results look quite satisfying, it should however be stated that the gap was not determined self-consistently, as should be, but rather passed as an input parameter in the TB code.

4.4.2 TB treatment of magnetism

The Hamiltonian given in (4.9) is quite general, and allows to model different types of magnetic textures, ranging from collinear configurations such as (anti)ferromagnets, to noncollinear configurations, such as skyrmions. In the following, a brief introduction to collinear and noncollinear magnetism will be given.

Collinear magnetism

The simplest way to take collinear magnetism into account is certainly through the Stoner model, in which the potential felt by electrons depends on their spin. This spin-dependent potential is taken into account in the exchange term, which depends on the magnetic moment of the d -electrons. Consequently, the exchange energy takes the form

$$\epsilon_{j\mu}^{\text{exc}} = I_{j\mu} \cdot m_j^d,$$

where $I_{j\mu}$ is the Stoner parameter for the j^{th} atom in the μ^{th} orbital. In the case of collinear magnetism, the magnetic moment m_j^d can be computed thanks to the relation $m_j = N_{i,d}^{\uparrow} - N_{i,d}^{\downarrow}$, where $N_{i,d}^{\sigma}$ ($\sigma = \uparrow, \downarrow$) is the number of d -electrons with spin σ . This exchange term has the effect to split the DOS according to the spin, as schematically shown in figure 4.6.

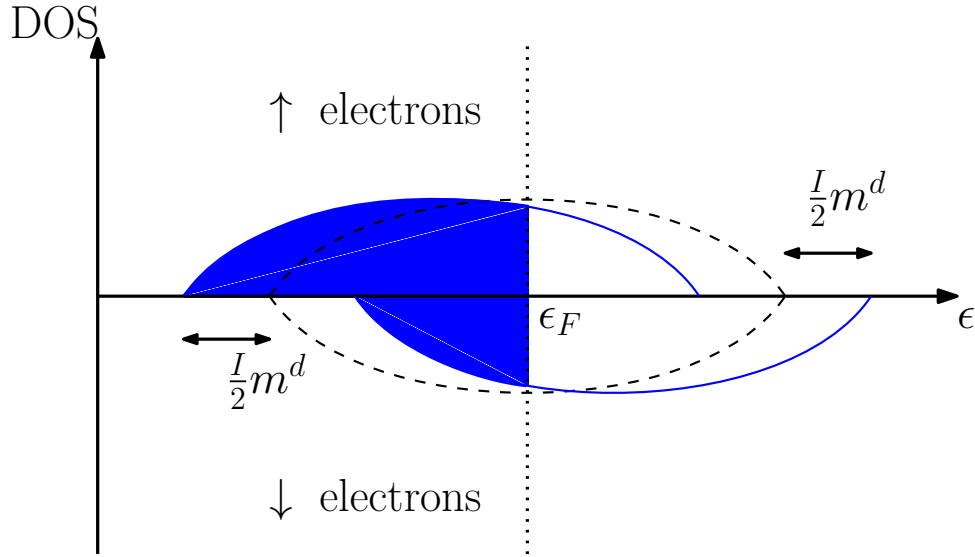


Figure 4.6 – Graphical representation of the DOS in the case where the magnetism is neglected (dashed lines), and where it is considered (full lines). Due to the Stoner exchange, the DOS is split according to the electron spin. The band filling (up to the Fermi energy ϵ_F) is different for $\uparrow$ and $\downarrow$ electrons, leaving a system with a net magnetisation.

In the case of collinear magnetism, the Stoner part of the total Hamiltonian in spin-space

has the form

$$[\mathbf{H}_{\text{mag}}]_{i,\mu}^{j,\nu} = \begin{bmatrix} -\frac{I_{i\mu}}{2} \cdot m_i^d & 0 \\ 0 & \frac{I_{i\mu}}{2} \cdot m_i^d \end{bmatrix} \delta_{ij} \delta_{\mu\nu}, \quad (4.11)$$

which shows that the Stoner interaction modifies only the onsite energies. The reason why only d -electrons are considered in the Stoner model is that magnetism originates mainly from d -electrons in transition metals, such as Fe¹. This can be shown from the Stoner criterion $I \cdot D(\epsilon_F) > 1$ for ferromagnetic materials, where $D(\epsilon_F)$ is the DOS at the Fermi energy [36].

The computation of the magnetic moments can be made thanks to the density matrix $[\boldsymbol{\rho}]$ which, for the j^{th} atom in the μ^{th} orbital, takes the form (in spin space with the z axis as quantisation axis)

$$[\boldsymbol{\rho}]_{j\mu} = \begin{bmatrix} \rho_{j\mu}^{\uparrow\uparrow} & \rho_{j\mu}^{\uparrow\downarrow} \\ \rho_{j\mu}^{\downarrow\uparrow} & \rho_{j\mu}^{\downarrow\downarrow} \end{bmatrix},$$

where the different components $\rho_{j\mu}^{\sigma\sigma'}$ ($\sigma, \sigma' = \uparrow, \downarrow$) are given by

$$\rho_{j\mu}^{\sigma\sigma'} = \sum_{n,\mathbf{k}} f(\epsilon_{\mathbf{k},n}, \epsilon_F) |\Psi_{nj\mu\sigma}(\mathbf{k})\rangle \langle \Psi_{nj\mu\sigma'}(\mathbf{k})|.$$

Moreover, the spatial component of the magnetisation can be derived from the density matrix, thanks to the relation

$$[\mathbf{m}_{j\mu}]_{\alpha} = \text{Tr} \left\{ [\boldsymbol{\rho}]_{j\mu} \cdot \hat{\sigma}_{\alpha} \right\}, \quad \alpha = x, y, z,$$

where the $\hat{\sigma}_{\alpha}$'s are the Pauli matrices. From there, the full-length expression of the different components of the magnetisation $\mathbf{m}_{j\mu}$ are given by

$$[\mathbf{m}_{j\mu}]_x = 2 \text{Re} \left\{ \rho_{j\mu}^{\uparrow\downarrow} \right\}, \quad [\mathbf{m}_{j\mu}]_y = 2 \text{Im} \left\{ \rho_{j\mu}^{\uparrow\downarrow} \right\}, \quad \text{and} \quad [\mathbf{m}_{j\mu}]_z = \rho_{j\mu}^{\uparrow\uparrow} - \rho_{j\mu}^{\downarrow\downarrow}.$$

Noncollinear magnetism

Quite often, a lot of interesting properties arise in systems which shows noncollinear magnetism, such as spin waves [18, 56] and skyrmions. To get a TB picture of noncollinear magnetism, two reference frames are needed, namely (i) an absolute one, in which the z -axis is chosen as quantisation axis, and (ii) a local one, in which the quantisation axis is chosen to be the magnetisation $\mathbf{m}$. To move a spin state $|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ from the global frame, to its representation $|\uparrow\rangle_{\mathbf{m}}$ in the local frame, a rotation matrix $\mathcal{U}$ can be defined, which expression is given by [38]

$$\mathcal{U}(\theta, \phi) = \begin{bmatrix} e^{-i\frac{\theta}{2}} \cos\left(\frac{\phi}{2}\right) & -e^{-i\frac{\theta}{2}} \sin\left(\frac{\phi}{2}\right) \\ e^{i\frac{\theta}{2}} \sin\left(\frac{\phi}{2}\right) & e^{i\frac{\theta}{2}} \cos\left(\frac{\phi}{2}\right) \end{bmatrix},$$

where θ and ϕ are the traditional spherical coordinates, illustrated in figure 4.7.

¹The DOS of s -electrons is usually small compared to that of d -electrons, hence their contribution to magnetism can safely be neglected.

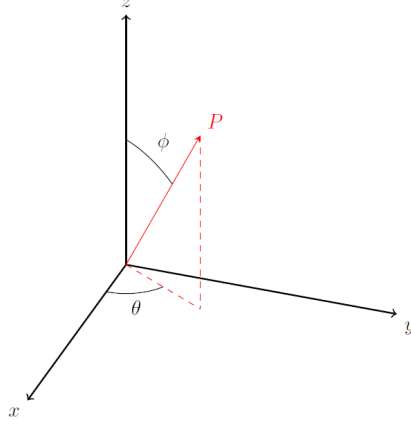


Figure 4.7 – Schematic representation of the spherical coordinate system.

Using the rotation matrix, the expression of the local spin $|\uparrow\rangle_{\mathbf{m}}$ takes the form

$$|\uparrow\rangle_{\mathbf{m}} = \mathcal{U}(\theta, \phi) |\uparrow\rangle = e^{-i\frac{\theta}{2}} \cos\left(\frac{\phi}{2}\right) |\uparrow\rangle + e^{i\frac{\theta}{2}} \sin\left(\frac{\phi}{2}\right) |\downarrow\rangle.$$

The former onsite Stoner Hamiltonian (4.11) can also be expressed in a local or global frame, with an expression looking (almost) unchanged. To see this, the expression appearing in (4.11) (which is expressed in the local frame) can be rewritten under the form

$$\begin{aligned} [\mathbf{H}_{\text{mag}}]_{i,\mu}^{j,\nu} &= \begin{bmatrix} -\frac{I_{i\mu}}{2} \cdot m_i^d & 0 \\ 0 & \frac{I_{i\mu}}{2} \cdot m_i^d \end{bmatrix} \delta_{ij} \delta_{\mu\nu} \\ &= -\frac{I_{i\mu}}{2} \mathbf{m}_i^d \cdot \hat{\boldsymbol{\sigma}} \delta_{ij} \delta_{\mu\nu}. \end{aligned}$$

That local expression can be changed in the global frame by applying the following transformation

$$[\mathbf{H}_{\text{mag}}^{\text{global}}] = \mathcal{U}(\theta_i, \phi_i) [\mathbf{H}_{\text{mag}}]_{i,\nu}^{j,\mu} \mathcal{U}^\dagger(\theta_i, \phi_i),$$

where θ_i and ϕ_i are the angles defining the local magnetic moment $\mathbf{m}_i^d$. Applying that definition, the expression of the Stoner Hamiltonian in the global frame takes the form

$$[\mathbf{H}_{\text{mag}}^{\text{global}}] = -\frac{I_{i\mu}}{2} \mathbf{m}_i^d \cdot \boldsymbol{\sigma},$$

which looks similar to the previous expression. There is, however, a subtlety: in the previous (local) expression (4.11), only one component of the magnetisation $\mathbf{m}$ was needed, while the whole expression is needed in the global reference frame.

4.4.3 The coupling

To check how the coupling of the BCS Hamiltonian interacts with an underlying structure, and to see how the different TB parameters influence each other, different magnetic textures can be tested, such as a simple ferromagnetic background, a spin spiral, or a skyrmion.

Ferromagnetic background

A ferromagnetic (FM) background corresponds to all the magnetic moments pointing in the same direction. To check the influence of the texture on the superconductor, the most important parameter is the J_{sd} coupling: it is expected that the superconducting behaviour of the system will be preserved as long as the value of the coupling parameter does not exceed a critical value. This can be checked in the DOS, represented in figure 4.8: as long as there is a gap, the system remains superconducting.

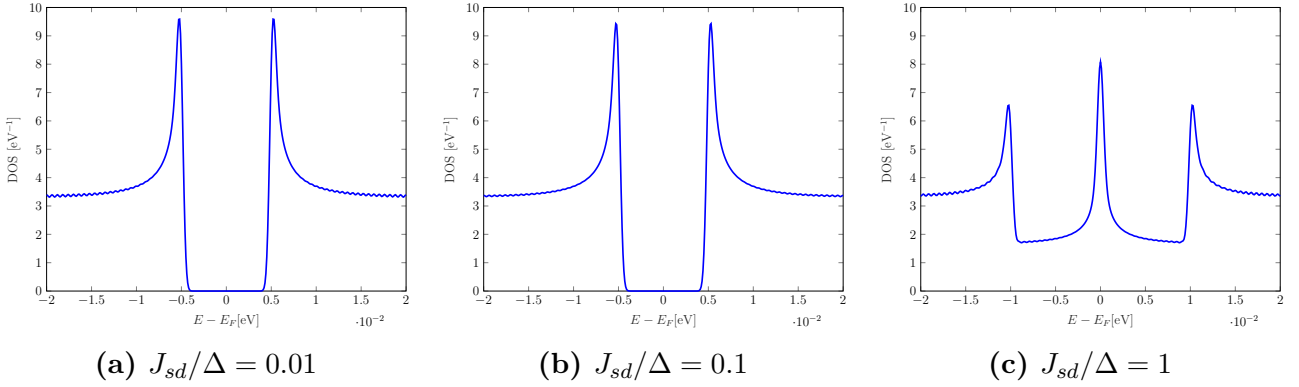


Figure 4.8 – DOS for the 1D system coupling a superconductor and a ferromagnetic SC background. The hopping parameter is kept at $t = 5 \cdot 10^{-2}[\text{eV}]$, and the superconducting gap $\Delta = 5 \cdot 10^{-3}[\text{eV}]$.

An interesting shape occurs for a coupling $J_{sd}/\Delta = 1$, represented in figure 4.8c, where the gap is closed and a peak appears around the Fermi energy. This could be linked to a splitting of the spin-up and spin-down electrons, which could be checked by plotting the local DOS. Unfortunately, this functionality is still not fully functional in the code, hence it stays at the level of simple hypothesis.

Spin spiral background

As its name suggest, a spin spiral is a configuration in which the spin of the different atoms form a spiral. Such a spin spiral is a periodic magnetic texture, in which the magnetic moment

at site i , $\mathbf{m}_i$, can be written under the form [37]

$$\mathbf{m}_i = M \begin{bmatrix} \cos(\mathbf{q} \cdot \mathbf{R}_i) \sin(\theta) \\ \sin(\mathbf{q} \cdot \mathbf{R}_i) \sin(\theta) \\ \cos(\theta) \end{bmatrix},$$

where M is the modulus of the magnetisation. In that expression, the angle θ is the angle between the magnetisation and the rotation axis of the spin spiral, and $\mathbf{q}$ represents the propagation of the spiral.

A first set of tests that can be done is to see the relative influence of the magnetic coupling on the superconductivity for different values of the $\mathbf{q}$ -vector, as illustrated in figure 4.9. As can be seen on that figure, the smaller the wavelength of the spiral, the bigger the ratio J_{sd}/Δ before the superconductivity is killed by the magnetism. This can be explained by the fact that if the spiral oscillates very slowly as compared to the size of the supercell in which it exists, the superconducting part does not “see” an appreciable difference in the magnetic texture from one site to the other, i.e. the background acts as if it were a ferromagnet.

Another set of tests that can be run is one in which both the hopping parameter and the superconducting gap are fixed, and the relative influence of the magnetic texture on the kinetic energy can be assessed. The results of such tests are presented in figure 4.10, in which different values for the $\mathbf{q}$ -vector are tested.

A final set of tests that can be made is to check how the system behaves when the ratio Δ/t is changed, once again for different values of the $\mathbf{q}$ -vector. The result of such a test is given in figure 4.11. As expected, the bigger the ratio, the bigger the gap. However, it is interesting to note that there seem to exist a critical value (somewhere between 0.1 and 0.2) below which the system is not superconducting anymore, since the gap disappears.

Skyrmion background

Another magnetic texture and its coupling to superconductivity can be studied: the magnetic skyrmion. The whole point is to find some values for the tight-binding parameters which allow to find some Majorana fermions inside those skyrmions, which would be visible in the DOS, as schematically shown in figure 4.12.

The whole point is thus to couple the skyrmion and the superconductor, and to plot the (local) DOS of that system. The result of such a coupling is presented in figure 4.13, from which it can be seen that there could potentially be Majorana fermions for a ratio J_{sd}/Δ lying in-between 0.1 and 1. In the same way as what was done for the spin spiral, different values for the ratios J_{sd}/t and Δ/t can be tested, to try to enlighten the relation between those parameters. However, by a lack of time, those tests could not be made. Moreover, the clear localisation of a peak in the DOS at 0 energy is best seen with the local DOS, which is still not functional in the code in presence of superconductivity. Still, some values for the ratio Δ/t have been tested, and the results are plotted in figure 4.14. For some values of the ratio, there is a clear peak at 0

energy, but an extensive set of tests is lacking, which means that it cannot be concluded that the peak is a manifestation of Majorana fermions.

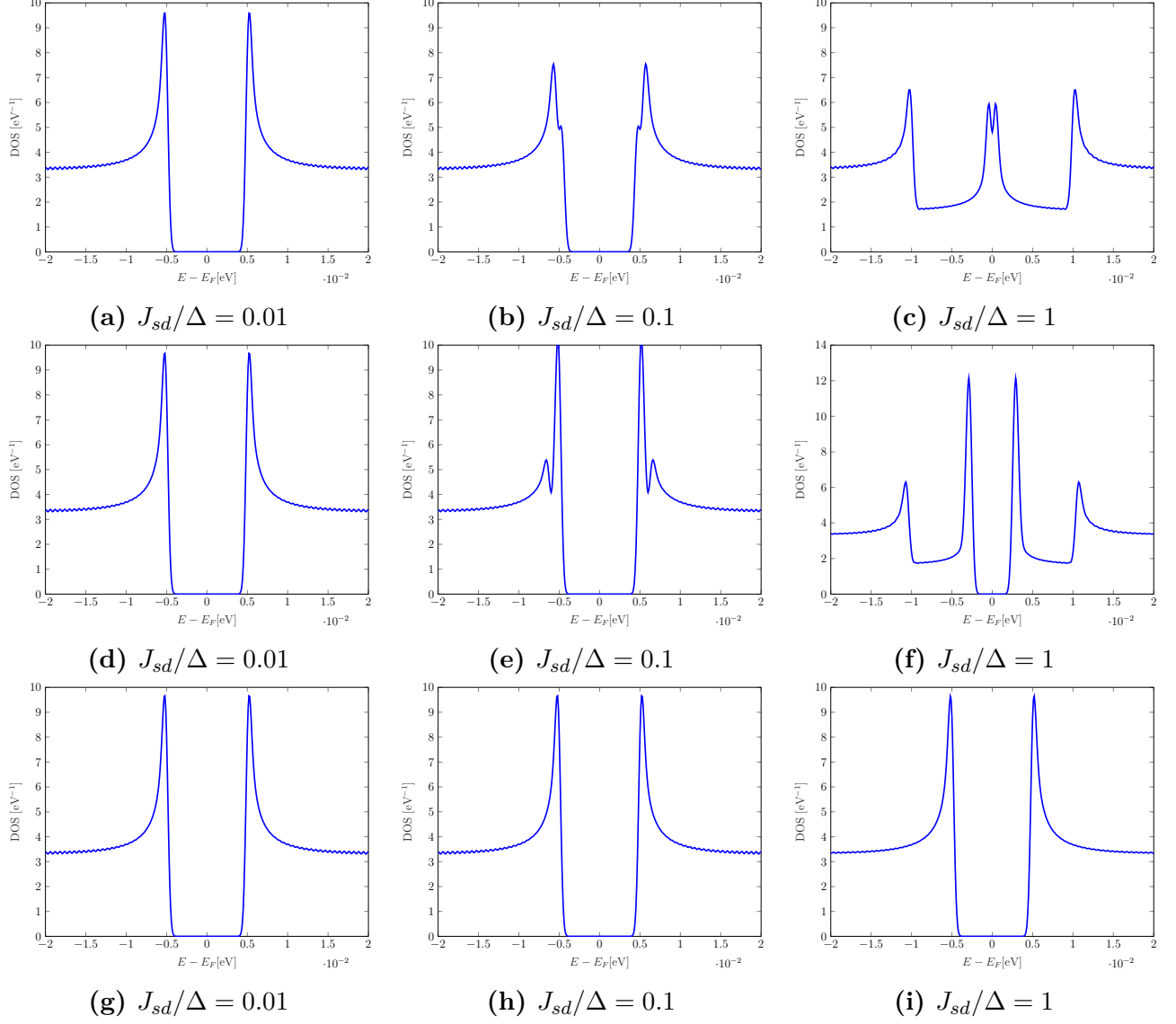


Figure 4.9 – DOS for the coupling between a superconductor and a spin spiral. The hopping parameter is kept at $t = 5 \cdot 10^{-2}[\text{eV}]$, and the superconducting gap at $\Delta = 5 \cdot 10^{-3}[\text{eV}]$. The 3 rows are for a spin spiral having, from top to bottom, a $\|\mathbf{q}\|$ of 1000, 100, and $1 \text{ \AA}^{-1}$.

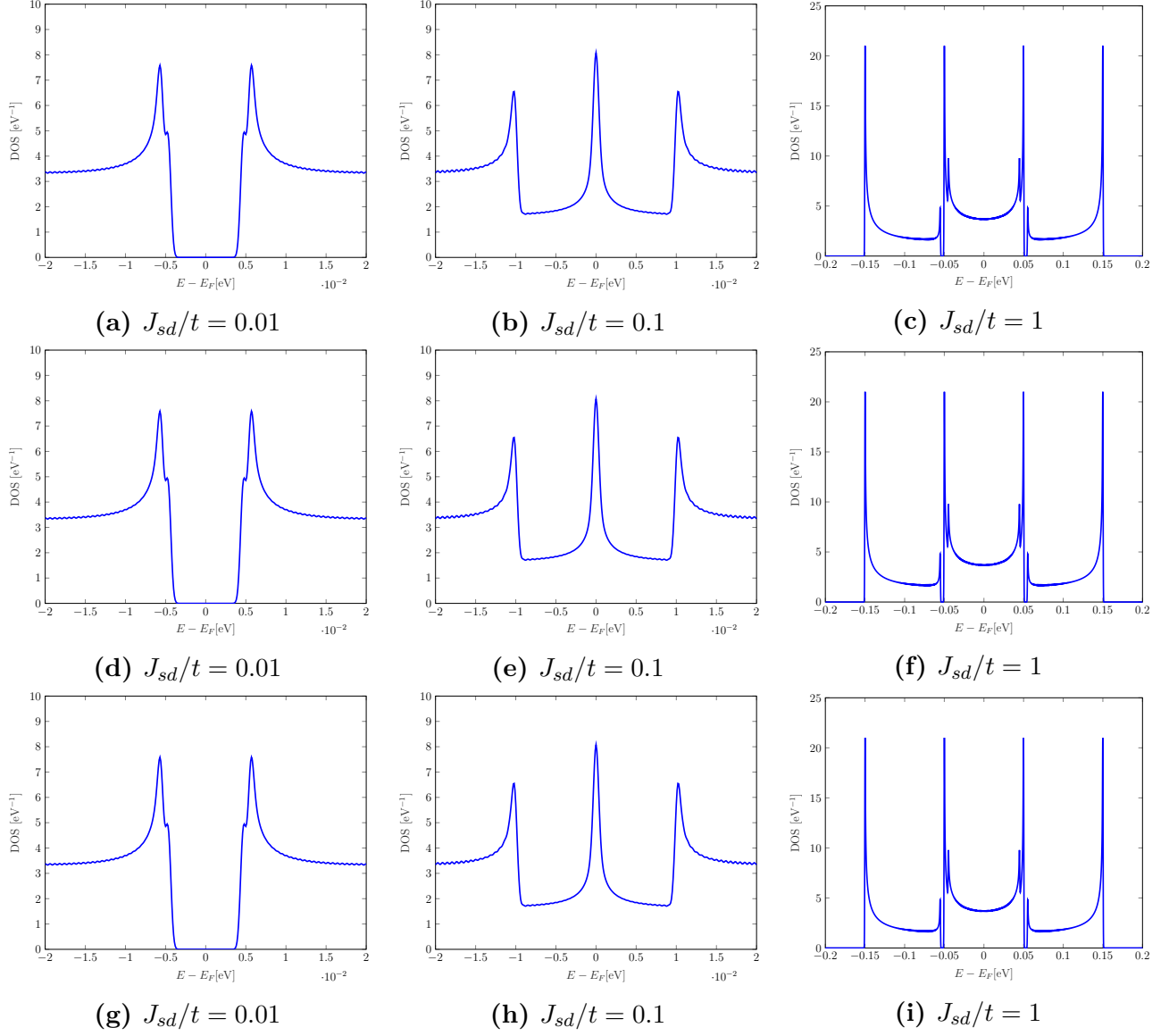


Figure 4.10 – DOS for the coupling between a superconductor and a spin spiral. The hopping parameter is kept at $t = 5 \cdot 10^{-2}$ [eV], and the superconducting gap at $\Delta = 5 \cdot 10^{-3}$ [eV]. The 3 rows are for a spin spiral having, from top to bottom, a $\|\mathbf{q}\|$ of 1000, 100, and $1 \text{ \AA}^{-1}$.

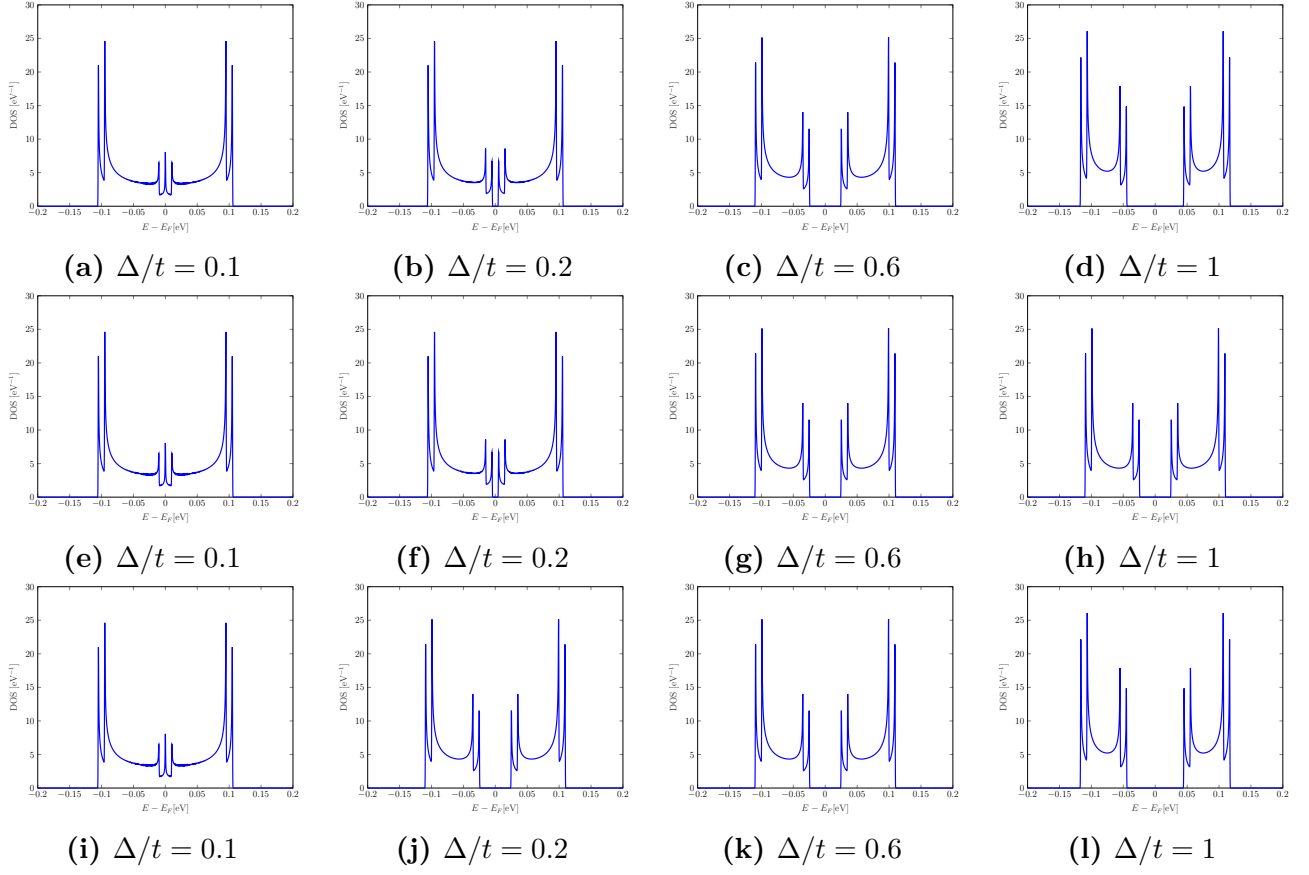


Figure 4.11 – DOS for the coupling between a superconductor and a spin spiral. The hopping parameter is kept at $t = 5 \cdot 10^{-2}[\text{eV}]$, and the coupling constant at $J_{sd} = 5 \cdot 10^{-3}[\text{eV}]$. The 3 rows are for a spin spiral having, from top to bottom, a wavelength of 1000, 100, and 1 site(s).

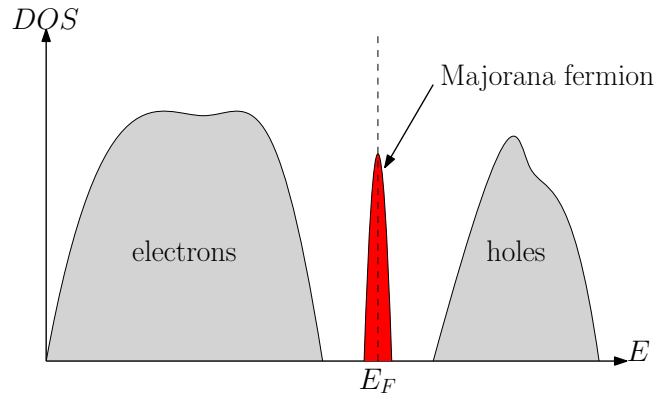
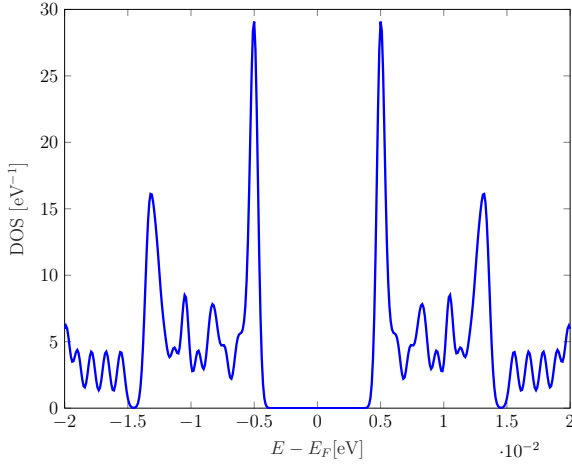
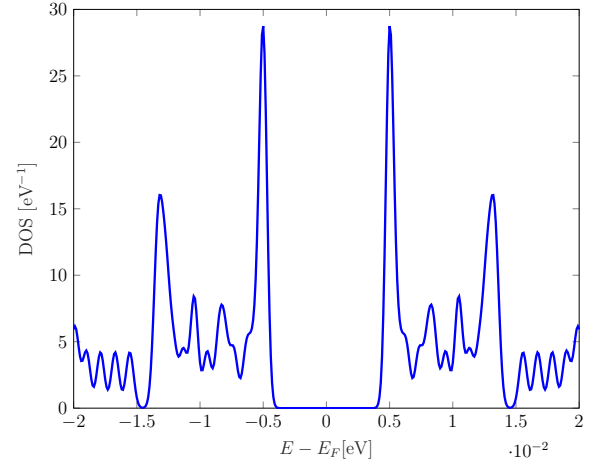


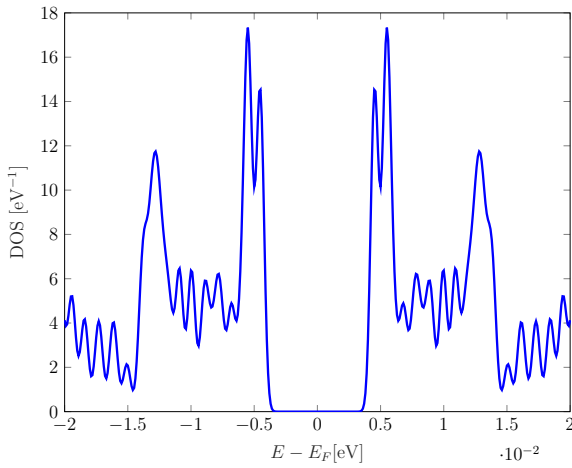
Figure 4.12 – Graphical representation of the DOS of a system hosting Majorana fermions.



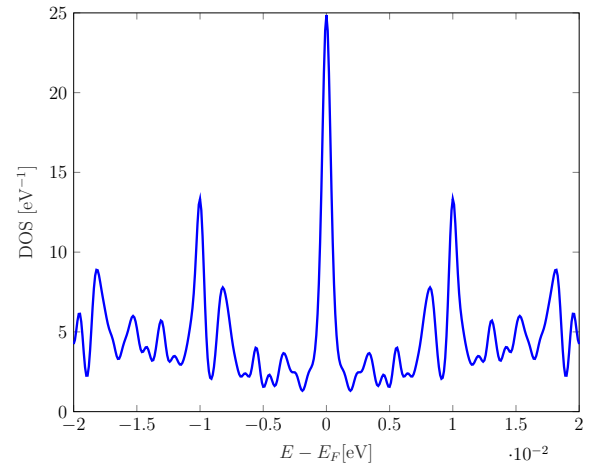
(a) $J_{sd}/\Delta = 0.001$



(b) $J_{sd}/\Delta = 0.01$

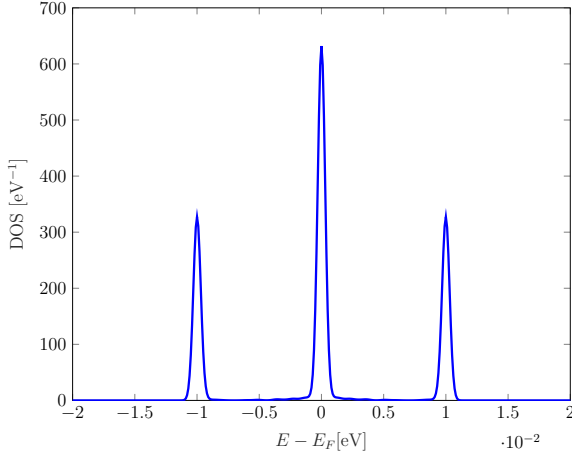


(c) $J_{sd}/\Delta = 0.1$

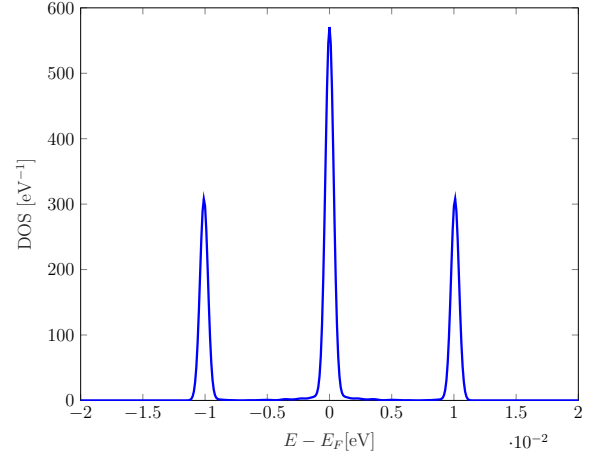


(d) $J_{sd}/\Delta = 1$

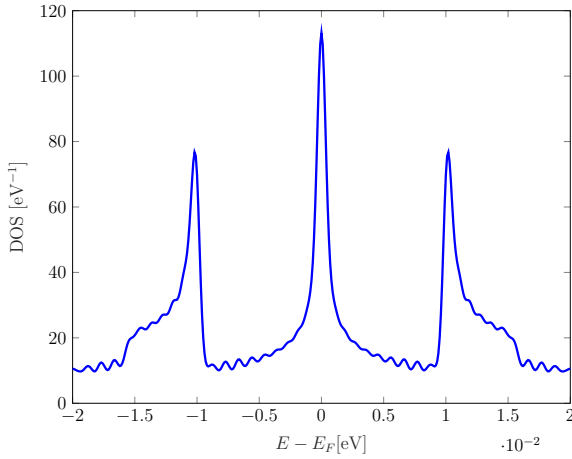
Figure 4.13 – DOS for the coupling between a superconductor and a skyrmion on a 2D SC lattice. The hopping parameter is kept at $t = 5 \cdot 10^{-2}[\text{eV}]$, and the superconducting gap at $\Delta = 5 \cdot 10^{-3}[\text{eV}]$.



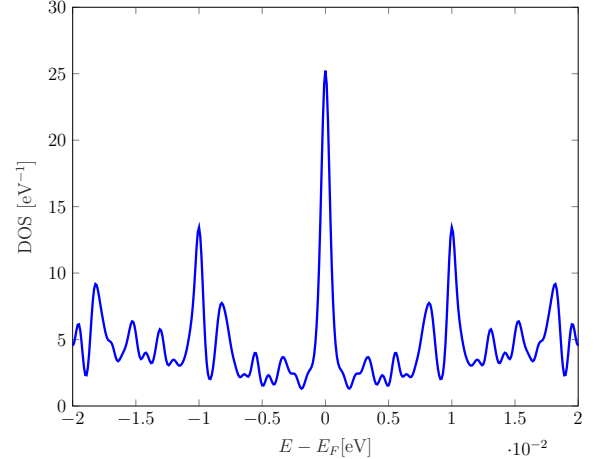
(a) $\Delta/t = 100$



(b) $\Delta/t = 10$



(c) $\Delta/t = 1$



(d) $\Delta/t = 0.1$

Figure 4.14 – DOS for the coupling between a superconductor and a skyrmion on a 2D SC lattice. The magnetic coupling is kept at $J_{sd} = 5 \cdot 10^{-3}[\text{eV}]$, and the superconducting gap at $\Delta = 5 \cdot 10^{-3}[\text{eV}]$.

Summary and outlook

In this work, several quite different concepts have been presented: on one side, some generalities about magnetic skyrmions were discussed. In particular, a small introduction to topology was given, which allowed to gain insight into the classification of various magnetic textures, as well as some potential technological applications of such “objets”. The discussion went on with a totally different concept: superconductivity. It was briefly explained that magnetism and superconductivity were phenomena opposing each other: indeed, it was argued, by a hand-waving explanation, that a too strong magnetic field would destroy the Cooper pairs responsible for superconductivity, by aligning the spins on the field. Continuing the discussion on superconductors, so-called topological superconductors were presented, with an emphasis on their potential to host Majorana fermions in the core of vortices, allowing to imagine some data-storage devices based on such exotic materials. This leads to the last chapter of this work, which consisted in the creation of a tight-binding model allowing to study the coupling between magnetism and superconductivity, with the objective to find ranges of value for different parameters allowing for Majorana fermions to exist in the core of magnetic skyrmions.

This ambitious goal, i.e. find the regime(s) in which skyrmions could host Majorana fermions, could not be fulfilled, for different reasons: first, and foremost the lack of time the author has faced to realise an extensive enough set of tests to find some intervals for the parameters involved in the problem. Another issue is that the code is still under development, and thus some tests could not be properly undertaken.

To briefly conclude this work, a tight-binding is being set-up to study the possibility to host Majorana fermions inside magnetic skyrmions, and use that coupling to realise some stable qubits. The fulfilment of that ambitious goal is still ongoing work.

Equivalence between the different forms of the Landau-Lifschitz-Gilbert equation

The aim of this appendix is to show that the two forms of the Landau-Lifschitz-Gilbert equation are equivalent. Those two different forms read

$$\frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) = -\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t) + \alpha \mathbf{m}(\mathbf{r}, t) \times \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) \quad (\text{A.1})$$

and

$$\frac{1 + \alpha^2}{\gamma\mu_0} \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) = -\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t) - \alpha \mathbf{m}(\mathbf{r}, t) \times [\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t)]. \quad (\text{A.2})$$

In order to go from equation (A.1) to equation (A.2), some algebra is needed. Taking the cross product of the magnetization with its time derivative given in equation (A.1) leads to

$$\begin{aligned} \mathbf{m}(\mathbf{r}, t) \times \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) &= -\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times [\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t)] \\ &\quad + \alpha \mathbf{m}(\mathbf{r}, t) \times \left[\mathbf{m}(\mathbf{r}, t) \times \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) \right]. \end{aligned} \quad (\text{A.3})$$

From there, the vectorial relation

$$\mathbf{a} \times [\mathbf{b} \times \mathbf{c}] = (\mathbf{a} \cdot \mathbf{c}) \mathbf{b} - (\mathbf{a} \cdot \mathbf{b}) \mathbf{c}$$

can be used in equation (A.3), leading to

$$\begin{aligned} \mathbf{m}(\mathbf{r}, t) \times \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) &= -\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t) \\ &\quad + \alpha \left[\left(\mathbf{m}(\mathbf{r}, t) \cdot \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) \right) \mathbf{m}(\mathbf{r}, t) - \|\mathbf{m}(\mathbf{r}, t)\|^2 \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) \right] \\ &= -\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t) - \alpha \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t). \end{aligned}$$

To go from the first to the second line, the key assumption that the magnetization vector has constant unit norm, i.e. $\|\mathbf{m}(\mathbf{r}, t)\| = 1$, was used. Indeed, in this case that vector is orthogonal to its time derivative, which cancels the first term between the square brackets. Injecting the last expression back into the original expression equation (A.1) leads to

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) &= -\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t) \\ &\quad + \alpha \left\{ -\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times [\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t)] - \alpha \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t) \right\} \\ &= -\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t) - \alpha\gamma\mu_0 \mathbf{m}(\mathbf{r}, t) \times [\mathbf{m}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t)] - \alpha^2 \frac{\partial}{\partial t} \mathbf{m}(\mathbf{r}, t), \end{aligned}$$

which, once reordered, is the form announced in equation (A.2). As a final note, it can be noted that the LLG equation is norm preserving. This can be easily checked by computing $\partial_t \|\mathbf{m}(\mathbf{r}, t)\|^2 = 2\mathbf{m}(\mathbf{r}, t) \cdot \partial_t \mathbf{m}(\mathbf{r}, t) = 0$, since all the terms in the LHS of the LLG consist in cross products of $\mathbf{m}(\mathbf{r}, t)$ with another vector field. This shows that the Landau-Lifshitz-Gilbert equation is a norm-preserving equation.

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