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Ultrafast manipulation of Heisenberg exchange and Dzyaloshinskii–Moriya interactions in antiferromagnetic insulators

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Chapter 1

AFM spinotronics

1.1 History and background

Antiferromagnetism was first studied by L. Néel who introduced a thermodynamic theory following the Weiss's model of a local molecular field. This made it possible to explain the antiferromagnetic order and it predicted the existence of a temperature above which this order vanishes. This temperature is known as Néel temperature. Later Néel proposed the picture of a magnetic order where two sublattices were magnetised in opposite directions. During the same period, Lev Landau developed a phenomenological model using a combination of two antiferromagnetically coupled ferromagnetic layers.

The discovery of the giant magnetoresistance effect by P. Grünberg [1] and A. Fert [2] in the 80s opened the gate for a new field of study known as spinotronics, in which electron spin is exploited in improved electronic devices. Magnetoresistive random-access memory (MRAM) is an example of a new type of memory in which data is stored in magnetic elements [3]. Newer techniques include thermal assisted switching (TA-MRAM) [4] and spin transfer torque (SPRAM) [5].

However, so far, in most current spinotronic devices antiferromagnets play only a minor role. During several decades after the discovery of antiferromagnetics, these materials were percived as useless from a practical point of view. On contrast, ferromagnets have been widely studied historically for its technical applications. However, the development of information technology demands devices with high storage density, high energy efficiency and high write-read speeds. Therefore, controlling magnetically ordered systems on subpicosecond timescales is currently a widely studied area. Antiferromagnets aim to complement or even replace ferromagnets due to their rigidity to external magnetic field, and the abscence of stray field.

It has been shown that spin-transfer torques and giant magnetoresistance effects can occur in circuits containing only normal and antiferromagnetic materials [6]. Additionally, spin axis reorientation by a lateral electrical current can be used to offer ultra-fast electrical writing and reading in AFM devices [7].

Our goal in this project is to investigate the techniques to manipulate the magnetic state in an antiferromagnetic insulator, which could potantially lead to applications for ultra-fast writing devices. For ferromagnetic materials it has already been shown that short laser pulses can induce an effective magnetic field that can reach an amplitude of a few Tesla ([8], [9]).

Chapter 2

Basic models for solid state

Many properties of solids can be understood using one-electron models, that is, non-interacting models. When the interaction between the ions and the valence electrons can be mostly neglected one can adapt the free electron approximation. This model is mostly limited to the study of metals and despite its simplicity it successfully explains phenomena related with electrical conductivity and heat capacity. In the opposite limit, we can consider systems in which the ion potential is so large that the electrons are bound in the cores with occasional jumps from site to site. This is known as tight binding model and it can be used to study a wide variety of solids. It is typically used for calculations of the electronic band structure.

Despite the success of the single particle models, there are several phenomena which cannot be explained neglecting electron correlations. For example, high temperature superconductivity cannot be understood with these models. The Hubbard model is the simplest model including electron correlations and despite its simplicity it is not fully understood yet. In this Chapter we will outline the main features of the tight binding model and the Hubbard model, which are basic tools for any condensed matter researcher.

2.1 Tight binding

When the electrons are strongly localized in the atom cores, the wavefunction describing such an electron is similar to the corresponding atomic orbital. Therefore it is natural to consider linear superposition of atomic orbitals as an anstatz for the crystal electron states.

Let $\phi_i(r)$ be the i-*th* eigenstate of the atomic Hamiltonian $\hat{H}_a(r) = -\frac{\hbar^2 p^2}{2m} + V_a(r - bsr_n)$ with energy E_i and where $V_a(r)$ is the atomic potential. The crystal Hamiltonian is:

$$\hat{H} = -\frac{\hbar^2 p^2}{2m} + \sum_n V_a(r - r_n) \tag{2.1}$$

An electron localized around the atom at r_n will mainly feel the potential of that atom, and the potential of the rest of the atoms will be a perturbation to the free atom problem. That is, we can spit 2.1 into:

$$\hat{H} = \hat{H}_a + v(r - r_n) \tag{2.2}$$

Where $v(r - r_n) = \sum_{m \neq n} V_a(r - r_m)$ is a small perturbation. We can expect the crystal electron to retain the properties of the free atom electron, and so, it is natural to describe the crystal electron as a superposition of atomic orbitals. Thus, we will try to find solutions of the form:

$$\psi_i(\boldsymbol{r}) = \sum_n b_i(\boldsymbol{r}_n)\phi_i(\boldsymbol{r} - \boldsymbol{r}_n) \tag{2.3}$$

Now, the Bloch theorem states that an eigenfunction of the crystal Hamiltonian should only change by a phase from site to site, that is $\psi_i(\boldsymbol{r} + \boldsymbol{r}_m) = e^{ik \cdot \boldsymbol{r}_m}\psi_i(\boldsymbol{r})$, where $\boldsymbol{k}$ is the crystal momentum of the Bloch wave. We can see that see implies $b_i(\boldsymbol{r}_m) = e^{ik \cdot \boldsymbol{r}_m} b_i(0)$, by normalizing $\psi_i(\boldsymbol{r})$ we find $b_i(0) = \frac{1}{\sqrt{N}}$, where N is the number of atoms in the crystal. We therefore obtain:

$$\psi_{ik}(\boldsymbol{r}) = \frac{1}{\sqrt{N}}\sum_n e^{ik \cdot \boldsymbol{r}_n}\phi_i(\boldsymbol{r} - \boldsymbol{r}_n) \tag{2.4}$$

The energy of this state is $E_i(\boldsymbol{k}) = \langle\psi_{ik}|\hat{H}|\psi_{ik}\rangle$, using 2.2 this can be written as:

$$E_i(\boldsymbol{k}) = \frac{1}{N}\sum_{n,m} e^{ik \cdot (\boldsymbol{r}_n - \boldsymbol{r}_m)}\int \phi_i^*(\boldsymbol{r} - \boldsymbol{r}_m)(E_i + v(\boldsymbol{r} - \boldsymbol{r}_n))\phi_i(\boldsymbol{r} - \boldsymbol{r}_n)d\boldsymbol{r} \tag{2.5}$$

Assuming that ϕ_i is spherically symmetric, and neglecting the perturbation $v(\boldsymbol{r} - \boldsymbol{r}_n)$ further away than nearest neighbors, we can simplify this expression to:

$$E_i(\boldsymbol{k}) = E_i - A - B\sum_\delta e^{ik \cdot \delta} \tag{2.6}$$

Where $A = -\langle\phi_i(\boldsymbol{r} - \boldsymbol{r}_n)|v(\boldsymbol{r} - \boldsymbol{r}_n)|\phi_i(\boldsymbol{r} - \boldsymbol{r}_n)\rangle$ and $B = -\langle\phi_i(\boldsymbol{r} - \boldsymbol{r}_m)|v(\boldsymbol{r} - \boldsymbol{r}_n)|\phi_i(\boldsymbol{r} - \boldsymbol{r}_n)\rangle$ and where δ are the NN vectors. A measures the amount of energy reduced when the atom forms a crystal, B is a measure of the width of the band. In second quantization formalism we can write the tight binding single band Hamiltonian as:

$$\hat{H} = -t\sum_{\langle i,j\rangle\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \tag{2.7}$$

Where $\hat{c}_{i\sigma}^\dagger$ ($\hat{c}_{i\sigma}$) creates (annihilates) an electron in site i and spin state σ. The quantity t is the hopping amplitude, and plays the same role B in the first quantization formalism. We can obtain back 2.6 by changing basis to momentum space $\hat{c}_{k\sigma} = \frac{1}{\sqrt{N}}\sum_j e^{-ik \cdot \boldsymbol{r}_j}\hat{c}_{j\sigma}$.

2.2   The Hubbard model

As we discuss earlier, even tough the tight binding model is successful in describing the band structure of most solids, it fails in some cases. In strongly correlated electron systems, the effect of electron-electron Coulomb interactions is important, and this effect is neglected in 2.7. The simplest way to take this effect into account is to consider the interaction of electrons in the same site only, that is, adding a term of the form $U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$:

$$\hat{H} = -t\sum_{\langle i,j\rangle\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{2.8}$$

This new term will add an energy $+U$ when a site is double occupied ($\hat{n}_{i\uparrow} = \hat{n}_{i\downarrow} = 1$) and will not contribute in the more normal case, that $\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} = 1$. The half-filled case is most commonly studied, this is the situation where the system has one electron per site (or it has half the maximum allowed number). This situation is simpler in many ways and it exhibits a lot of interesting phenomena (Mott insulating

behavior, antiferromagnetic order, etc.). However, other cases have also been widely studied.

Notice that if we set U = 0 in 2.8 we recover the tight binding Hamiltonian, therefore we can say that the Hubbard model is an expansion of the tight binding model. The opposite limit $t = 0$ is more interesting. In the half-filling case, for U > 0 the ground state will be any state with exactly one electron per site. Since each electron can be in two spin states there is a 2^N degeneracy. The subspace spaned by these states is referred to as low energy subspace, and in this case is has energy $E_0 = 0$. If we switch $0 \neq t \ll$ U this hopping term will allow an even further decrease in energy by allowing virtual processes $i \to j \to i$ that delocalized the electrons withing their neighbor sites. For $t \ll$ U the dynamics of the system can be described withing the low energy subspace only, by doing so we can obtain an effective spin Hamiltonian $\hat{H}_{\text{eff}} = \sum \langle i, j \rangle J S_i \cdot S_j$ where $J > 0$ describing an antiferromagnetic system. A rigurous derivation of this will be ofered in the next Chapter, however we can intuitively understand this result in the following way: the virtual processes $i \to j \to i$ will be allowed when the electrons at sites i and j have opposite spin (otherwise it would contradict the Pauli principle), therefore states where neighbor sites have opposite spins will have a lower energy due to the delocalization mechanism. Additionally, the constant J will be proportional to the amplitude of the process $i \to j \to i$. We can already see that this amplitude is $2\frac{t^2}{U}$, t^2 due to two hoppings, $\frac{1}{U}$ due to the energy of the intermediate state and the factor 2 due to the two spin possibilities.

Chapter 3

Effective Spin Hamiltonian

In this chapter we will start with a Hamiltonian

$$\hat{H} = \sum_{i=1}^{N_e} \hat{H}^{(1)}(\mathbf{r}_i) + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N_e} v(\mathbf{r}_i - \mathbf{r}_j) \tag{3.1}$$

where v is the electron-electron interaction and where $\hat{H}^{(1)}$ is the single particle Hamiltonian:

$$\hat{H}^{(1)}(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + U(\mathbf{r}) + \lambda\sigma \cdot \boldsymbol{\nabla} V(\mathbf{r}) \times \mathbf{p} \tag{3.2}$$

Where $\lambda = \frac{\hbar^2}{4m^2c^2}$ is the spin orbit coupling constant and $U(r)$ is a periodic potential. The second quantized form of this Hamiltonian can be approximated by a version of the Hubbard model. The original Hubbard model, was developed to describe the single-band magnetism [10], it also describes the transition between conducting and insulating systems, predicting the existence of Mott insulators, materials which should be conducting according to band theory, but they are insulating due to electron-electron interactions.

We will consider a half filled system in the strong coupling limit. Ignoring electron hopping and spin orbit interaction, the ground state of this system is massively degenerated. We will find an effective Hamiltonian considering that the hopping term and the spin interaction term act on this subspace. This effective Hamiltonian will be the sum of three spin interactions: an exchange interaction $J\mathbf{S}_i \cdot \mathbf{S}_j$ with $J > 0$, a Dzyaloshinkii-Moriya interaction $\mathbf{D}\mathbf{S}_i \times \mathbf{S}_j$ and an anisotropic interaction $\mathbf{S}_i \boldsymbol{\Gamma} \mathbf{S}_j$ known as pseudodipolar interaction [11].

3.1 Single particle in a periodic potential

First we will define a suitable basis for the single particle wavefunctions. To do so, we will consider the single particle Hamiltonian without the spin orbit interaction term:

$$\hat{H}_{\text{NSOI}}^{(1)}(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + U(\mathbf{r}) \tag{3.3}$$

Where $U(r)$ has the symmetry of the lattice, i.e. $U(r + R) = U(r)$ for all Bravais lattice vectors R(A). Let $\hat{H}_{\text{NSOI}}^{(1)}$ act on a Hilbert space $\mathcal{H}$ and let $|\phi\rangle \in \mathcal{H}$, then, the group of translation symmetries defined by $\langle r| T_R |\phi\rangle = \langle r + R|\phi\rangle$ is an abelian group, therefore its irreducible representations are one-dimensional, that is, within

an energy level n the wavefunctions of that level transform according to the representation they belong. If Γ^k is a one dimensional representation and $|\phi_n, \boldsymbol{k}\rangle$ is a wavefunction in the energy level n belonging to that representation then $T_{\boldsymbol{R}} |\phi_{n,k}\rangle = \Gamma^k(\boldsymbol{R}) |\phi_{n,k}\rangle$. Now, imposing periodic boundary conditions, $\Gamma^k(\boldsymbol{a}_\mu)^{L_\mu} = 1$, where $\boldsymbol{a}_\mu$ are the primitive translations and L_μ is the number of lattice sites in the μ direction as defined in A. This can be accomplished if we label the representation with a vector of the first Brillouin zone and have $\Gamma^k(R) = e^{ik\cdot R}$. Therefore, for a wavefunction in a periodic lattice we have:

$$\langle \boldsymbol{r} + \boldsymbol{R} | \phi_{n,\mathbf{k}}\rangle = e^{ik\cdot R} \langle \boldsymbol{r} | \phi_{n,\mathbf{k}}\rangle \tag{3.4}$$

Which is the well-known Bloch function form. Here, n is called the band index, and $\mathbf{k}$ is the quasimomentum. The energy of this wavefunction is $\epsilon_{n\mathbf{k}}$. Notice that both $\phi_{n,\mathbf{k}}$ and $\epsilon_{n\mathbf{k}}$ are periodic functions of $\mathbf{k}$ in the reciprocal lattice.

The Bloch function is extended over the whole crystal volume V. We would like to work with a localized basis. An alternative orthonormal basis are the Wannier functions $|\psi_{in}\rangle$, defined in terms of the Bloch functions as:

$$\langle \boldsymbol{r} | \phi_{nk}\rangle = \frac{1}{\sqrt{M}} \sum_{\boldsymbol{R}} e^{ik\cdot R} \langle \boldsymbol{r} | \psi_{\boldsymbol{R}n}\rangle \tag{3.5}$$

$$\langle \boldsymbol{r} | \psi_{in}\rangle = \frac{1}{\sqrt{M}} \sum_{\boldsymbol{k}\in BZ} e^{-ik\cdot R_i} \langle \boldsymbol{r} | \phi_{nk}\rangle \tag{3.6}$$

Where M is the number of lattice sites as defined in A. Using 3.4 we see that $\psi_{in}(\mathbf{r}) = \psi_{0n}(\mathbf{r} - \mathbf{r}_i) \equiv \psi_n(\mathbf{r} - \mathbf{r}_i)$, so we only need to define one Wannier function for each band and the others are obtained by translations. From now on we will restrict ourselves to a fixed band, so we will drop the band index. Additionally, we will include the spin state, therefore the basis states will have two quantum numbers one for the site and one for the spin state. We will adopt the notation $|i\sigma\rangle$ for the basis state of site i with spin state $\sigma = \uparrow, \downarrow$, or just $|i\rangle$ when the spin state is irrelevant. Fock space states with small number of particles will be denoted as $|i\sigma, j\sigma'\rangle$, for a state with a particle at site i with spin σ and a particle at j with spin σ', or $|ij\rangle$ when spin is irrelevant.

3.2 Derivation of the single-band Hubbard model

In this section we will derive the second quantized form of 3.1 using the Wannier function basis. Let $\hat{c}_{j\sigma}^\dagger$ and $\hat{c}_{j\sigma}$ create and annihilate a particle in the state $|j\sigma\rangle$. In this basis, the second quantized form of 3.1 is:

$$\hat{H} = \sum_{i,j,\sigma,\sigma'} \langle i\sigma| \hat{H}^{(1)} |j\sigma'\rangle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} + \frac{1}{2} \sum_{i,j,k,l,\sigma,\sigma'} \langle ij| \hat{v} |kl\rangle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'}^\dagger \hat{c}_{l\sigma'} \hat{c}_{k\sigma} \tag{3.7}$$

Where we assumed $\hat{v}$ to be spin independent. This can be rewritten as:

$$\hat{H} = - \sum_{i,j,\sigma,\sigma'} (\delta_{\sigma,\sigma'} t_{ij} + \boldsymbol{\Delta}_{ij} \cdot \sigma_{\sigma,\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} + \frac{1}{2} \sum_{i,j,k,l,\sigma,\sigma'} \langle ij| \hat{v} |kl\rangle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'}^\dagger \hat{c}_{l\sigma'} \hat{c}_{k\sigma} \tag{3.8}$$

Where $t_{ij} = - \langle i| - \frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + \mathrm{U}(\mathbf{r}) |j\rangle$ and $\boldsymbol{\Delta}_{ij} = - \langle i| \lambda \boldsymbol{\nabla} V(\mathbf{r}) \times \mathbf{p} |j\rangle$. Notice that $\boldsymbol{\Delta}_{ij} = -\boldsymbol{\Delta}_{ji}$, for example, in the x component:

$$\Delta_{ij,x} = - \langle i| \lambda (\partial_y V(\boldsymbol{r}) p_z - \partial_z V(\boldsymbol{r}) p_y) |j\rangle = i\hbar\lambda \int d\boldsymbol{r} \phi_i(\boldsymbol{r})^* (\partial_y V(\boldsymbol{r})\partial_z - \partial_z V(\boldsymbol{r})\partial_y)\phi_j(\boldsymbol{r}) =$$

$$= -i\hbar\lambda \int d\boldsymbol{r} \left[\partial_z(\phi_i(\boldsymbol{r})^* \partial_y V(\boldsymbol{r}) - \partial_y(\phi_i(\boldsymbol{r})^* \partial_z V(\boldsymbol{r}) \right] \phi_j(\boldsymbol{r}) =$$

$$= -i\hbar\lambda \int d\boldsymbol{r} \left[\partial_z \phi_i(\boldsymbol{r})^* \partial_y V(\boldsymbol{r}) - \partial_y \phi_i(\boldsymbol{r})^* \partial_z V(\boldsymbol{r}) \right] \phi_j(\boldsymbol{r}) =$$

$$= \int d\boldsymbol{r} \phi_j(\boldsymbol{r}) \lambda (\boldsymbol{\nabla} V(\boldsymbol{r}) \times \boldsymbol{p})_x \phi_i(\boldsymbol{r})^* = -\Delta_{ji,x}$$

Therefore $\Delta_{ii} = 0$. Notice also that Δ_{ij} is purely imaginary. We can impose that $t_{ii} = t(0) = 0$. For a system of strongly correlated electrons we can assume that:

- A property of the Wannier functions Φ_j is that they have exponentially decreasing overlaps, therefore t_{ij} and Δ_{ij} will decay rapidly with the distance $|\mathbf{r}_i - \mathbf{r}_j|$. In an isotropic system we can approximate:

$$t_{ij} = \begin{cases} t, & \text{for } (i,j) \text{ nearest neighbous} \\ 0, & \text{otherwise} \end{cases} \tag{3.9}$$

and

$$\Delta_{ij} = \begin{cases} \Delta_{ij}, & \text{for } (i,j) \text{ nearest neighbours} \\ 0, & \text{otherwise} \end{cases} \tag{3.10}$$

Hubbard models with hopping terms further than nearest neighbors are also interesting and will be considered in next chapter.

- Taking into account the locality of the Wannier functions and the Coulomb interaction, the dominant contribution of $\langle ij| \hat{v} |kl\rangle$ will come from $i = j = k = l$. Terms with $i = k$ and $j = l$ also contribute when i, j are nearest neighbours. Therefore we approximate:

$$\langle ij| \hat{v} |kl\rangle = \begin{cases} U, & \text{if } i = j = k = l \\ V, & \text{if } i = k \text{ and } j = l \text{ where } (i,j) \text{ nearest neighbours} \\ 0, & \text{otherwise} \end{cases} \tag{3.11}$$

Where we defined:

$$U = \frac{1}{2} \int d\boldsymbol{r} d\boldsymbol{r}' \phi(\boldsymbol{r})^* \phi(\boldsymbol{r}')^* \hat{v}(\boldsymbol{r} - \boldsymbol{r}') \phi(\boldsymbol{r}') \phi(\boldsymbol{r}) \tag{3.12}$$

$$V = \int d\boldsymbol{r} d\boldsymbol{r}' \phi(\boldsymbol{r})^* \phi(\boldsymbol{r}' - \boldsymbol{R}_1)^* \hat{v}(\boldsymbol{r} - \boldsymbol{r}') \phi(\boldsymbol{r}' - \boldsymbol{R}_1) \phi(\boldsymbol{r}) \tag{3.13}$$

Where $\phi(\boldsymbol{r})$ is the Wannier function centered at the origin and $\boldsymbol{R}_1$ is a nearest neighbour lattice vector. Notice that we made explicit use of the translational invariance of the system. Also, for $i = j = k = l$ the Pauli principle requires $\sigma' = -\sigma$.
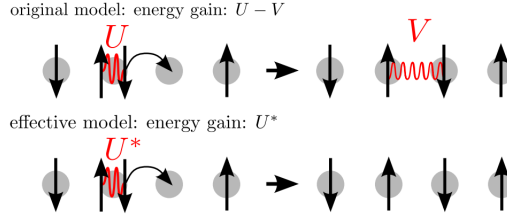
FIGURE 3.1: Image from [12]. In a half-filled system decreasing the number of double occupancies increases the number of adjacent occupied sites, and so the energy difference is reduced to U − V.

Taking these approximations and writing $\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'}^\dagger \hat{c}_{j\sigma'} \hat{c}_{i\sigma} = \hat{n}_{i\sigma} \hat{n}_{j\sigma'}$, we obtain:

$$\hat{H} = -\sum_{\langle i,j \rangle, \sigma, \sigma'} (\delta_{\sigma,\sigma'} t_{ij} + \mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma,\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} + \mathrm{U} \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \mathrm{V} \sum_{i,j,\sigma,\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} \qquad (3.14)$$

Now, in a half filling system this Hamiltonian can be well approximated by an effective Hamiltonian without non local Coulomb interactions:

$$\hat{H} = -\sum_{\langle i,j \rangle, \sigma, \sigma'} (\delta_{\sigma,\sigma'} t_{ij} + \mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma,\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} + \mathrm{U}^* \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad (3.15)$$

Where $\mathrm{U}^* = \mathrm{U} - \mathrm{V}$. The physical reason for this is that the energy difference when the Coulomb interaction pushes an electron from a double occupied site to an empty site is U − V in 3.14, because the number of double occupied sites is reduced by one but the number of adjacent occupied sites is increased by one. This is illustred in Figure 3.1. A more rigouros derivation of this effective model can be found in [12]. Although V < U, they can be comparable in magnitude, and U^* can be reduced by a factor of 0.5 or more.

Now, abusing the notation and writing $\mathrm{U} = \mathrm{U}^*$ we arrive at the model that we will use in the next sections:

$$\hat{H} = -\sum_{\langle i,j \rangle, \sigma, \sigma'} (\delta_{\sigma,\sigma'} t_{ij} + \mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma,\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} + \mathrm{U} \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad (3.16)$$

3.2.1 Hubbard model

In the absence of spin-orbit interaction the model 3.16 becomes the well-known Hubbard model: $\hat{H} = -\sum_{\langle i,j \rangle, \sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \mathrm{U} \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$. This model has been extensively studied since its proposal in 1963 by Hubbard [10]. Despite its simplicity the ground state has no analytic form in more than one dimensions, and different computational methods must be used to study it. Originally the Hubbard model was proposed to describe electron correlations in d or f bands in transition metals. The result was a simplified model to predict metal-insulator transitions. However, it exhibits much richer phenomena. It can be considered an impoved tight binding model, describing Mott insulators, which cannot be described by band theory (i.e. they should be conductors according to band theory, but electron-electron interactions keep away from). Also, the attractive Hubbard model (where U < 0) can be considered an effective model relevant for understanding high temperature superconductivity [13].

3.3 Effective Hamiltonian for half-filling system

At half filling and in the $t << U$ limit, which correspond to the strong coupling limit, we can apply perturbation theory to obtain the Heisenberg model from the Hubbard Hamiltonian 3.16. First notice that in the case $t = 0$ the ground state corresponds to having all sites single-occupied. There are two possible spin orientations for each sites, so there is a 2^M degeneracy. The ground state energy is 0. The first exited states are obtained by moving one electron from one site to another, thus leaving one empty site and one double-occupied site. The energy of one of these states is U. Now, if we turn the kinetic term on as a perturbation, having two neighbors electrons with antiparallel spin will allow them to hop and reduce the kinetic energy, whereas while being parallel this hopping is not allowed and there is no energy reduction. Therefore, we can see that when turning the kinetic term on antiparallel alignment will be favored.

Let us write $\hat{H} = \hat{H}_0 + \hat{H}_t$, where $\hat{H}_0$ is the Hamiltonian for $t = 0$ i.e. $\hat{H}_0 = U \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ and $\hat{H}_t = -\sum_{\langle i,j \rangle, \sigma, \sigma'} (\delta_{\sigma,\sigma'} t + \mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma,\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'}$. Let $|\phi\rangle$ and $|\phi'\rangle$ be states from the ground state of $\hat{H}_0$, then we know $\langle \phi'| \hat{H}_0 |\phi\rangle = 0$ and in first order in t $\langle \phi'| \hat{H} |\phi\rangle = \langle \phi'| \hat{H}_t |\phi\rangle = 0$ since $\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}$ moves an electron from site j to i thus leaving i doubly occupied, therefore $\hat{H}_t |\phi\rangle$ has no superposition with ϕ'. In second order we have:

$$\langle \phi'| \hat{H} |\phi\rangle = \sum_s \frac{\langle \phi'| \hat{H}_t |s\rangle \langle s| \hat{H}_t |\phi\rangle}{E_0 - E_s} \tag{3.17}$$

The sum being over all excited states. Since $\hat{H}_t |\phi\rangle$ is a superposition of states with exactly one double occupied site and one empty site, we see that only excited states with one double occupied site will contribute. These states have energy $E_s = U$ therefore we have $\langle \phi'| \hat{H} |\phi\rangle = -\frac{1}{U} \sum_s \langle \phi'| \hat{H}_t |s\rangle \langle s| \hat{H}_t |\phi\rangle = \langle \phi'| -\frac{\hat{H}_t^2}{U} |\phi\rangle$. This means that within the subspace generated by the ground states of $\hat{H}_0$, $\hat{H}$ acts as an effective Hamiltonian $\hat{H}_{\text{eff}} = -\frac{\hat{H}_t^2}{U}$. Now,

$$\langle \phi'| -\frac{\hat{H}_t^2}{U} |\phi\rangle =$$

$$= -\frac{1}{U} \langle \phi'| \sum_{\langle i,j \rangle, \sigma_1, \sigma_2} \sum_{\langle i',j' \rangle, \sigma_3, \sigma_4} (\delta_{\sigma_1,\sigma_2} t + \mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_1,\sigma_2})(\delta_{\sigma_3,\sigma_4} t + \mathbf{\Delta}_{i'j'} \boldsymbol{\sigma}_{\sigma_3,\sigma_4}) \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{i'\sigma_3}^\dagger \hat{c}_{j'\sigma_4} |\phi\rangle =$$

$$= -\frac{1}{U} \langle \phi'| \sum_{\langle i,j \rangle, \sigma_1, \sigma_2, \sigma_3, \sigma_4} (\delta_{\sigma_1,\sigma_2} t + \mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_1,\sigma_2})(\delta_{\sigma_3,\sigma_4} t - \mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_3,\sigma_4}) \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4} |\phi\rangle =$$

$$-\frac{1}{U} \langle \phi'| \sum_{\langle i,j \rangle, \sigma_1, \sigma_2, \sigma_3, \sigma_4} (t^2 \delta_{\sigma_1\sigma_2} \delta_{\sigma_3\sigma_4} + t\mathbf{\Delta}_{ij}(\delta_{\sigma_3\sigma_4} \boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1\sigma_2} \boldsymbol{\sigma}_{\sigma_3\sigma_4}) - (\mathbf{\Delta}_{ij} \boldsymbol{\sigma}_{\sigma_1\sigma_2})(\mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_3\sigma_4})) \hat{c}_{i\sigma_1}^\dagger \hat{c}_{i\sigma_4} \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger |\phi\rangle =$$

$$\langle \phi'| \hat{H}_J + \hat{H}_D + \hat{H}_P |\phi\rangle \tag{3.18}$$

In the second line we imposed $i = j'$ and $j = i'$ since that's the only way $\hat{H}_t^2 |\phi\rangle$ has no double occupied sites and so the matrix element does not vanish. We also used $\mathbf{\Delta}_{ij} = -\mathbf{\Delta}_{ji}$. We defined:

$$\hat{H}_J = -\frac{t^2}{U} \sum_{\langle i,j \rangle, \sigma, \sigma'} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma'} \hat{c}_{j\sigma} \hat{c}_{j\sigma'}^\dagger \tag{3.19}$$

$$\hat{H}_D = -\frac{t}{U} \sum_{\langle i,j \rangle, \sigma_1, \sigma_2, \sigma_3, \sigma_4} \boldsymbol{\Delta}_{ij}(\delta_{\sigma_3\sigma_4}\boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_3\sigma_4})\hat{c}_{i\sigma_1}^\dagger \hat{c}_{i\sigma_4} \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \tag{3.20}$$

$$\hat{H}_P = \frac{1}{U} \sum_{\langle i,j \rangle, \sigma_1, \sigma_2, \sigma_3, \sigma_4} (\boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_1\sigma_2})(\boldsymbol{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_3\sigma_4})\hat{c}_{i\sigma_1}^\dagger \hat{c}_{i\sigma_4} \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \tag{3.21}$$

Let us now introduce the on-site spin operators:

$$S_i = \frac{1}{2} \sum_{\sigma, \sigma'} \hat{c}_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma,\sigma'} \hat{c}_{i\sigma'} \tag{3.22}$$

Which satisfy:

$$\hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma'} = \delta_{\sigma\sigma'}\frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) + S_i \cdot \boldsymbol{\sigma}_{\sigma',\sigma} \tag{3.23}$$

$$\hat{c}_{i\sigma} \hat{c}_{i\sigma'}^\dagger = \delta_{\sigma\sigma'}\frac{1}{2}(2 - n_{i\uparrow} - n_{i\downarrow}) - \cdot S_i \boldsymbol{\sigma}_{\sigma,\sigma'} \tag{3.24}$$

In the half-filling case we have $n_{i\uparrow} + n_{i\downarrow} = 1$ and we can show two important relations. First:

$$\sum_{\sigma\sigma'} \left(\frac{1}{2}\delta_{\sigma\sigma'} + S_i \cdot \boldsymbol{\sigma}_{\sigma'\sigma}\right)\left(\frac{1}{2}\delta_{\sigma\sigma'} - S_j \cdot \boldsymbol{\sigma}_{\sigma\sigma'}\right) = \sum_{\sigma\sigma'}\left\{\frac{1}{4}\delta_{\sigma\sigma'} - \sum_{ab}S_i^a S_j^b \boldsymbol{\sigma}_{\sigma'\sigma}^a \cdot \boldsymbol{\sigma}_{\sigma\sigma'}^b\right\} =$$

$$= \frac{1}{2} - \sum_{ab}S_i^a S_j^b 2\delta_{ab} = \frac{1}{2} - 2S_i \cdot S_j$$

Where we have neglected the term $\sum_{\sigma\sigma'} \frac{1}{2}\delta_{\sigma,\sigma'}(S_i \cdot \boldsymbol{\sigma}_{\sigma',\sigma} - S_j \cdot \boldsymbol{\sigma}_{\sigma,\sigma'})$ because eventually we will sum over all $\langle i, j \rangle$ and it will cancel out. We also used the well known property $tr(\sigma^a\sigma^b) = 2\delta_{a,b}$. And second:

$$\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} \mathbf{\Delta}_{ij} \cdot (\delta_{\sigma_3\sigma_4}\boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_3\sigma_4}) \left(\frac{1}{2}\delta_{\sigma_1\sigma_4} + \mathbf{S}_i \cdot \boldsymbol{\sigma}_{\sigma_4\sigma_1}\right) \left(\frac{1}{2}\delta_{\sigma_2\sigma_3} - \mathbf{S}_j \cdot \boldsymbol{\sigma}_{\sigma_2\sigma_3}\right) =$$

$$= \{ \overbrace{0}^{\uparrow\uparrow\uparrow\uparrow} + \overbrace{(-\Delta_{ij}^+)S_i^-(\frac{1}{2} - S_j^z)}^{\uparrow\uparrow\downarrow\uparrow} + \overbrace{(-\Delta_{ij}^-)(\frac{1}{2} + S_i^z)(-S_j^+)}^{\uparrow\uparrow\downarrow\uparrow} + \overbrace{2\Delta_{ij}^z S_i^-(-S_j^+)}^{\uparrow\uparrow\downarrow\downarrow} +$$

$$\overbrace{\Delta_{ij}^+(\frac{1}{2} + S_i^z)(-S_j^-)}^{\uparrow\downarrow\uparrow\uparrow} + \overbrace{0}^{\uparrow\downarrow\uparrow\downarrow} + \overbrace{0}^{\uparrow\downarrow\downarrow\uparrow} + \overbrace{\Delta_{ij}^+ S_i^-(\frac{1}{2} + S_j^z)}^{\uparrow\downarrow\downarrow\downarrow} +$$

$$\overbrace{\Delta_{ij}^- S_i^+(\frac{1}{2} - S_j^z)}^{\downarrow\uparrow\uparrow\uparrow} + \overbrace{0}^{\downarrow\uparrow\uparrow\downarrow} + \overbrace{0}^{\downarrow\uparrow\downarrow\uparrow} + \overbrace{\Delta_{ij}^-(\frac{1}{2} - S_i^z)(-S_j^+)}^{\downarrow\uparrow\downarrow\downarrow} +$$

$$\overbrace{(-2\Delta_{ij}^z)S_i^+(-S_j^-)}^{\downarrow\downarrow\uparrow\uparrow} + \overbrace{(-\Delta_{ij}^+)(\frac{1}{2} - S_i^z)(-S_j^-)}^{\downarrow\downarrow\uparrow\downarrow} + \overbrace{(-\Delta_{ij}^-)S_i^+(\frac{1}{2} + S_j^z)}^{\downarrow\downarrow\downarrow\uparrow} + \overbrace{0}^{\downarrow\downarrow\downarrow\downarrow} \} =$$

$$= 2\left\{\Delta_{ij}^+(S_i^- S_j^z - S_i^z S_j^-) + \Delta_{ij}^-(S_i^z S_j^+ - S_i^+ S_j^z) + \Delta_{ij}^z(S_i^+ S_j^- - S_i^- S_j^+)\right\} =$$

$$= -2i\left\{\Delta_{ij}^+(\mathbf{S}_i \times \mathbf{S}_j)^- + \Delta_{ij}^-(\mathbf{S}_i \times \mathbf{S}_j)^+ + 2\Delta_{ij}^z(\mathbf{S}_i \times \mathbf{S}_j)^z\right\} = -4i\mathbf{\Delta}_{ij} \cdot \mathbf{S}_i \times \mathbf{S}_j$$

Where in the second line we expand the sum in the spin states (overbrace indicates the spin state σ_1, σ_2, σ_3, σ_4 respectively). We also used that for any vector $\vec{v}$ we can define $\sigma_{12}\vec{v} = v^x + iv^y = v^+$, $\sigma_{21}\vec{v} = v^x - iv^y = v^-$, $\sigma_{11}\vec{v} = v^z$ and $\sigma_{22}\vec{v} = -v^z$. Also, for any two vectors $\vec{a}$ and $\vec{b}$, the following applies $a^-b^z - a^z b^- = -i(\vec{a} \times \vec{b})^-$, $a^z b^+ - a^+ b^z = -i(\vec{a} \times \vec{b})^+$, $a^+ b^- - a^- b^+ = -2i(\vec{a} \times \vec{b})^z$ and $a^+ b^- + a^- b^+ = 2(a^x b^x + a^y b^y)$.

Also:

$$\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} (\mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_1\sigma_2})(\mathbf{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_3\sigma_4}) \left(\frac{1}{2}\delta_{\sigma_1\sigma_4} + \mathbf{S}_i \cdot \boldsymbol{\sigma}_{\sigma_4\sigma_1} \right) \left(\frac{1}{2}\delta_{\sigma_2\sigma_3} - \mathbf{S}_j \cdot \boldsymbol{\sigma}_{\sigma_2\sigma_3} \right) =$$

$$= \overbrace{\Delta_{ij}^z \Delta_{ij}^z (\frac{1}{2} + S_i^z)(\frac{1}{2} - S_j^z)}^{\uparrow\uparrow\uparrow\uparrow} + \overbrace{\Delta_{ij}^z \Delta_{ij}^+ S_i^- (\frac{1}{2} - S_j^z)}^{\uparrow\uparrow\uparrow\downarrow} + \overbrace{\Delta_{ij}^z \Delta_{ij}^- (\frac{1}{2} + S_i^z)(-S_j^+)}^{\uparrow\uparrow\downarrow\uparrow} + \overbrace{\Delta_{ij}^z (-\Delta_{ij}^z) S_i^- (-S_j^+)}^{\uparrow\uparrow\downarrow\downarrow} +$$

$$\overbrace{\Delta_{ij}^+ \Delta_{ij}^z (\frac{1}{2} + S_i^z)(-S_j^-)}^{\uparrow\downarrow\uparrow\uparrow} + \overbrace{\Delta_{ij}^+ \Delta_{ij}^+ S_i^- (-S_j^-)}^{\uparrow\downarrow\uparrow\downarrow} + \overbrace{\Delta_{ij}^+ \Delta_{ij}^- (\frac{1}{2} + S_i^z)(\frac{1}{2} + S_j^z)}^{\uparrow\downarrow\downarrow\uparrow} + \overbrace{\Delta_{ij}^+ (-\Delta_{ij}^z) S_i^- (\frac{1}{2} + S_j^z)}^{\uparrow\downarrow\downarrow\downarrow} +$$

$$\overbrace{\Delta_{ij}^- \Delta_{ij}^z S_i^+ (\frac{1}{2} - S_j^z)}^{\downarrow\uparrow\uparrow\uparrow} + \overbrace{\Delta_{ij}^- \Delta_{ij}^+ (\frac{1}{2} - S_i^z)(\frac{1}{2} - S_j^z)}^{\downarrow\uparrow\uparrow\downarrow} + \overbrace{\Delta_{ij}^- \Delta_{ij}^- S_i^+ (-S_j^+)}^{\downarrow\uparrow\downarrow\uparrow} + \overbrace{\Delta_{ij}^- (-\Delta_{ij}^z)(\frac{1}{2} - S_i^z)(-S_j^+)}^{\downarrow\uparrow\downarrow\downarrow} +$$

$$\overbrace{(-\Delta_{ij}^z)\Delta_{ij}^z S_i^+ (-S_j^-)}^{\downarrow\downarrow\uparrow\uparrow} + \overbrace{(-\Delta_{ij}^z)\Delta_{ij}^+ (\frac{1}{2} - S_i^z)(-S_j^-)}^{\downarrow\downarrow\uparrow\downarrow} + \overbrace{(-\Delta_{ij}^z)\Delta_{ij}^- S_i^+ (\frac{1}{2} + S_j^z)}^{\downarrow\downarrow\downarrow\uparrow} +$$

$$+ \overbrace{(-\Delta_{ij}^z)(-\Delta_{ij}^z)(\frac{1}{2} - S_i^z)(\frac{1}{2} + S_j^z)}^{\downarrow\downarrow\downarrow\downarrow} =$$

$$= \frac{(\Delta_{ij}^z)^2 + \Delta_{ij}^+ \Delta_{ij}^-}{2} + S_i^z S_j^z (-2(\Delta_{ij}^z)^2 + 2\Delta_{ij}^+ \Delta_{ij}^-) + S_i^z S_j^+ (-2\Delta_{ij}^z \Delta_{ij}^-) + S_i^z S_j^- (-2\Delta_{ij}^z \Delta_{ij}^+) +$$

$$+ S_i^+ S_j^z (-2\Delta_{ij}^z \Delta_{ij}^-) + S_i^+ S_j^+ (-\Delta_{ij}^- \Delta_{ij}^-) + S_i^+ S_j^- (\Delta_{ij}^z)^2 +$$

$$+ S_i^- S_j^z (-2\Delta_{ij}^z \Delta_{ij}^+) + S_i^- S_j^+ (\Delta_{ij}^z)^2 + S_i^- S_j^- (-(\Delta_{ij}^+)^2) =$$

$$= \frac{(\Delta_{ij}^z)^2 + \Delta_{ij}^+ \Delta_{ij}^-}{2} + S_i^z S_j^z (-2(\Delta_{ij}^z)^2 + 2(\Delta_{ij}^x)^2 + 2(\Delta_{ij}^y)^2 + S_i^z S_j^y (-4\Delta_{ij}^z \Delta_{ij}^y) + S_i^z S_j^x (-4\Delta_{ij}^z \Delta_{ij}^x) +$$

$$+ S_i^y S_j^z (-4\Delta_{ij}^y \Delta_{ij}^z) + S_i^y S_j^y (2(\Delta_{ij}^z)^2 - 2(\Delta_{ij}^y)^2 + 2(\Delta_{ij}^x)^2) + S_i^y S_j^x (-4\Delta_{ij}^y \Delta_{ij}^x) +$$

$$+ S_i^x S_j^z (-4\Delta_{ij}^x \Delta_{ij}^z) + S_i^x S_j^y (-4\Delta_{ij}^x \Delta_{ij}^y) + S_i^x S_j^x (2(\Delta_{ij}^z)^2 + 2(\Delta_{ij}^y)^2 - 2(\Delta_{ij}^x)^2) =$$

$$= \frac{(\Delta_{ij}^z)^2 + \Delta_{ij}^+ \Delta_{ij}^-}{2} + \begin{pmatrix} S_i^x & S_i^y & S_i^z \end{pmatrix}$$

$$\begin{pmatrix} 2(\Delta_{ij}^z)^2 + 2(\Delta_{ij}^y)^2 - 2(\Delta_{ij}^x)^2 & -4\Delta_{ij}^x \Delta_{ij}^y & -4\Delta_{ij}^x \Delta_{ij}^z \\ -4\Delta_{ij}^y \Delta_{ij}^x & +2(\Delta_{ij}^x)^2 - 2(\Delta_{ij}^y)^2 + 2(\Delta_{ij}^z)^2 & -4\Delta_{ij}^y \Delta_{ij}^z \\ -4\Delta_{ij}^z \Delta_{ij}^x & -4\Delta_{ij}^z \Delta_{ij}^y & 2(\Delta_{ij}^x)^2 + 2(\Delta_{ij}^y)^2 - 2(\Delta_{ij}^z)^2 \end{pmatrix} \begin{pmatrix} S_j^x \\ S_j^y \\ S_j^z \end{pmatrix} =$$

$$\frac{(\Delta_{ij}^z)^2 + \Delta_{ij}^+ \Delta_{ij}^-}{2} + \sum_{\alpha,\beta} S_i^\alpha (4\Delta_{ij}^\alpha \Delta_{ij}^\beta - \delta_{\alpha\beta} 2\mathbf{\Delta}_{ij}^2) S_j^\beta$$

These three relations are important and will be used in the next chapter:

$$\sum_{\sigma\sigma'} \left(\frac{1}{2}\delta_{\sigma\sigma'} + \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma'\sigma} \right) \left(\frac{1}{2}\delta_{\sigma\sigma'} - \boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\sigma\sigma'} \right) =$$

$$= \frac{1}{2} - \sum_{ab} S_i^a S_j^b 2\delta_{ab} = \frac{1}{2} - 2\boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{3.25}$$

$$\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} \boldsymbol{\Delta}_{ij} \cdot (\delta_{\sigma_3\sigma_4}\boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_3\sigma_4}) \left(\frac{1}{2}\delta_{\sigma_1\sigma_4} + \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma_4\sigma_1} \right) \left(\frac{1}{2}\delta_{\sigma_2\sigma_3} - \boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\sigma_2\sigma_3} \right) =$$

$$= -4i\boldsymbol{\Delta}_{ij} \cdot \boldsymbol{S}_i \times \boldsymbol{S}_j \tag{3.26}$$

$$\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} (\boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_1\sigma_2})(\boldsymbol{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_3\sigma_4})\boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma_4\sigma_1} \left(-\boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\sigma_2\sigma_3} \right) =$$

$$= \sum_{\alpha,\beta} S_i^\alpha (\delta_{\alpha\beta} 2\boldsymbol{\Delta}_{ij}^2 - 4\Delta_{ij}^\alpha\Delta_{ij}^\beta) S_j^\beta \tag{3.27}$$

Now introducing the spin operators into $\hat{H}_J$ with $n_{i\uparrow} + n_{i\downarrow} = 1$ and using 3.25 we obtain:

$$\hat{H}_J = -\frac{t^2}{U} \sum_{\langle i,j \rangle, \sigma\sigma'} \left(\frac{1}{2}\delta_{\sigma\sigma'} + \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma'\sigma} \right) \left(\frac{1}{2}\delta_{\sigma\sigma'} - \boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\sigma\sigma'} \right) =$$

$$- \frac{t^2}{U} \sum_{\langle i,j \rangle} \left(\frac{1}{2} - 2\boldsymbol{S}_i \cdot \boldsymbol{S}_j \right)$$

The constant term can be neglected leaving:

$$\hat{H}_J = \frac{2t^2}{U} \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j = \sum_{\langle i,j \rangle} J_{ij}^0 \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{3.28}$$

Which is the Heisenberg model for antiferromagnets with $J_{ij}^0 = \frac{2t^2}{U} > 0$. Likewise, for $\hat{H}_D$, using 3.26:

$$\hat{H}_D = -\frac{t}{U} \sum_{\langle i,j \rangle, \sigma_1,\sigma_2,\sigma_3,\sigma_4} \boldsymbol{\Delta}_{ij} \cdot (\delta_{\sigma_3\sigma_4}\boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_3\sigma_4}) \left(\frac{1}{2}\delta_{\sigma_1\sigma_4} + \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma_4\sigma_1} \right) \left(\frac{1}{2}\delta_{\sigma_2\sigma_3} - \boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\sigma_2\sigma_3} \right) =$$

$$= +\frac{4it}{U} \sum_{\langle i,j \rangle} \boldsymbol{\Delta}_{ij} \cdot \boldsymbol{S}_i \times \boldsymbol{S}_j = \sum_{\langle i,j \rangle} \boldsymbol{D}_{ij}^0 \cdot \boldsymbol{S}_i \times \boldsymbol{S}_j$$

Where $\boldsymbol{D}_{ij}^0 = \frac{4it}{U}\boldsymbol{\Delta}_{ij}$, notice that being $\boldsymbol{\Delta}_{ij}$ purely imaginary, $\boldsymbol{D}_{ij}^0$ is a real vector. Lastly, using 3.27, the term proportional to $\boldsymbol{\Delta}_{ij}^2$ leads to:

$$\hat{H}_P = \frac{1}{U} \sum_{\langle i,j \rangle, \sigma_1,\sigma_2,\sigma_3,\sigma_4} (\boldsymbol{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_1\sigma_2})(\boldsymbol{\Delta}_{ij} \cdot \boldsymbol{\sigma}_{\sigma_3\sigma_4}) \left(\frac{1}{2}\delta_{\sigma_1\sigma_4} + \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma_4\sigma_1} \right) \left(\frac{1}{2}\delta_{\sigma_2\sigma_3} - \boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\sigma_2\sigma_3} \right) =$$

$$\frac{1}{U} \sum_{\langle i,j \rangle} \sum_{\alpha,\beta} S_i^\alpha (\delta_{\alpha\beta} 2\boldsymbol{\Delta}_{ij}^2 - 4\Delta_{ij}^\alpha\Delta_{ij}^\beta) S_j^\beta = \sum_{\langle i,j \rangle} \boldsymbol{S}_i \boldsymbol{\Gamma}_{ij} \boldsymbol{S}_j$$

With $\boldsymbol{\Gamma}_{ij}^{\alpha\beta} = \frac{1}{U}(\delta_{\alpha\beta} 2\boldsymbol{\Delta}_{ij}^2 - 4\Delta_{ij}^\alpha\Delta_{ij}^\beta)$. The total effective Hamiltonian is:

$$\hat{H}_{\text{eff}} = \sum_{\langle i,j \rangle} \left(J_{ij}^0 \mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{D}_{ij}^0 \cdot \mathbf{S}_i \times \mathbf{S}_j + \mathbf{S}_i \mathbf{\Gamma}_{ij} \mathbf{S}_j \right) \tag{3.29}$$

With:

$$J_{ij}^0 = \frac{2t^2}{U} \tag{3.30}$$

$$\mathbf{D}_{ij}^0 = \frac{4it}{U} \mathbf{\Delta}_{ij} \tag{3.31}$$

$$\mathbf{\Gamma}_{ij}^{\alpha\beta} = \frac{1}{U} (\delta_{\alpha\beta} 2\Delta_{ij}^2 - 4\Delta_{ij}^\alpha \Delta_{ij}^\beta) \tag{3.32}$$

The $J_{ij}^0 \mathbf{S}_i \cdot \mathbf{S}_j$ term is known as exchange interaction, in the $\mathbf{\Delta}_{ij} = 0$ limit (no SOI) we see that 3.29 reduces to the Heisenberg model. Since $J_{ij}^0 > 0$ this model describes an antiferromagnetic material. However, the Hubbard model can also lead to ferromagnetic and paramagnetic magnetic behavior in non half-filled systems as shown in [14] with a mean-field theory approach. $\mathbf{D}_{ij}^0 \cdot \mathbf{S}_i \times \mathbf{S}_j$ is known as Dzyaloshinskii-Moriya interaction (DMI), the symmetries of the crystal will restrict the direction of $\mathbf{D}_{ij}^0$ [11]. In the next chapter we will examine this further. Lastly $\mathbf{S}_i \mathbf{\Gamma}_{ij} \mathbf{S}_j$ is an anisotropic term known as pseudodipolar interaction [11] and it is usually neglected since it is proportional to $\mathbf{\Delta}_{ij}^2$.

3.3.1 Next-nearest neighbor hopping

This analysis can be easily extended to electronic Hamiltonians including next-nearest neighbor (NNN) hopping term. The simplest example of such a Hamiltonian is:

$$\hat{H} = - \sum_{\langle i,j \rangle, \sigma} t_1 \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} - \sum_{\langle\langle i,j \rangle\rangle, \sigma} t_2 \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{3.33}$$

Where $\langle\langle i,j \rangle\rangle$ denotes sum over NNN. If we follow the procedure as before we will obtain an effective spin Hamiltonian:

$$\hat{H}_{\text{eff}} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{3.34}$$

Where $J_1 = \frac{t_1^2}{U}$ and $J_2 = \frac{t_2^2}{U}$. This Hamiltonian is known as $J_1 - J_2$ Heisenberg model. This model has been extensively studied, and the $J_1 - J_2 - J_3$ is also of interest [15].

Notice that we can also obtain a $J_1 - J_2$ Heisenberg model starting simply from a NN hamiltonian $\hat{H} = -\sum_{\langle i,j \rangle, \sigma} t_1 \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$. This is because the NNN exchange interaction comes from the possibility of the process $i\sigma \to j\sigma \to i\sigma$ being i, j NNN. This process is available when sites i, j have opposite spins (otherwise it would violate the Pauli principle). Now, when i, j are NNN, we can consider the fourth order process $i\sigma \to k\sigma \to j\sigma \to k\sigma \to i\sigma$, where k is a site between i and j. The resulting effective spin Hamiltonian has exchange couplings $J_1 = 2\frac{t_1^2}{U} - 8\frac{t_1^4}{U^3}$ and $J_2 = 2\frac{t_1^4}{U}$. A rigorous derivation can be found in [16].

3.3.2   Introducing disorder

It is possible to consider a disordered Hubbard model by adding random uncorrelated on-site energies. We neglect the SOI term for simplicity, then the disordered Hubbard model can be written as:

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \sum_{i\sigma} \epsilon_i \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma} + \mathrm{U} \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{3.35}$$

Where ϵ_i are random variable $\epsilon_i \in [-W, W]$. At half filling we can derive an effective Hamiltonian using the same procedure as before. The second order virtual hopping $i\sigma \rightarrow j\sigma \rightarrow i\sigma$ will give rise to an exchange spin interaction. In this case, however, the intermediate energy is $\mathrm{U} + (\epsilon_j - \epsilon_i)$. Therefore the spin Hamiltonian will be:

$$\hat{H}_{\text{eff}} = \sum_{\langle i,j \rangle} \frac{2t^2}{\mathrm{U} + (\epsilon_j - \epsilon_i)} S_i \cdot S_j = \sum_{\langle i,j \rangle} \frac{2t^2 \mathrm{U}}{\mathrm{U}^2 - (\epsilon_j - \epsilon_i)^2} S_i \cdot S_j = \sum_{\langle i,j \rangle} J_{ij} S_i \cdot S_j \tag{3.36}$$

Where in the second step we added the contributions of $\langle i, j \rangle$ and $\langle j, i \rangle$ and where $J_{ij} = \frac{2t^2 \mathrm{U}}{\mathrm{U}^2 - (\epsilon_j - \epsilon_i)^2}$. This model is relevant for studying many-body localization phenomena [17].

3.4   AFM dynamics

In this section we will show how a continuum one dimensional model can be obtained from the discrete Heisenberg Hamiltonian in order to describe the AFM order and its dynamics [18]. We write the Heisenberg Hamiltonian as $\hat{H} = J \sum_{\langle i,j \rangle} S_i S_j - K \sum_i S_{iz}^2$ with $J > 0$ and K is the anisotropy energy. Let the lattice be a one dimensional chain with $2N$ sites, such lattice can be described by the repetition of N unit cells consisting of two sites α and β for the left and right site respectively. Then the ground state of this Hamiltonian is double degenerated and is obtained by aligning the spins in the α sites in the $\hat{z}$ direction and the β spins in the $-\hat{z}$ direction or vice versa. Let us introduce the parameters:

$$m_i = \frac{S_\alpha^i + S_\beta^i}{2S} \tag{3.37}$$

$$l_i = \frac{S_\alpha^i - S_\beta^i}{2S} \tag{3.38}$$

Where S is the spin angular momentum in units of $\hbar$. Inverting these relations, introducing them into the Hamiltonian and neglecting edge terms we obtain:

$$\hat{H} = JS^2 \sum_i^{N-1} (\boldsymbol{m}_i - \boldsymbol{l}_i)(\boldsymbol{m}_i + \boldsymbol{l}_i + \boldsymbol{m}_{i+1} + \boldsymbol{l}_{i+1}) - KS^2 \sum_i^N \left[(\boldsymbol{m}_{iz} + \boldsymbol{l}_{iz})^2 + (\boldsymbol{m}_{iz} - \boldsymbol{l}_{iz})^2 \right] =$$

$$2JS^2 \sum_i^N (\boldsymbol{m}_i^2 - \boldsymbol{l}_i^2) + \frac{JS^2}{2} \sum_i^{N-1} \left[(\boldsymbol{l}_{i+1} - \boldsymbol{l}_i)^2 - (\boldsymbol{m}_{i+1} - \boldsymbol{m}_i)^2 \right]$$

$$+ JS^2 \sum_i^{N-1} \left[\boldsymbol{m}_i (\boldsymbol{l}_{i+1} - \boldsymbol{l}_i) - \boldsymbol{l}_i (\boldsymbol{m}_{i+1} - \boldsymbol{m}_i) \right] - 2KS^2 \sum_i^N (\boldsymbol{m}_{iz}^2 + \boldsymbol{l}_{iz}^2) \tag{3.39}$$

Now we can take the continuum limit with:

$$\boldsymbol{m}_i \to \boldsymbol{m}(x)$$
$$\boldsymbol{l}_i \to \boldsymbol{l}(x)$$
$$2d \sum_i \to \int dx$$
$$\hat{H} \to \int \frac{dx}{2d} \mathcal{H}(\boldsymbol{l}, \boldsymbol{m})$$

This, together with $\boldsymbol{m}_i - \boldsymbol{l}_i = 2\boldsymbol{m}_i - 1$ and $\boldsymbol{m}_{i+1} \to \boldsymbol{m}(x) + 2d\partial_x \boldsymbol{m}(x)$ gives:

$$\mathcal{H}(\boldsymbol{l}, \boldsymbol{m}) = JS^2 \left\{ 4|\boldsymbol{m}|^2 + |\partial_x \boldsymbol{l}'|^2 - |\partial_x \boldsymbol{m}'|^2 + (\boldsymbol{m}\partial_x \boldsymbol{l} - \boldsymbol{l}\partial_x \boldsymbol{m}) \right\} - KS^2 \left\{ (\boldsymbol{l}\hat{z})^2 + (\boldsymbol{m}\hat{z})^2 \right\} \tag{3.40}$$

Chapter 4

Perturbing the lattice

In this chapter we will derive an effective spin Hamiltonian for different models in the presence of a high frequency electromagnetic perturbation. The goal is to manipulate J and $\boldsymbol{D}_{ij}$ in 3.29 separately. This has already been done for the case of Mott insulators ([19], [20]) where the starting Hamiltonian is the Hubbard model:

$$\hat{H} = -t_0 \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + U \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

In this model, since SOI is not taken into account, only the exchange interaction J plays a role. The electromagnetic perturbation is then introduced via the Peierls substitution. We reproduce the result in section 4.2. In the following sections we extend the analysis to different systems with spin orbit interaction thereby modulating $\boldsymbol{D}_{ij}$ or other spin interactions. The simplest model with spin orbit interaction is 3.16:

$$\hat{H} = - \sum_{\langle i,j \rangle, \sigma, \sigma'} (\delta_{\sigma,\sigma'} t_0 + \boldsymbol{\Delta}_{ij} \boldsymbol{\sigma}_{\sigma,\sigma'}) \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma'} + U \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Which is the same Hubbard model plus a spin dependent hopping term, which represents Rashba SOI for $\boldsymbol{\Delta}_{ij} = i\Delta_R(R_{ij}^y, -R_{ij}^x, 0)$ or Dresselhaus SOI for $\boldsymbol{\Delta}_{ij} = i\Delta_R(R_{ij}^x, -R_{ij}^y, 0)$. In section 4.3 we show how the exchange interaction and the DMI couplings are modulated in presence of an electromagnetic field.

In the case of graphene or other coplanar honeycomb lattice structures, nearest neighbor Rashba terms are not allowed by symmetry, and only next nearest neighbor (NNN) spin conserving terms contribute [21], this term opens a gap in the band structure describing a topological insulator. For this case we examine the Kane-Mele-Hubbard model. The effective spin model of this Hamiltonian contains the usual exchange interaction and DMI and, in addition, it exhibits anisotropic exchange interaction arising from the intrinsic SOI term. This new term has already been obtained in [22] without taking into account any electromagnetic field.

Non-coplanar honeycomb lattice may exhibit intrinsic Rashba interactions between NNN [23], this, together with a NNN hopping (which would arise from direct overlapping of the next nearest neighbor Wannier functions or from second order processes) will lead to NNN DMI.

4.1   Time dependent effective Hamiltonian

First we will start we a general Hamiltonian of the type:

$$\hat{H} = -\hat{T} + U\hat{D} \tag{4.1}$$

Where $\hat{D} = \sum_{i=1}^{M} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the doublon number operator and $\hat{T}$ is any hopping operator. The only assumption we will make about $\hat{T}$ is that it is proportional to any power of $\hat{p}$ in which case we can apply the Peierls substitution (B) to introduce to take into account the effect of the electromagnetic perturbation in the lattice. The strength of the on-site interaction U is much larger than the hopping amplitude, therefore, in a half filling system the zero double occupancies subspace $d = 0$ can be taken as the low energy subspace in which the effective Hamiltonian will act.

In terms of on-site creation and annihilation operators we can write the hopping operator as $\hat{T} = \sum_{i,j,\sigma,\sigma'} t_{ij}^{\sigma\sigma'} \hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma'}$. In the simplest case, for example, the sum would be restricted to nearest neighbors and the hopping amplitude would be diagonal in the spin state. With this notation, in presence of a vector potential $\vec{A}(t)$ (which we assume to not vary noticeably in the scale of the lattice) the Peierls substitution leads to an extra time dependent phase in the hopping amplitude:

$$t_{ij}^{\sigma\sigma'}(t) = t_{ij}^{\sigma\sigma'} e^{ie\mathbf{R}_{ij}A(t)} \tag{4.2}$$

Where $\mathbf{A}$ is the vector potential and $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$. We write the electric field as $\mathbf{E}(t) = \frac{1}{2}(\vec{E}e^{-i\omega t} + \vec{E}^*e^{i\omega t})$, where $\vec{E} = E_0\hat{e}$ and $\hat{e} = \frac{1}{\sqrt{1+\lambda_{POL}^2}}(\hat{e}_x + i\lambda_{POL}\hat{e}_y)$ is the polarization vector and $\lambda_{POL} = 0, \pm 1$ for plane polarized, right handed and left handed circular polarized field respectively. The vector potential takes the form $\mathbf{A}(t) = \frac{1}{2}(\vec{A}e^{-i\omega t} + \vec{A}^*e^{i\omega t})$, with $\vec{A} = \frac{iE_0}{\omega}\hat{e}$.

Let us define:

$$e\mathbf{R}_{ij}\vec{A} = \alpha_{ij}e^{i\theta_{ij}} \tag{4.3}$$

With $\alpha_{ij} = \pm|e\mathbf{R}_{ij}\vec{A}|$ in such a way that:

$$\alpha_{ij} = -\alpha_{ji} \tag{4.4}$$
$$\theta_{ij} = \theta_{ji} \tag{4.5}$$

and $\theta_{ij} \in [0, \pi)$. Then we can apply the Jacobi–Anger expansion:

$$t_{ij}^{\sigma\sigma'}(t) = t_{ij}^{\sigma\sigma'} e^{ie\mathbf{R}_{ij}A(t)} = t_{ij}^{\sigma\sigma'} e^{i\alpha_{ij}\cos(\omega t - \theta_{ij})} = t_{ij}^{\sigma\sigma'} \sum_m e^{i(\frac{\pi}{2}-\theta_{ij})m} \mathcal{J}_m(\alpha_{ij})e^{im\omega t} = \sum t_{ij,m}^{\sigma\sigma'}e^{im\omega t}$$

Where we defined

$$t_{ij,m}^{\sigma\sigma'} = t_{ij}^{\sigma\sigma'} e^{i(\frac{\pi}{2}-\theta_{ij})m} \mathcal{J}_m(\alpha_{ij}) \tag{4.6}$$

Which is the mth Fourier mode of the hopping term and $\mathcal{J}_m(x)$ is the mth Bessel function [20]. Correspondingly we can write $\hat{T}(t) = \sum_m \hat{T}_m e^{im\omega t}$ where $\hat{T}_m$ is the sum of all the mth Fourier mode of the hopping terms. We can further decompose the hopping operator into:

$$\hat{T}(t) = \sum_m (\hat{T}_{-1,m} + \hat{T}_{0,m} + \hat{T}_{1,m})e^{im\omega t} \tag{4.7}$$

Where $\hat{T}_{dm}(t)$ changes the doublon number by d, for example, if $\hat{P}_d$ is the projection operator into the subspace with doublon number d, then $\hat{T}_{dm}(t) = \sum_i \hat{P}_{i+d}\hat{T}_m(t)\hat{P}_i$.

In order to derive the form of the effective Hamiltonian let us introduce a time dependent unitary transformation $\hat{U}(t) = e^{-i\hat{S}(t)}$. The transformed Hamiltonian is:

$$\hat{H}'(t) = e^{i\hat{S}(t)}\hat{H}(t)e^{-i\hat{S}(t)} - e^{i\hat{S}(t)}id_te^{-i\hat{S}(t)} \tag{4.8}$$

We perform the unitary transformation perturbatively in the hopping operator, we can formally write $\hat{T}(t) = \eta\hat{T}(t)$, where η will play the role of a bookkeeping parameter in the perturbative expansion. We expand $\hat{S}(t) = \sum_\nu \eta^\nu \hat{S}^{(\nu)}(t)$ and $\hat{H}'(t) = \sum_\nu \eta^\nu \hat{H}'^{(\nu)}(t)$. In order for the new Hamiltonian to be periodic we impose the unitary transformation to have the periodicity of the Hamiltonian, so that we can expand $\hat{S}^{(\nu)}(t) = \sum_m e^{im\omega t}\hat{S}^{(\nu)}_m$. Additionally we can impose the transformed Hamiltonian to be block diagonal in the doublon number d. With these conditions the unitary transformation can be uniquely determined if we impose that $\hat{S}(t)$ does not contain block-diagonal terms, i.e. we can write:

$$\hat{S}^{(\nu)}(t) = \sum_{d\neq 0}\sum_m \eta^\nu \hat{S}^{(\nu)}_{d,m}e^{im\omega t} \tag{4.9}$$

where $\hat{S}^{(\nu)}_{d,m}$ changes the double occupancy number by d.
Now we can use the identity:

$$id_te^{-i\hat{S}(t)} = \sum_n \frac{1}{(n+1)!}\text{ad}^n_{-i\hat{S}(t)}(d_t\hat{S}(t))e^{-i\hat{S}(t)} \tag{4.10}$$

Derived in appendix C, where $\text{ad}_A(B) = [A,B]$ to rewrite the transformed Hamiltonian as:

$$\hat{H}'(t) = e^{i\hat{S}(t)}\left(\hat{H}(t) - \sum_n \frac{1}{(n+1)!}\text{ad}^n_{-i\hat{S}(t)}(d_t\hat{S}(t))\right)e^{-i\hat{S}(t)} \tag{4.11}$$

Using the Baker–Campbell–Hausdorff expansion we can write the transformed Hamiltonian as:

$$\hat{H}'(t) = \sum_m \frac{1}{m!}\text{ad}^m_{i\hat{S}(t)}\left(\hat{H}(t) - \sum_n \frac{1}{(n+1)!}\text{ad}^n_{-i\hat{S}(t)}(d_t\hat{S}(t))\right) \tag{4.12}$$

Now, in this expression we have to expand $\hat{S}(t) = \sum_\nu \eta^\nu \hat{S}^{(\nu)}(t)$ and $\hat{H}'(t) = \sum_\nu \eta^\nu \hat{H}'^{(\nu)}(t)$ and determine $\hat{S}^{(\nu)}(t)$ iteratively in ν so that $\hat{H}'^{(\nu)}(t)$ is diagonal in the doublon number. Notice that we do not expand $\hat{H}(t)$ as an infinite series since $\hat{H}(t) = -\eta\hat{T}(t) + U\hat{D}$. Now, notice also that if we take $i\hat{S}^{(0)}(t) = 0$ in 4.12, then, to zeroth order in η only terms in $m = 0$ and $n = 0$ contribute obtaining:

$$\hat{H}'^{(0)}(t) = U\hat{D} \tag{4.13}$$

Which is indeed diagonal in the doublon number, and therefore we can take $i\hat{S}^{(0)}(t) = 0$. With this equating terms of the same order in 4.12 is greatly simplified, since terms with high m, n will correspond to terms with high η. Since we are only interested in orders up to second order, we can truncate 4.12 up to $m = 2$:

$$\hat{H}'(t) = \hat{H}(t) - \sum_n \frac{1}{(n+1)!}\text{ad}^n_{-i\hat{S}(t)}(d_t\hat{S}(t)) + [i\hat{S}(t), \hat{H}(t) - \sum_n \frac{1}{(n+1)!}\text{ad}^n_{-i\hat{S}(t)}(d_t\hat{S}(t))] +$$

$$+ \frac{1}{2}[i\hat{S}(t), [i\hat{S}(t), \hat{H}(t) - \sum_n \frac{1}{(n+1)!}\text{ad}^n_{-i\hat{S}(t)}(d_t\hat{S}(t))]] \tag{4.14}$$

This equation holds up to order η^2. In first order we obtain:

$$\hat{H}'^{(1)}(t) = -\hat{T}(t) - d_t\hat{S}^{(1)}(t) + \left[i\hat{S}^{(1)}(t), U\hat{D}\right] \qquad (4.15)$$

Now we expanding in m, d and use $\left[\hat{D}, \hat{S}_{dm}^{(v)}\right] = d\hat{S}_{dm}^{(v)}$ because $\hat{S}_{dm}^{(v)}$ changes the doublon number by d:

$$\hat{H}'^{(1)}(t) = -\hat{T}(t) - \sum_{d\neq 0}\sum_m (Ud + m\omega)i\hat{S}_{dm}^{(1)}e^{im\omega t} \qquad (4.16)$$

Therefore:

$$i\hat{S}_d^{(1)}(t) = -\sum_m \frac{\hat{T}_{d,m}}{Ud + m\omega}e^{im\omega t} \qquad (4.17)$$

$$\hat{H}'^{(1)}(t) = -\sum_m \hat{T}_{0,m}(t)e^{im\omega t} \qquad (4.18)$$

To second order we find:

$$\hat{H}'^{(2)}(t) = -d_t\hat{S}^{(2)}(t) - \frac{1}{2}\left[-i\hat{S}^{(1)}(t), d_t\hat{S}^{(1)}(t)\right] + \left[i\hat{S}^{(1)}(t), -\hat{T}(t) - \frac{1}{2}d_t\hat{S}^{(1)}(t)\right] +$$

$$+ \left[i\hat{S}^{(2)}(t), U\hat{D}\right] + \frac{1}{2}\left[i\hat{S}^{(1)}(t), \left[i\hat{S}^{(1)}(t), U\hat{D}\right]\right] =$$

$$= \left[i\hat{S}^{(2)}(t), U\hat{D}\right] - \left[i\hat{S}^{(1)}(t), \hat{T}(t)\right] + \frac{1}{2}\left[i\hat{S}^{(1)}(t), \left[i\hat{S}^{(1)}(t), U\hat{D}\right]\right] - d_t\hat{S}^{(2)}(t) \qquad (4.19)$$

Using 4.15 and using $\left[i\hat{S}^{(1)}(t), d_t\hat{S}^{(1)}(t)\right] = 0$ due to different Fourier modes of the hopping operator being equal up to a constant (explain better), we can rewrite:

$$\hat{H}'^{(2)}(t) = \left[i\hat{S}^{(2)}(t), U\hat{D}\right] - \frac{1}{2}\left[i\hat{S}^{(1)}(t), \hat{T}(t) - \hat{H}'^{(1)}(t)\right] - d_t\hat{S}^{(2)}(t) \qquad (4.20)$$

Using 4.17 and 4.18, the middle term is:

$$\left[i\hat{S}^{(1)}(t), \hat{T}(t) - \hat{H}'^{(1)}(t)\right] = -\left[\sum_m \left(\frac{\hat{T}_{1m}}{U + m\omega} - \frac{\hat{T}_{-1m}}{U - m\omega}\right)e^{im\omega t}, \sum_n \left(\hat{T}_{-1n} + 2\hat{T}_{0n} + \hat{T}_{1n}\right)e^{in\omega t}\right]$$

$$= -\sum_{mn}\left\{\frac{2\left[\hat{T}_{1m}, \hat{T}_{0n}\right]}{U + m\omega} + \frac{\left[\hat{T}_{1m}, \hat{T}_{-1n}\right]}{U + m\omega} - \frac{\left[\hat{T}_{-1m}, \hat{T}_{1n}\right]}{U - m\omega} - \frac{2\left[\hat{T}_{-1m}, \hat{T}_{0n}\right]}{U - m\omega}\right\}e^{i(m+n)\omega t}$$

$$= -\sum_{mn}\left\{\frac{2\left[\hat{T}_{1n}, \hat{T}_{0(m-n)}\right]}{U + n\omega} + \frac{\left[\hat{T}_{1n}, \hat{T}_{-1(m-n)}\right]}{U + n\omega} - \frac{\left[\hat{T}_{-1n}, \hat{T}_{1(m-n)}\right]}{U - n\omega} - \frac{2\left[\hat{T}_{-1n}, \hat{T}_{0(m-n)}\right]}{U - n\omega}\right\}e^{im\omega t}$$

Altogether:

$$\hat{H}'^{(2)}(t) = \sum_{mn} \left\{ \frac{\left[\hat{T}_{1n}, \hat{T}_{0(m-n)}\right]}{U+n\omega} + \frac{\left[\hat{T}_{1n}, \hat{T}_{-1(m-n)}\right]}{2(U+n\omega)} - \frac{\left[\hat{T}_{-1n}, \hat{T}_{1(m-n)}\right]}{2(U-n\omega)} - \frac{\left[\hat{T}_{-1n}, \hat{T}_{0(m-n)}\right]}{U-n\omega} \right\} e^{im\omega t}$$
$$- \sum_{d\neq 0} \sum_{m} (Ud+m\omega) i\hat{S}_{dm}^{(2)} e^{im\omega t}$$

We obtain:

$$i\hat{S}_{dm}^{(2)} = \sum_{n} \frac{\left[\hat{T}_{dn}, \hat{T}_{0(m-n)}\right]}{(Ud+n\omega)(Ud+m\omega)} \tag{4.21}$$

$$\hat{H}'^{(2)}(t) = \frac{1}{2} \sum_{mn} \left(\frac{\left[\hat{T}_{1n}, \hat{T}_{-1(m-n)}\right]}{U+n\omega} - \frac{\left[\hat{T}_{-1n}, \hat{T}_{1(m-n)}\right]}{U-n\omega} \right) e^{im\omega t} \tag{4.22}$$

Now the effective Hamiltonian acts on the subspace of $\hat{P}_0$, therefore we are only interested on $\hat{P}_0 \hat{H}'^{(2)}(t) \hat{P}_0$ (notice that $\hat{P}_0 \hat{H}'^{(1)}(t) \hat{P}_0 = 0$). In this subspace we can write:

$$\hat{H}_{\text{eff}}(t) = \hat{P}_0 \hat{H}'^{(2)}(t) \hat{P}_0 = -\frac{1}{2} \sum_{mn} \left(\frac{\hat{P}_0 \hat{T}_{-1(m-n)} \hat{T}_{1n} \hat{P}_0}{U+n\omega} + \frac{\hat{P}_0 \hat{T}_{-1n} \hat{T}_{1(m-n)} \hat{P}_0}{U-n\omega} \right) e^{im\omega t}$$
$$= -\frac{1}{2} \sum_{mn} \left\{ \frac{\hat{P}_0 (\hat{T}_{-1(m-n)} \hat{T}_{1n} + \hat{T}_{-1-n} \hat{T}_{1(m+n)}) \hat{P}_0}{U+n\omega} \right\} e^{im\omega t} \tag{4.23}$$

Now, since the hopping operators act on the subspace $d = 0$ and must remain within that subspace, therefore $\hat{P}_0 \hat{T}_{-1a} \hat{T}_{1b} \hat{P}_0$ will be a sum of all possible hoppings between two different sites:

$$\hat{P}_0 \hat{T}_{-1a} \hat{T}_{1b} \hat{P}_0 = \sum_{i,j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} t_{ij,a}^{\sigma_1\sigma_2} t_{ji,b}^{\sigma_3\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4}$$

Where a and b are any two Fourier modes. Inserting this into 4.24 and using the definition of $t_{ij,m}^{\sigma\sigma'} = t_{ij}^{\sigma\sigma'} e^{i(\frac{\pi}{2}-\theta_{ij})m} \mathcal{J}_m(\alpha_{ij})$ and using that $\theta_{ji} = \theta_{ij}$ and $\alpha_{ji} = -\alpha_{ij}$ and the properties $\mathcal{J}_{-m}(x) = (-1)^m \mathcal{J}_m(x)$ and $\mathcal{J}_m(-x) = (-1)^m \mathcal{J}_m(x)$ we can write 4.24 as:

$$\hat{H}_{\text{eff}}(t) = \hat{P}_0 \hat{H}'^{(2)}(t) \hat{P}_0 = -\frac{1}{2} \sum_{mn} \sum_{i,j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4} \frac{t_{ij,m-n}^{\sigma_1\sigma_2} t_{ji,n}^{\sigma_3\sigma_4} + t_{ij,-n}^{\sigma_1\sigma_2} t_{ji,m+n}^{\sigma_3\sigma_4}}{U+n\omega} e^{im\omega t}$$

$$= -\frac{1}{2} \sum_{mn} \sum_{i,j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4} t_{ij}^{\sigma_1\sigma_2} t_{ji}^{\sigma_3\sigma_4} e^{i(\frac{\pi}{2}-\theta_{ij})m} \frac{\mathcal{J}_{m-n}(\alpha_{ij})\mathcal{J}_n(\alpha_{ji}) + \mathcal{J}_{-n}(\alpha_{ij})\mathcal{J}_{m+n}(\alpha_{ji})}{U+n\omega} e^{im\omega t}$$

$$= -\frac{1}{2} \sum_{mn} \sum_{i,j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4} t_{ij}^{\sigma_1\sigma_2} t_{ji}^{\sigma_3\sigma_4} e^{i(\frac{\pi}{2}-\theta_{ij})m} (-1)^m \frac{\mathcal{J}_{n-m}(\alpha_{ij})\mathcal{J}_n(\alpha_{ij}) + \mathcal{J}_n(\alpha_{ij})\mathcal{J}_{m+n}(\alpha_{ij})}{U+n\omega} e^{im\omega t}$$

$$= -\frac{1}{2} \sum_{i,j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4} t_{ij}^{\sigma_1\sigma_2} t_{ji}^{\sigma_3\sigma_4} \mathcal{M}(\alpha_{ij}, U, \omega, t) \tag{4.24}$$

Where we defined:

$$\mathcal{M}(\alpha_{ij}, U, \omega, t) = \sum_{mn} e^{-i(\frac{\pi}{2}+\theta_{ij})m} \left\{ \frac{\mathcal{J}_{n-m}(\alpha_{ij})\mathcal{J}_n(\alpha_{ij}) + \mathcal{J}_n(\alpha_{ij})\mathcal{J}_{m+n}(\alpha_{ij})}{U + n\omega} \right\} e^{im\omega t}$$
(4.25)

In the following sections we will apply what we have derived here for different models of the hopping operator.

4.1.1 Time independent field

We would like to investigate the case in which the electric field is time independent. In that case we can restrict the analysis to the one dimensional case, since in second order the electric field will only affect the bonds parallel to the field. Let us denote $\vec{E} = E_0 \hat{e}_x$, then the Peiels transformed hopping amplitudes can be written as:

$$t_{ij}^{\sigma\sigma'}(t) = t_{ij}^{\sigma\sigma'} e^{ie\vec{R}_{ij}\vec{E}t}$$
(4.26)

Therefore, there will be only two Fourier modes with frequency $\omega_0 = e\vec{R}_{ij}\vec{E} = \pm eaE_0$, where the sign $+(-)$ corresponds to the case $\vec{R}_{ij} = \pm a\hat{e}_x$. Notice that this frequency ω_0 does not correspond to a field frequency ($\vec{E}$ is time independent), but to the Fourier mode in the hopping amplitudes (which is induced by the time independent field). From this point we can apply the same procedure as in the general case up to 4.23. We can greatly simplify this by considering that:

- n can only take values $n = \pm 1$ (there are no additional Fourier modes).

- When restricted to the low energy subspace a product $\hat{T}_{-1a}\hat{T}_{1b}$ will only contribute when a and b have opposite signs ($a = 1, b = -1$ or viceversa). This is because, in the low energy subspace $\hat{T}_{-1a}\hat{T}_{1b}$ can only represent a hopping from a site i to a site j and the hopping back to i, we can see from 4.26 that these two amplitudes will be in opposite Fourier modes.

Taking this into consideration we see that only $m = 0$ terms will remain, which is consistent with the fact that the two phases cancel out in the process $i \to j \to i$. We can thus rewrite 4.23 as:

$$\hat{H}_{\text{eff}} = -\hat{P}_0 \left\{ \frac{\hat{T}_{-1,1}\hat{T}_{1,-1}}{U - \omega_0} + \frac{\hat{T}_{-1,-1}\hat{T}_{1,1}}{U + \omega_0} \right\} \hat{P}_0$$
(4.27)

Now, the first fraction represents a hopping process $i \to j \to i$ where j lies left to i, whereas in the second fraction j lies right to i:

$$\hat{P}_0\hat{T}_{-1,1}\hat{T}_{1,-1}\hat{P}_0 = \sum_{i>j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} t_{ij}^{\sigma_1\sigma_2} t_{ji}^{\sigma_3\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4}$$

$$\hat{P}_0\hat{T}_{-1,-1}\hat{T}_{1,1}\hat{P}_0 = \sum_{i<j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} t_{ij}^{\sigma_1\sigma_2} t_{ji}^{\sigma_3\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4}$$

We can rewrite this in the more compact form:

$$\hat{H}_{\text{eff}} = -\sum_{i,j,\sigma_1,\sigma_2,\sigma_3,\sigma_4} \frac{t_{ij}^{\sigma_1\sigma_2} t_{ji}^{\sigma_3\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4}}{U + \text{sgn}(j-i)\omega_0}$$
(4.28)

This is the same effective Hamiltonian obtained in the previous section without an electric field but with a shift in the intermediate state energy by $\pm\omega_0 = \pm eaE_0$. We will analyze the corresponding spin Hamiltonian of this effective Hamiltonian when we consider the Kane-Mele-Hubbard model in Section 4.4.

4.2 Hubbard model without SOI

We start by considering the simplest hopping operator, as in the Hubbard model:

$$\hat{H} = -t_0 \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_{i=1}^{M} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{4.29}$$

Which is the Hamiltonian 3.16 without DMI interaction. We see that the hopping amplitudes introduced in the previous section take the form $t_{ij}^{\sigma\sigma'} = \delta_{\sigma\sigma'} t_0$ for i, j being nearest neighbors, and $t_{ij}^{\sigma\sigma'} = 0$ otherwise. With this we can directly apply 4.24 to obtain:

$$\hat{H}_{\text{eff}}(t) = -\frac{t_0^2}{2} \sum_{\langle i,j \rangle, \sigma, \sigma'} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \hat{c}_{j\sigma'}^\dagger \hat{c}_{i\sigma'} \mathcal{M}(\alpha_{ij}, U, \omega, t) \tag{4.30}$$

Now, introducing the spin operators 3.23 and 3.24 and summing over the spin states as in 3.25:

$$\sum_{\sigma,\sigma'} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \hat{c}_{j\sigma'}^\dagger \hat{c}_{i\sigma'} = \sum_{\sigma,\sigma'} \left(\frac{\delta_{\sigma\sigma'}}{2} + S_i \sigma_{\sigma'\sigma} \right) \left(\frac{\delta_{\sigma\sigma'}}{2} - S_j \sigma_{\sigma\sigma'} \right) = -2S_i S_j$$

Where we neglected the constant term. The effective spin Hamiltonian is thus:

$$\hat{H}_{\text{eff}}(t) = \sum_{\langle i,j \rangle} J_{ij} S_i S_j \tag{4.31}$$

With

$$
\begin{aligned}
J_{ij} &= t_0^2 \mathcal{M}(\alpha_{ij}, U, \omega, t) \\
&= \sum_{mn} t_0^2 e^{-i(\frac{\pi}{2} + \theta_{ij})m} \left(\frac{\mathcal{J}_{n-m}(\alpha_{ij}) \mathcal{J}_n(\alpha_{ij}) + \mathcal{J}_n(\alpha_{ij}) \mathcal{J}_{n+m}(\alpha_{ij})}{U + n\omega} \right) e^{im\omega t}
\end{aligned} \tag{4.32}
$$

After time average this reduces to the $m = 0$ term:

$$\mathcal{M}(\alpha_{ij}, U, \omega, t) \approx \sum_n 2 \frac{\mathcal{J}_n(\alpha_{ij})^2}{U + n\omega} \tag{4.33}$$

For $\omega >> U$ we can truncate this to the three smallest values of n, i.e. $n = 0, \pm 1$. We can also use that $\alpha_{ij} << 1$ because α_{ij} is proportional to $\vec{A}$ which is proportional to ω^{-1}. Therefore we can use $\mathcal{J}_n(x) \approx x^n$ for $n > 0$ and $x << 1$ to obtain:

$$\mathcal{M}(\alpha_{ij}, U, \omega, t) \approx 2 \left(\frac{\alpha_{ij}^2}{U + \omega} + \frac{1}{U} + \frac{\alpha_{ij}^2}{U - \omega} \right) \tag{4.34}$$

And the exchange interaction coupling becomes:

$$J_{ij} \approx J_{ij}^0 + 2t_0^2 \alpha_{ij}^2 \left(\frac{1}{U+\omega} + \frac{1}{U-\omega} \right) \tag{4.35}$$

The lattice structure is contained in $\alpha_{ij} = \pm|e\boldsymbol{R}_{ij}\vec{A}|$. For a square lattices aligned with the coordinate system so that $\vec{a}_1 = \hat{e}_x$ and $\vec{a}_2 = \hat{e}_y$, we will have $\boldsymbol{R}_{ij} = \pm a\hat{e}_x, \pm a\hat{e}_y$, where a is the lattice constant. Using $\vec{A} = \frac{iE_0}{\omega\sqrt{1+\lambda^2}}(\hat{e}_x + i\lambda\hat{e}_y)$ we have:

$$\alpha_{ij} = \begin{cases} \pm\frac{eaE_0}{\omega\sqrt{1+\lambda^2}} = \pm\frac{\mathcal{E}}{\sqrt{1+\lambda^2}}, & \text{for } \boldsymbol{R}_{ij} = \pm\hat{e}_x \\ \pm\lambda\frac{eaE_0}{\omega\sqrt{1+\lambda^2}} = \pm\frac{\lambda\mathcal{E}}{\sqrt{1+\lambda^2}}, & \text{for } \boldsymbol{R}_{ij} = \pm\hat{e}_y \end{cases} \tag{4.36}$$

Where $\mathcal{E} = \frac{eaE_0}{\omega}$.

For plane polarized light ($\lambda = 0$) the exchange interaction only changes in the direction of the polarization, that is:

$$J_{ij}^{PP} = \begin{cases} J_{ij}^0 + 2t_0^2\mathcal{E}^2\left(\frac{1}{U+\omega} + \frac{1}{U-\omega}\right) & \text{for } \boldsymbol{R}_{ij} = \pm\hat{e}_x \\ J_{ij}^0 & \text{for } \boldsymbol{R}_{ij} = \pm\hat{e}_y \end{cases} \tag{4.37}$$

For circular polarized light ($\lambda = \pm1$) in this approximation the exchange interaction changes in the same way in all the directions:

$$J_{ij}^{CP} = J_{ij}^0 + t_0^2\mathcal{E}^2 \left(\frac{1}{U+\omega} + \frac{1}{U-\omega} \right) \tag{4.38}$$

4.2.1 Honeycomb lattice

Now consider a honeycomb lattice structure, so that the α_{ij} values are given by $\alpha_{ij} = \pm|e\boldsymbol{R}_{ij}\vec{A}|$ where $\boldsymbol{R}_{ij}$ are the displacement vectors in a honeycomb lattice. There are six such vectors:

$$\boldsymbol{R}_1^\pm = \pm a\hat{e}_x \tag{4.39}$$

$$\boldsymbol{R}_2^\pm = \pm a\frac{1}{2}(\hat{e}_x + \sqrt{3}\hat{e}_y) \tag{4.40}$$

$$\boldsymbol{R}_3^\pm = \pm a\frac{1}{2}(\hat{e}_x - \sqrt{3}\hat{e}_y) \tag{4.41}$$

These six possible directions will lead to $\alpha_a^\pm = \pm|e\boldsymbol{R}_a\vec{A}|$ where $\vec{A} = \frac{iE_0}{\omega\sqrt{1+\lambda^2}}(\hat{e}_x + i\lambda\hat{e}_y)$:

$$\alpha_1^\pm = \pm\frac{eaE_0}{\omega\sqrt{1+\lambda^2}} \tag{4.42}$$

$$\alpha_2^\pm = \alpha_3^\pm = \pm\frac{eaE_0}{2\omega}\sqrt{\frac{1+3\lambda^2}{1+\lambda^2}} = \pm\frac{eaE_0}{2\omega}\sqrt{1 + \frac{2\lambda^2}{1+\lambda^2}} \tag{4.43}$$

From here we can see that if we take the same approximation as in 4.35 we will obtain the same form of exchange interaction for circular polarized light ($\lambda = \pm1$) 4.38 with possibly a different lattice constant a.

4.2.2 Dielectric permittivity

Using the approximation for the exchange coupling constant for circular polarized light derived in 4.38 we can write the free energy of the system Φ as:

$$
\begin{aligned}
\Phi &= \Phi_0 + \sum_{\langle i,j \rangle} J_{ij} S_i S_j = \\
&= \Phi_0 + \sum_{\langle i,j \rangle} J_{ij}^0 S_i S_j + |\vec{E}_0|^2 \frac{t_0^2 e^2 a^2}{\omega} \left(\frac{1}{U + \omega} + \frac{1}{U - \omega} \right) \sum_{\langle i,j \rangle} S_i S_j
\end{aligned}
\tag{4.44}
$$

Then, the dielectric permittivity is $\epsilon_{kl} = \frac{\partial^2 \Phi}{\partial E_k \partial E_l}$, i.e., the dielectric permittivity is isotropic $\epsilon_{kl} = \epsilon$ and:

$$
\epsilon = \epsilon^0 + 2 \frac{t_0^2 e^2 a^2}{\omega} \left(\frac{1}{U + \omega} + \frac{1}{U - \omega} \right) \sum_{\langle i,j \rangle} S_i S_j
\tag{4.45}
$$

Where $\epsilon^0 = \frac{\partial^2 \Phi_0}{\partial E_k \partial E_l}$. The refractive index will therefore depend on the magnetization of the antiferromagnet, this was already demonstrated experimentally in the 80's [24].

4.3 Hubbard model with SOI

Now, let's investigate the effect of the electric field for the Hubbard model with SOI, i.e. 3.16, in this case the hopping operator gets an extra spin-dependent term:

$$
\hat{T} = \sum_{\langle i,j \rangle, \sigma, \sigma'} (\delta_{\sigma,\sigma'} t_0 + \mathbf{\Delta}_{ij} \boldsymbol{\sigma}_{\sigma,\sigma'}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'}
\tag{4.46}
$$

The vector $\mathbf{\Delta}_{ij}$ can describe Rashba or Dresselhaus SOI, $\mathbf{\Delta}_{ij} = i\Delta_R(R_{ij}^y, -R_{ij}^x, 0)$ for Rashba SOI and $\mathbf{\Delta}_{ij} = i\Delta_R(R_{ij}^x, -R_{ij}^y, 0)$ for Dresselhaus SOI. In this case the hopping amplitudes are:

$$
t_{ij}^{\sigma\sigma'} = \begin{cases} (\delta_{\sigma\sigma'} t_0 + \mathbf{\Delta}_{ij} \boldsymbol{\sigma}_{\sigma,\sigma'}) & \text{for } i, j \text{ nearest neighbors} \\ 0 & \text{otherwise} \end{cases}
\tag{4.47}
$$

And as before $\hat{H} = -\hat{T} + U\hat{D}$. In the presence of an electromagnetic field we can apply the Peierls substitution as we did before, and the effective Hamiltonian will be given by 4.24. inserting the spin operators 3.23 and 3.24 we get:

$$
\begin{aligned}
\hat{H}_{\text{eff}}(t) &= -\frac{1}{2} \sum_{\langle i,j \rangle, \sigma_1, \sigma_2, \sigma_3, \sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_3}^\dagger \hat{c}_{i\sigma_4} t_{ij}^{\sigma_1\sigma_2} t_{ji}^{\sigma_3\sigma_4} \mathcal{M}(\alpha_{ij}, U, \omega, t) \\
&= -\frac{1}{2} \sum_{\langle i,j \rangle, \sigma_1, \sigma_2, \sigma_3, \sigma_4} \left(\frac{\delta_{\sigma_1\sigma_4}}{2} + S_i \boldsymbol{\sigma}_{\sigma_4\sigma_1} \right) \left(\frac{\delta_{\sigma_2\sigma_3}}{2} - S_j \boldsymbol{\sigma}_{\sigma_2\sigma_3} \right) \\
&\quad (\delta_{\sigma_1\sigma_2} t_0 + \mathbf{\Delta}_{ij} \boldsymbol{\sigma}_{\sigma_1,\sigma_2})(\delta_{\sigma_3\sigma_4} t_0 + \mathbf{\Delta}_{ji} \boldsymbol{\sigma}_{\sigma_3,\sigma_4}) \mathcal{M}(\alpha_{ij}, U, \omega, t)
\end{aligned}
\tag{4.48}
$$

Using $\mathbf{\Delta}_{ji} = -\mathbf{\Delta}_{ij}$:

$$(\delta_{\sigma_1\sigma_2}t_0 + \boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_1,\sigma_2})(\delta_{\sigma_3\sigma_4}t_0 + \boldsymbol{\Delta}_{ji}\boldsymbol{\sigma}_{\sigma_3,\sigma_4}) =$$
$$\delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4}t_0^2 + t_0\boldsymbol{\Delta}_{ij}(\delta_{\sigma_3\sigma_4}\boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_3\sigma_4}) - (\boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_1,\sigma_2})(\boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_3,\sigma_4})$$

The term proportional to t_0^2 will lead to the modified exchange interaction, as in the previous section. The term proportional to $t_0\boldsymbol{\Delta}_{ij}$ will lead to the modified DMI interaction and the term proportional to $\boldsymbol{\Delta}_{ij}^2$ will lead to the pseudodipolar interaction.

Now we can rewrite 4.48 as:

$$\hat{H}_{\text{eff}}(t) = -\frac{1}{2}\sum_{\langle i,j\rangle,\sigma_1,\sigma_2,\sigma_3,\sigma_4}\left(\frac{\delta_{\sigma_1\sigma_4}}{2} + \boldsymbol{S}_i\boldsymbol{\sigma}_{\sigma_4\sigma_1}\right)\left(\frac{\delta_{\sigma_2\sigma_3}}{2} - \boldsymbol{S}_j\boldsymbol{\sigma}_{\sigma_2\sigma_3}\right)$$

$$\left[\delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4}t_0^2 + t_0\boldsymbol{\Delta}_{ij}(\delta_{\sigma_3\sigma_4}\boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_3\sigma_4}) - (\boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_1,\sigma_2})(\boldsymbol{\Delta}_{ji}\boldsymbol{\sigma}_{\sigma_3,\sigma_4})\right]\mathcal{M}(\alpha_{ij},\text{U},\omega,t)$$

$$= -\frac{t_0^2}{2}\sum_{\langle i,j\rangle\sigma,\sigma'}\left(\frac{1}{2}\delta_{\sigma\sigma'} + \boldsymbol{S}_i\boldsymbol{\sigma}_{\sigma'\sigma}\right)\left(\frac{1}{2}\delta_{\sigma\sigma'} - \boldsymbol{S}_j\boldsymbol{\sigma}_{\sigma\sigma'}\right)\mathcal{M}(\alpha_{ij},\text{U},\omega,t) -$$

$$-\frac{t_0}{2}\sum_{\langle i,j\rangle\sigma_1,\sigma_2,\sigma_3,\sigma_4}\left(\frac{1}{2}\delta_{\sigma_1\sigma_4} + \boldsymbol{S}_i\boldsymbol{\sigma}_{\sigma_4\sigma_1}\right)\left(\frac{1}{2}\delta_{\sigma_2\sigma_3} - \boldsymbol{S}_j\boldsymbol{\sigma}_{\sigma_2\sigma_3}\right)\times$$

$$\boldsymbol{\Delta}_{ij}(\delta_{\sigma_3,\sigma_4}\boldsymbol{\sigma}_{\sigma_1\sigma_2} - \delta_{\sigma_1,\sigma_2}\boldsymbol{\sigma}_{\sigma_3\sigma_4})\mathcal{M}(\alpha_{ij},\text{U},\omega,t) +$$

$$+\frac{1}{2}\sum_{\langle i,j\rangle\sigma_1,\sigma_2,\sigma_3,\sigma_4}\left(\frac{1}{2}\delta_{\sigma_1\sigma_4} + \boldsymbol{S}_i\boldsymbol{\sigma}_{\sigma_4\sigma_1}\right)\left(\frac{1}{2}\delta_{\sigma_2\sigma_3} - \boldsymbol{S}_j\boldsymbol{\sigma}_{\sigma_2\sigma_3}\right)$$

$$(\boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_1,\sigma_2})(\boldsymbol{\Delta}_{ij}\boldsymbol{\sigma}_{\sigma_3,\sigma_4})\mathcal{M}(\alpha_{ij},\text{U},\omega,t) =$$

$$= \sum_{\langle i,j\rangle}\left(t_0^2\boldsymbol{S}_i\boldsymbol{S}_j + 2it_0\boldsymbol{\Delta}_{ij}\boldsymbol{S}_i\times\boldsymbol{S}_j + \sum_{\alpha,\beta}S_i^\alpha(\delta_{\alpha\beta}2\Delta_{ij}^2 - 4\Delta_{ij}^\alpha\Delta_{ij}^\beta)S_j^\beta\right)\mathcal{M}(\alpha_{ij},\text{U},\omega,t) =$$

$$= \sum_{\langle i,j\rangle}\left\{J_{ij}\boldsymbol{S}_i\boldsymbol{S}_j + \boldsymbol{D}_{ij}\boldsymbol{S}_i\times\boldsymbol{S}_j + \boldsymbol{S}_i\boldsymbol{\Gamma}_{ij}\boldsymbol{S}_j\right\}$$

Where we used relations 3.25, 3.26 and 3.27. We have:

$$J_{ij} = t_0^2\mathcal{M}(\alpha_{ij},\text{U},\omega,t) \tag{4.49}$$

$$\boldsymbol{D}_{ij} = 2it_0\boldsymbol{\Delta}_{ij}\mathcal{M}(\alpha_{ij},\text{U},\omega,t) \tag{4.50}$$

$$\Gamma_{ij}^{\alpha\beta} = (\delta_{\alpha\beta}\Delta_{ij}^2 - 2\Delta_{ij}^\alpha\Delta_{ij}^\beta)\mathcal{M}(\alpha_{ij},\text{U},\omega,t) \tag{4.51}$$

We can see that since we only considered NN hopping processes, all the terms in the spin Hamiltonian are renormalized in the same way by the laser field (as in [25]). In order to obtain different dependencies with the field we should consider NNN hopping processes.

4.4 Including next nearest neighbor hopping

In the previous sections we have seen that the second order perturbation effective Hamiltonian will contain the following terms:

- Exchange interaction $J_{ij}\boldsymbol{S}_i\boldsymbol{S}_j$, arising from the kinetic hopping - kinetic hopping terms.

- DMI $\boldsymbol{D}_{ij}\boldsymbol{S}_i \times \boldsymbol{S}_j$, arising from the kinetic hopping - SOI hopping terms.

- Anisotropic or pseudodipolar interaction $\boldsymbol{S}_i\boldsymbol{\Gamma}_{ij}\boldsymbol{S}_j$, arising from the SOI hopping - SOI hopping terms.

And all these coupling factors will be renormalized by the laser field. This renormalization depends only on the field and the sites i, j, it does not depend on the nature of the interaction. With this in mind we will introduce a model with additional NNN hopping terms:

$$\hat{H} = - \sum_{\langle i,j\rangle,\sigma,\sigma'} (\delta_{\sigma,\sigma'}t_1 + \boldsymbol{\Delta}_{1,ij}\boldsymbol{\sigma}_{\sigma,\sigma'})\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} - \sum_{\langle\langle i,j\rangle\rangle,\sigma,\sigma'} (\delta_{\sigma,\sigma'}t_2 + \boldsymbol{\Delta}_{2,ij}\boldsymbol{\sigma}_{\sigma,\sigma'})\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} + \mathrm{U}\hat{D}$$

(4.52)

Where sum over next-nearest neighbors is denoted by $\langle\langle ij\rangle\rangle$. This Hamiltonian is the same we studied in section 4.3 plus a NNN hopping and SOI term. The hopping amplitudes thus are:

$$t_{ij}^{\sigma\sigma'} = \begin{cases} (\delta_{\sigma\sigma'}t_1 + \boldsymbol{\Delta}_{1,ij}\boldsymbol{\sigma}_{\sigma,\sigma'}) & \text{for } i,j \text{ nearest neighbors} \\ (\delta_{\sigma\sigma'}t_2 + \boldsymbol{\Delta}_{2,ij}\boldsymbol{\sigma}_{\sigma,\sigma'}) & \text{for } i,j \text{ next nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

(4.53)

The effective Hamiltonian will be the same as in section 4.3, with the corresponding NNN terms. This is because in second order perturbation NN hopping terms do not mix with NNN hopping terms. Thus, the effective spin Hamiltonian will be:

$$\hat{H}_{\text{eff}}(t) = \sum_{\langle i,j\rangle} \left\{ J_{1,ij}\boldsymbol{S}_i\boldsymbol{S}_j + \boldsymbol{D}_{1,ij}\boldsymbol{S}_i \times \boldsymbol{S}_j + \boldsymbol{S}_i\boldsymbol{\Gamma}_{1,ij}\boldsymbol{S}_j \right\} +$$
$$\sum_{\langle\langle i,j\rangle\rangle} \left\{ J_{2,ij}\boldsymbol{S}_i\boldsymbol{S}_j + \boldsymbol{D}_{2,ij}\boldsymbol{S}_i \times \boldsymbol{S}_j + \boldsymbol{S}_i\boldsymbol{\Gamma}_{2,ij}\boldsymbol{S}_j \right\}$$

(4.54)

Where:

$$J_{n,ij} = t_n^2 \mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t) \tag{4.55}$$

$$\boldsymbol{D}_{n,ij} = 2it_n\boldsymbol{\Delta}_{n,ij}\mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t) \tag{4.56}$$

$$\Gamma_{n,ij}^{\alpha\beta} = (\delta_{\alpha\beta}\Delta_{n,ij}^2 - 2\Delta_{n,ij}^\alpha\Delta_{n,ij}^\beta)\mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t) \tag{4.57}$$

NNN interaction coupling factors will be normalized according to $\mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t)$, where i, j are NNN sites, whereas NN interaction coupling factors will be normalized according to $\mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t)$ where i, j are NN sites. Therefore the dependence on the field will differ. For example, if we take the time independent approximation 4.34, and use $\lambda = \pm 1$ for circular polarized light, and $\alpha_{ij} = \pm\frac{\mathcal{E}|\boldsymbol{R}_{ij}|}{a\sqrt{2}}$, where $\mathcal{E} = \frac{eaE_0}{\omega}$. Then the exchange interaction will be:

$$J_{1,ij} = J_1^0 + t_1^2 \frac{\mathcal{E}^2}{2} \left(\frac{1}{U+\omega} + \frac{1}{U-\omega} \right) = J_1^0 + J_1^0 \frac{\mathcal{E}^2}{2} \left(\frac{1}{1+\frac{\omega}{U}} + \frac{1}{1-\frac{\omega}{U}} \right)$$

$$J_{2,ij} = J_2^0 + t_2^2 \frac{3\mathcal{E}^2}{2} \left(\frac{1}{U+\omega} + \frac{1}{U-\omega} \right) = J_2^0 + J_2^0 \frac{3\mathcal{E}^2}{2} \left(\frac{1}{1+\frac{\omega}{U}} + \frac{1}{1-\frac{\omega}{U}} \right)$$

Where $J_n^0 = \frac{t_n^2}{U}$ and where we used that $|\boldsymbol{R}_{ij}| = a$ for NN and $|\boldsymbol{R}_{ij}| = \sqrt{3}a$ for NNN in a honeycomb lattice. The other coupling factors in 4.56 and 4.57 can be approximated in the same way.

In section 4.5 we will investigate this numerically. The reason for this is that in a hopping process, the electron picks up a phase $e^{ie\boldsymbol{R}_{ij}A(t)}$ (assuming flat field approximation). This phase will be larger for NNN hopping than for NN hopping and this will therefore translate in the corresponding spin interactions.

Next we will show several well-known models which are described by 4.52.

4.4.1 Kane-Mele-Hubbard model

The first model to describe topological insulators was introduced by Kane and Mele [21] to describe quantum spin Hall effect in graphene. In a honeycomb lattice time reversal symmetry and inversion symmetry allow only next-nearest neighbor spin orbit coupling, which is known as intrinsic spin orbit coupling. In these circumstances the system can be modeled by the Kane-Mele-Hubbard model:

$$\hat{H}_{\text{KMH}} = -t_1 \sum_{\langle ij \rangle \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + i\Delta \sum_{\langle\langle ij \rangle\rangle \sigma\sigma'} \hat{c}_{i\sigma}^\dagger \nu_{ij} \sigma_{\sigma\sigma'}^z \hat{c}_{j\sigma'} + U\hat{D} \tag{4.58}$$

Where Δ is the intrinsic spin orbit coupling constant. $\nu_{ij} = \pm 1$ depending on whether the electron traversing from i to j makes a right ($+1$) or a left turn (-1). This Hamiltonian is described by 4.52 if we set $\boldsymbol{\Delta}_{1,ij} = 0$, $t_2 = 0$ and $\boldsymbol{\Delta}_{2,ij} = -i\Delta\nu_{ij}\hat{e}_z$. Then, the effective spin model will be:

$$\hat{H}_{\text{KMH}}^{\text{eff}}(t) = \sum_{\langle i,j \rangle} J_{ij}\boldsymbol{S}_i\boldsymbol{S}_j + \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i\boldsymbol{\Gamma}_{ij}\boldsymbol{S}_j \tag{4.59}$$

With and:

$$J_{ij} = t_1^2 \mathcal{M}(\alpha_{ij}, U, \omega, t)$$

$$\boldsymbol{\Gamma}_{ij} = \Delta^2 \text{diag}(-1,-1,1)\mathcal{M}(\alpha_{ij}, U, \omega, t)$$

according to 4.55 and 4.57. Notice that:

$$\boldsymbol{S}_i\boldsymbol{\Gamma}_{ij}\boldsymbol{S}_j = \Delta^2 \mathcal{M}(\alpha_{ij}, U, \omega, t) \left(S_i^z S_j^z - S_i^x S_j^x - S_i^y S_j^y \right)$$

This describes a type of anisotropic exchange interaction known as XXZ Heisenberg model for next nearest neighbors. Notice that the anisotropic term breaks the SU(2) symmetry of the bare Heisenberg model. The same spin model is obtained in [22] without the laser perturbation, this model has a much richer phase diagram than the $J_1 - J_2$ Heisenberg model [26]. If the laser field is not too strong so that
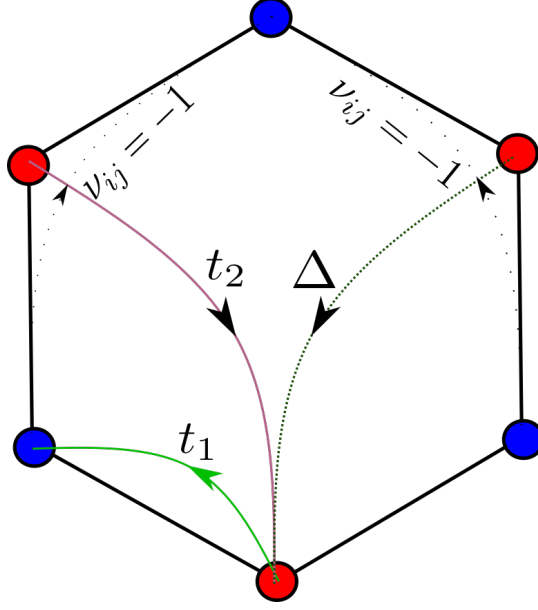
FIGURE 4.1: A honycomb cell with NN hopping t_1, NNN hopping t_2 and intrinsic SOI Δ. $\nu_{ij} = \pm 1$ depending on whether the electron traversing from i to j makes a right ($+1$) or a left turn (-1).

we can assume $\mathcal{M}(\alpha_{ij}, U, \omega, t) > 0$, then $\Gamma_{ij}^{zz} > 0$. Therefore we see that this interaction favors antiferromagnetic order in the $\hat{e}_z$ direction and ferromagnetic order in the $\hat{e}_x - \hat{e}_y$ plane. The exchange interaction J_{ij} will favor antiferromagnetic order for nearest neighbors, so that next nearest neighbors will tend to be aligned. Therefore, Γ_{ij}^{zz} will compete against J_{ij} in the $\hat{e}_z$ direction. In the $\hat{e}_x - \hat{e}_y$ plane, $\boldsymbol{\Gamma}_{ij}$ will favor ferromagnetic order between next nearest neighbors, which adds to the effect of J_{ij}. In general the strength of the exchange interaction will be larger and the net effect of $\boldsymbol{\Gamma}_{ij}$ will be a tilting of the spins towards the $\hat{e}_x$-$\hat{e}_y$ plane.

4.4.2 Modified Kane-Mele-Hubbard model

As we saw in the previous section the effective Hamiltonian 4.59 does not contain NNN DMI terms. The reason for this is because in the original Hamiltonian $t_2 = 0$. Next we will study the same Hamiltonian adding a finite NNN hopping terms t_2. In general this is more accurate than imposing $t_2 = 0$, and it can be understood as a second order NN hopping process (the direct NNN hopping integral would usually be much smaller). Our next Hamiltonian is thus:

$$\hat{H} = -t_1 \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \sum_{\langle\langle i,j \rangle\rangle, \sigma} (t_2 + i\Delta\nu_{ij}\sigma_{\sigma,\sigma}^z)\hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma} + U\hat{D} \tag{4.60}$$

This corresponds to the case $\boldsymbol{\Delta}_{1,ij} = 0$ and $\boldsymbol{\Delta}_{2,ij} = (0, 0, i\nu_{ij}\Delta)$ in 4.52. The Hamiltonian parameters are sketched in Figure 4.1. With this, the effective Hamiltonian will be:

$$\hat{H}_{\text{eff}}(t) = \sum_{\langle i,j \rangle} J_{1,ij}\boldsymbol{S}_i\boldsymbol{S}_j + \sum_{\langle\langle i,j \rangle\rangle} \left\{ J_{2,ij}\boldsymbol{S}_i\boldsymbol{S}_j + \boldsymbol{D}_{2,ij}\boldsymbol{S}_i \times \boldsymbol{S}_j + \boldsymbol{S}_i\boldsymbol{\Gamma}_{ij}\boldsymbol{S}_j \right\} \tag{4.61}$$

Where:

$$J_{1,ij} = t_1^2 \mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t)$$
$$J_{2,ij} = t_2^2 \mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t)$$
$$\boldsymbol{D}_{2,ij} = -2\nu_{ij} t_2 \Delta \hat{e}_z \mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t)$$
$$\boldsymbol{\Gamma}_{2,ij} = \Delta^2 \mathrm{diag}(-1,-1,1) \mathcal{M}(\alpha_{ij}, \mathrm{U}, \omega, t)$$

Such a Hamiltonian was first proposed by S. A. Owerre to model honeycome topological magnon insulators [27] [28]. Experimental results regarding topological properties of spin waves in honeycomb ferromagnet CrI_3 can only be understood by considering this Hamiltonian [29]. This model is also relevant for the study of Spin Hall effects of Weyl magnons [30] [31].

Now, a Hamiltonian with the form $\hat{H} = \sum_{\langle i,j \rangle} J_1 \boldsymbol{S}_i \boldsymbol{S}_j + \sum_{\langle\langle i,j \rangle\rangle} J_2 \boldsymbol{S}_i \boldsymbol{S}_j$ is known as the J_1-J_2 Heisenberg model and in a 2D honeycomb lattice it exhibits Néel order for $J_2 < J_1/6$ and for $J_2 > J_1/6$ spin density waves (SDW) appear [32]. In the presence of DMI alone there will always be SDW in the plane perpendicular to $\boldsymbol{D}$ [33]. In Hamiltonian 4.61 we expect SDW to appear in the ground state and the SDW wavevector will be determined by a function of the parameters of this model. In the next section we will do a numerical of study on how modifying the ratio between NN and NNN spin interaction factors can change the spin state of the system.

4.4.3 Time independent electric field in the NN + NNN Hamiltonian

Now, let us examine the case in which the applied electric field is time independent. In this case the effective Hamiltonian is 4.28, which is the same Hamiltonian obtained when no electric field is applied except for a shift in the intermediate energy by $\pm\omega_0 = e\vec{R}_{ij}\vec{E}_0$. In this case, if we consider a Hamiltonian such as 4.52, we can follow the same procedure done before: we plug in the hopping amplitudes 4.53 into 4.28 and apply 3.25 to sum over the spin states and obtain the corresponding spin Hamiltonian. We obtain:

$$\hat{H}_{\mathrm{eff}}(t) = \sum_{\langle i,j \rangle^*} \left\{ J_{1,ij} \boldsymbol{S}_i \boldsymbol{S}_j + \boldsymbol{D}_{1,ij} \boldsymbol{S}_i \times \boldsymbol{S}_j + \boldsymbol{S}_i \boldsymbol{\Gamma}_{1,ij} \boldsymbol{S}_j \right\} +$$
$$\sum_{\langle\langle i,j \rangle\rangle^*} \left\{ J_{2,ij} \boldsymbol{S}_i \boldsymbol{S}_j + \boldsymbol{D}_{2,ij} \boldsymbol{S}_i \times \boldsymbol{S}_j + \boldsymbol{S}_i \boldsymbol{\Gamma}_{2,ij} \boldsymbol{S}_j \right\} \qquad (4.62)$$

$\langle i,j \rangle^*$ denotes sum over NN avoiding repeating the same two sites. The coupling factors are:

$$J_{n,ij} = 4\frac{t_n^2}{U_{ij}^*} \qquad (4.63)$$

$$\boldsymbol{D}_{n,ij} = 8\frac{t_n i \boldsymbol{\Delta}_{n,ij}}{U_{ij}^*} \qquad (4.64)$$

$$\Gamma_{n,ij}^{\alpha\beta} = \frac{4}{U_{ij}^*}(\delta_{\alpha\beta} \boldsymbol{\Delta}_{n,ij}^2 - 2\Delta_{n,ij}^\alpha \Delta_{n,ij}^\beta) \qquad (4.65)$$

Where:

$$\frac{1}{U_{ij}^*} = \frac{1}{2}\left(\frac{1}{U - e\vec{R}_{ij}\vec{E}_0} + \frac{1}{U + e\vec{R}_{ij}\vec{E}_0}\right) \tag{4.66}$$

4.5 Numeric results

4.5.1 One dimensional system

We will start with a one dimensional chain with hamiltonian $\hat{H} = \sum_{\langle i,j\rangle} |J_1|S_iS_j - \sum_{\langle\langle i,j\rangle\rangle} \nu_{ij}|D_2|\hat{e}_z S_i \times S_j$. This approximated Hamiltonian with no NNN exchange interaction is very simple, but in some systems where it has even been observed that $|D_{2,ij}| > |J_{2,ij}|$ [29] it can be a good approximation. We write the absolute values in $|J_1|$ and $|D_2|$ to limit the analysis to the range in which the field does not change the sign of these factors. In this case we can write $S(r) = S(\cos(kr), \sin(kr), 0)$, where the real number k plays the role of the wavevector, and $\theta = ka - \pi$ is the deviation from the Néel state. This form assumes spiral order, with Néel state being the special case $\theta = 0$ (or $k = \pi$). From now we will use θ instead of k. Then the classical energy per site is given by:

$$\frac{E(\theta)}{2S^2} = -|J_1|\cos(\theta) - |D_2|\sin(2\theta) \tag{4.67}$$

and the energy is minimized for $\theta^* = \arcsin\left(\frac{-\frac{J_1}{D_2} + \sqrt{(\frac{J_1}{D_2})^2 + 32}}{8}\right)$, i.e. $\theta^* = \theta^*(\frac{J_1}{D_2})$.

This is the correct minimization for $J_1, D_2 > 0$. Next we will show numerically that the ratio between the NN and NNN parameters, $\frac{J_1}{D_2}$, can be modulated by the intensity of the field, and therefore the field can be used to control the SDW wavevector.

We will use the time average approximation 4.33 so that we can write:

$$J_{1,ij} = J_{1,ij}^0 \sum_n \frac{\mathcal{J}_n(\alpha_{ij})^2}{1 + n\frac{\omega}{U}} \tag{4.68}$$

$$D_{2,ij} = D_{2,ij}^0 \sum_n \frac{\mathcal{J}_n(\alpha_{ij})^2}{1 + n\frac{\omega}{U}} \tag{4.69}$$

Where $\boldsymbol{D}_{2,ij} = \hat{e}_z D_{2,ij}$ and where $J_{1,ij}^0 = J_1^0 = \frac{2t_1^2}{U}$ and $D_{2,ij}^0 = -\frac{4t_2\Delta\nu_{ij}}{U}$. Since $\mathcal{J}_n(-x) = (-1)^n \mathcal{J}_n(x)$ the dependance is on $|\alpha_{ij}|$ only. Now, using 4.3, for circularly polarized light we have $|\alpha_{ij}| = \frac{1}{\sqrt{2}}e|\vec{R}_{ij}|\frac{E_0}{\omega} = \frac{1}{\sqrt{2}}ea\frac{E_0}{\omega}\frac{|\vec{R}_{ij}|}{a} = \frac{|\vec{R}_{ij}|}{\sqrt{2}a}\mathcal{E}$, where a is the lattice constant and $\mathcal{E} = \frac{eaE_0}{\omega}$. Now, for $J_{1,ij}$, i and j are NN and so we can write $|\vec{R}_{ij}| = a$, whereas for $D_{2,ij}$, i and j are NNN and so $|\vec{R}_{ij}| = 2a$. Thus:

$$J_{1,ij} = J_1 = J_1^0 \sum_n \frac{\mathcal{J}_n(\frac{1}{\sqrt{2}}\mathcal{E})^2}{1 + n\frac{\omega}{U}} \tag{4.70}$$

$$D_{2,ij} = D_{2,ij}^0 \sum_n \frac{\mathcal{J}_n(\sqrt{2}\mathcal{E})^2}{1 + n\frac{\omega}{U}} \tag{4.71}$$

In each case the absolute vale is independent of i, j. Now, in units $\hbar = t_1 = 1$ we measure energy in units of t_1 and frequency in units of $\frac{t_1}{\hbar}$. Then, for $t_2 = 0.1$, $\Delta = 0.5$,
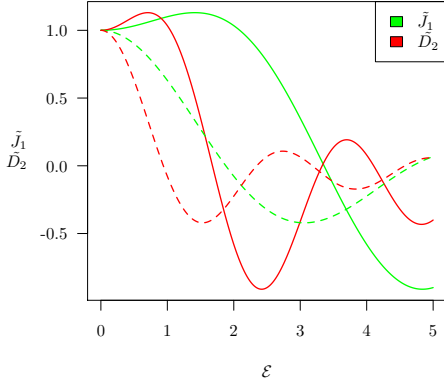
(A) $\frac{J_1}{J_1^0}$ and $\frac{D_{2,ij}}{D_{2,ij}^0}$ are plotted as function of $\mathcal{E}$. Similar results are obtained in [19] for J_1. Solid lines are for $\omega = 6$ and dashed lines are for $\omega = 16$.
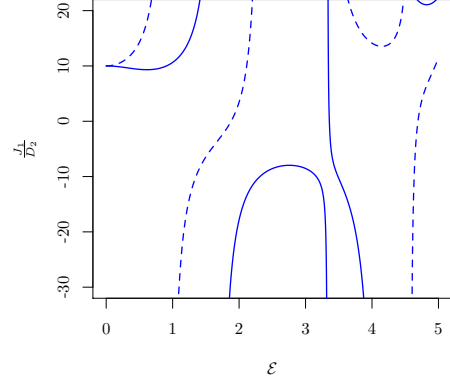
(B) $\frac{J_1}{D_{2,ij}}$ is plotted as function of $\mathcal{E}$, it diverges every time $D_{2,ij}$ changes sign. Solid lines are for $\omega = 6$ and dashed lines are for $\omega = 16$.

$U = 10$ and $\omega = 6, 16$ we obtain the plots in Figure 4.2a. The ratio $\frac{J_{1,ij}}{D_{2,ij}}$ is plotted in Figure 4.2b. The field can change the sign of J_1 and D_2 for strong amplitudes. Finally, in Figure 4.3 we plot the SDW NN angle θ limited to the case $J_1 > 0$ and $D_2 > 0$.

4.5.2 Two dimensional systems

In a honeycomb lattice described by the effective spin model 4.61 the usual approach is to write:

$$S_1(r) = S\left(\cos(Qr), \sin(Qr), 0\right) \tag{4.72}$$
$$S_2(r) = -S\left(\cos(Qr + \theta), \sin(Qr + \theta), 0\right) \tag{4.73}$$

The $1, 2$ subindex stands for the sublattice. The $\hat{e}_z$ component vanishes in order to minimize the contribution of the pseudodipolar interaction. Let $Q_a = Q\hat{a}$ and $Q_b = Q\hat{b}$, where $\hat{a}$ and $\hat{b}$ are the primitive cell vectors. Then, the classical energy per spin is given by:

$$\frac{E}{NS^2} = -\frac{J_1}{2}\left(\cos(\theta) + \cos(\theta - Q_a - Q_b) + \cos(\theta - Q_b)\right) + $$
$$+ (J_2 - \Gamma)\left(\cos(Q_a) + \cos(Q_b) + \cos(Q_a + Q_b)\right) + $$
$$+ D_2\left(\sin(Q_a) + \sin(Q_b) + \sin(Q_a + Q_b)\right) \tag{4.74}$$

Notice that when the spins are constrained in the $\hat{e}_x, \hat{e}_y$ plane, the anisotropic interaction $S_i \Gamma_{ij} S_j$ becomes a ferromagnetic interaction. The minimization of this energy will lead to an involved phase diagram in the J_1, J_2, D_2, Γ_2 space (or equivalently, in the t_1, t_2, Δ space). We will not attempt to describe this phase diagram. However, as we have shown in the one dimensional case, by modulating the laser amplitude we can control the ratio between the NN and NNN coupling factors, and thus the parameters Q and θ of the system state.
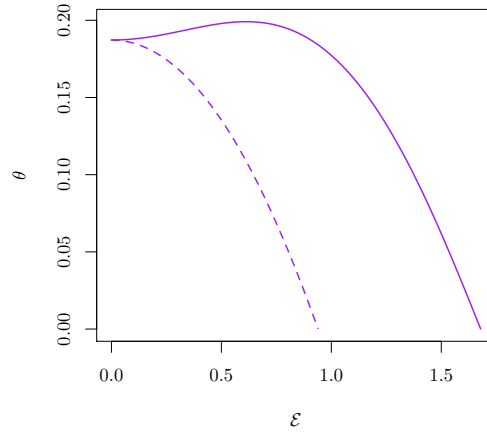
FIGURE 4.3: The spin wave density NN angle θ as a function of $\mathcal{E}$. The field modifies the ratio $\frac{J_1}{D_{2,ij}}$ thus modifying the wave vector. Solid lines are for $\omega = 6$ and dashed lines are for $\omega = 16$.

Appendix A

Crystal structure and reciprocal lattice

Here we will introduce some notation. The Bravais lattice in a crystal is the lattice generated by the primitive translations a_μ:

$$\boldsymbol{R} = \sum_{\mu=1}^{3} m_\mu \boldsymbol{a}_\mu \tag{A.1}$$

Where m_μ are integers. The volume of the unit cell is $v = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$. The crystal volume is $V = Mv$ where $M = L_1 L_2 L_3$ is the number of lattice sites. The primitive translations in the reciprocal lattice are defined as $\mathbf{b}_1 = \frac{2\pi}{v} \mathbf{a}_2 \times \mathbf{a}_3$, etc. With this notation the first Brillouin zone is:

$$\mathbf{k} = \sum_{\mu=1}^{3} \kappa_\mu \mathbf{b}_\mu \tag{A.2}$$

Where $\kappa_\mu = \frac{\nu_\mu}{L_\mu}, -\frac{L_\mu}{2} + 1 \leq \nu_\mu \leq \frac{L_\mu}{2}$ so that, $-\frac{1}{2} < \kappa_\mu \leq \frac{1}{2}$.

In the case of a cubic lattice we have $|\mathbf{a}_\mu| = a$ and $|b_\mu| = \frac{2\pi}{a}$ and the vectors of the first Brillouin zone have components $k_\mu = \frac{2\pi \nu_\mu}{aL}$.

In the next chapters we will also consider the two dimensional honecomb lattice. For this lattice we can choose the primitive translations to be:

$$a_1 = \frac{a_0}{2} \left(3, \sqrt{3} \right) \tag{A.3}$$

$$a_2 = \frac{a_0}{2} \left(3, -\sqrt{3} \right) \tag{A.4}$$

Where a_0 is the atom-atom distance (in the case of graphene $a_0 = 1.42$). Each unit cell contains two atoms, dividing the lattice into two sublattices, usually denoted A and B. The reciprocal lattice is defined by the vectors:

$$b_1 = \frac{2\pi}{3a_0} \left(1, \sqrt{3} \right) \tag{A.5}$$

$$b_2 = \frac{2\pi}{3a_0} \left(1, -\sqrt{3} \right) \tag{A.6}$$

These two vectors also span an hexagonal structure. The vectors connecting an atom in the A sublattice to its B sublattice nearest neighbors are:
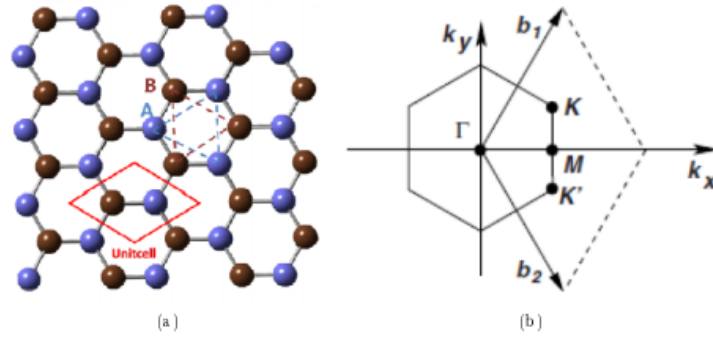
FIGURE A.1: Image from a web source. In Fig. (a) the unit cell is sketched and the sublattices A and B are shown in blue and red respectively. In Fig. (b) the reciprocal lattice is shown, toghether with the high symmetry points K, M and K'.

$$R_1^A = \frac{a_0}{2}\left(1, \sqrt{3}\right) \tag{A.7}$$

$$R_2^A = \frac{a_0}{2}\left(1, -\sqrt{3}\right) \tag{A.8}$$

$$R_3^A = a_0\left(-1, 0\right) \tag{A.9}$$

The vectors connecting an atom in the B sublattice to its A sublattice nearest neighbors are just $R_i^B = -R_i^A$

Appendix B

Peierls Substitution

In first quantization we can introduce a vector potential $A(r, t)$ by changing the Hamiltonian of the lattice 3.3 to:

$$\hat{H}'(r) = \frac{(p - eA)^2}{2m} + U(r) \tag{B.1}$$

Now the Bloch functions defined for 3.3 will not be eigenfunctions of this Hamiltonian. We define a new set of Wannier functions in terms of those defined in 3.6, and obtain the new Bloch functions.

$$\psi'_R(r) = e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\psi_R(r) \tag{B.2}$$

$$\phi'_k(r) = \frac{1}{\sqrt{M}}\sum_R e^{-ikR}\psi'_R(r) = \frac{1}{\sqrt{M}}\sum_R e^{-ikR}e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\psi_R(r) \tag{B.3}$$

Where we omitted the band number. The action of the new Hamiltonian is greatly simplified:

$$\hat{H}'(r)\psi'_R(r) = \left[\frac{(p - eA)^2}{2m} + U(r)\right]e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\psi_R(r) =$$

$$= e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\left[\frac{(p - i\hbar\boldsymbol{\nabla}_r(i\frac{e}{\hbar}\int_R^r dr' A(r',t)) - eA)^2}{2m} + U(r)\right] =$$

$$= e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\left[\frac{p^2}{2m} + U(r)\right]\psi_R(r) = e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\hat{H}(r)\psi_R(r)$$

And so, the matrix elements as in the case without field except for a phase:

$$t_{ij}(t) = \langle\psi'_{R_i}|\hat{H}'(r)|\psi'_{R_j}\rangle = e^{i\frac{e}{\hbar}\int_{R_j}^{R_i} dr' A(r',t)}\langle\psi_{R_i}|\hat{H}(r)|\psi_{R_j}\rangle \tag{B.4}$$

When the field can be approximated as constant along the lattice we have: $e^{i\frac{e}{\hbar}\int_{R_j}^{R_i} dr' A(r',t)} = e^{i\frac{e}{\hbar}(R_i - R_j)A(t)}$.

Notice that this substitution also applies if we add a Rashba Spin-Orbit interaction term to B.1, i.e., if $\hat{H}'(r) = \frac{(p - eA)^2}{2m} + U(r) + \alpha_R \hat{z}(\hat{\sigma} \times (p - eA))$, then

$$\alpha_R \hat{z}(\hat{\sigma} \times (p - eA))\psi'_R = \alpha_R(\hat{\sigma_x}(\hat{p}_y - eA) - \hat{\sigma_y}(\hat{p}_x - eA))e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\psi_R =$$

$$= e^{i\frac{e}{\hbar}\int_R^r dr' A(r',t)}\alpha_R \hat{z}\hat{\sigma} \times p\psi_R$$

Therefore relation B.4 still holds.

Appendix C

Identities

Let $Z(t)$ be an operator dependent on the parameter t. Then:

$$d_t e^Z = d_t \sum_{n=0}^{\infty} \frac{1}{n!} Z^n = \sum_{n=0}^{\infty} \sum_{m=0}^{n-1} \frac{1}{n!} Z^m \frac{\partial Z}{\partial t} Z^{n-m-1} =$$

$$= \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \frac{1}{(m+p+1)!} Z^m \frac{\partial Z}{\partial t} Z^p = \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \frac{m! p!}{(m+p+1)!} \frac{Z^m}{m!} \frac{\partial Z}{\partial t} \frac{Z^p}{p!} =$$

$$= \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \int_0^1 dx \, x^m (1-x)^p \frac{Z^m}{m!} \frac{\partial Z}{\partial t} \frac{Z^p}{p!} = \int_0^1 dx \, e^{Zx} \frac{\partial Z}{\partial t} e^{Z(1-x)} =$$

$$= \int_0^1 dx \sum_{n=0}^{\infty} \frac{1}{n!} \left[xZ, \ldots, \left[xZ, \frac{\partial Z}{\partial t} \right] \ldots \right] e^Z = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \left[Z, \ldots, \left[Z, \frac{\partial Z}{\partial t} \right] \ldots \right] e^Z$$

Where we used the Beta function $\int_0^1 dx \, x^m (1-x)^p = \frac{m! p!}{(m+p+1)!}$ and we also used the Baker-Campbell-Hausdorff expansion for $e^{xZ} \frac{\partial Z}{\partial t} e^{-xZ}$ and $\int_0^1 x^n = \frac{1}{n+1}$. Therefore we proved:

$$d_t e^Z = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \left[Z, \ldots, \left[Z, \frac{\partial Z}{\partial t} \right] \ldots \right] e^Z = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \text{ad}_Z^n \left(\frac{\partial Z}{\partial t} \right) e^Z \qquad \text{(C.1)}$$

Where $\text{ad}_A(B) = [A, B]$.

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