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

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This is the abstract.

MODEL AND CALCULATIONS

The first model to describe topological insulators was introduced by Kane and Mele [1] 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 which we write as a sum of a kinetic term, an interaction term and a SOI term:

$$\hat{H}^0 = \hat{\mathcal{H}}_t + \hat{\mathcal{H}}_{\text{SOI}} + \hat{\mathcal{H}}_{\text{int}} \tag{1}$$

Where:

$$\hat{\mathcal{H}}_t = -\sum_{\langle i,j\rangle,\sigma} t_1 \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} - \sum_{\langle\langle i,j\rangle\rangle,\sigma} t_2 \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} \tag{2}$$

$$\hat{\mathcal{H}}_{\text{SOI}} = \sum_{\langle\langle i,j\rangle\rangle,\sigma} i\Delta\nu_{ij}\sigma^z_{\sigma,\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} \tag{3}$$

$$\hat{\mathcal{H}}_{\text{int}} = \mathrm{U}_{00}\sum_{i=1}^{M}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \frac{1}{2}\sum_{\langle i,j\rangle,\sigma\sigma'}\mathrm{U}_{ij}\hat{n}_{i\sigma}\hat{n}_{j\sigma'} \tag{4}$$

Where $\hat{c}^\dagger_{i\sigma}$ ($\hat{c}_{i\sigma}$) creates (anihilates) an electron at site i in spin state σ, U_{00} and U_{ij} are the on-site and NN Coulomb interactions. t_1, t_2 are the hopping amplitudes originating from both kinetic hopping. 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). σ^z is the third Pauli matrix. In practice the NN Coulomb interaction can be effectively approximated by a reduced on-site interaction $\mathrm{U} = \mathrm{U}_{00} - \bar{\mathrm{U}}$ where $\bar{\mathrm{U}}$ is an average of the NN Coulomb interacion [2], we therefore can take:

$$\hat{\mathcal{H}}_{\text{int}} \approx \mathrm{U}\sum_{i=1}^{M}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{5}$$

With $\mathrm{U} = \mathrm{U}_{00} - \bar{\mathrm{U}}$.

Let us define $\hat{D} = \sum_{i=1}^{M}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ the doublon number operator so that $\hat{\mathcal{H}}_{\text{int}} \approx \mathrm{U}\hat{D}$ with eigenvalues d and projection operators $\hat{P}_d$. We will assume a half filling system in which the strength of the on-site interaction U is much larger than the hopping amplitudes. In the strong coupling limit any state with a nonzero number of double occupancies ($d \neq 0$) will have much larger energy than those with $d = 0$. We can therfore obtain an effective Hamiltonian acting on the $d = 0$ subspace by standard second

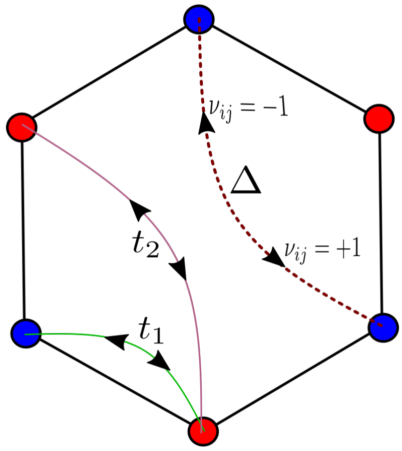

FIG. 1: A honycomb cell with NN hopping t_1, NNN hopping t_2 and intrinsic SOI Δ. $\nu_{ij} = \pm 1$ depending on whether the electron traversing from i to j makes a right $(+1)$ or a left turn (-1).

order perturbation techniques in the hopping terms. We can then obtain the effective spin Hamiltonian by using the relations:

$$\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma'} = \delta_{\sigma\sigma'}\frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) + \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma',\sigma} \tag{6}$$

$$\hat{c}_{i\sigma}\hat{c}^\dagger_{i\sigma'} = \delta_{\sigma\sigma'}\frac{1}{2}(2 - n_{i\uparrow} - n_{i\downarrow}) - \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma,\sigma'} \tag{7}$$

Following this procedure we obtain the following effective spin Hamiltonian:

$$\begin{aligned}\hat{H}_{\text{eff}} = &\sum_{\langle i,j\rangle} J_{1,ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \\ &+ \sum_{\langle\langle i,j\rangle\rangle}\{J_{2,ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \boldsymbol{D}_{2,ij}\cdot\boldsymbol{S}_i \times \boldsymbol{S}_j + \boldsymbol{S}_i\boldsymbol{\Gamma}_{ij}\boldsymbol{S}_j\}\end{aligned} \tag{8}$$

Where:

$$\begin{aligned}J_{1,ij} &= 2t_1^2 \\ J_{2,ij} &= 2t_2^2 \\ \boldsymbol{D}_{2,ij} &= -4\nu_{ij}t_2\Delta\hat{e}_z \\ \boldsymbol{\Gamma}_{2,ij} &= 2\Delta^2\mathrm{diag}(-1,-1,1)\end{aligned}$$

Introducing laser perturbation. In the prescence of an laser perturbation we can use the Peirls substitution to include the effect of the field trough the hopping amplitudes. We can write the electric field as $\boldsymbol{E}(t) = \frac{1}{2}(\vec{E}e^{-i\omega t} + \vec{E}^* e^{i\omega t})$, $\vec{E} = E_0\hat{e}$ and $\hat{e} = \frac{1}{\sqrt{1+\lambda^2_{POL}}}(\hat{e}_x +$

$i\lambda_{POL}\hat{e}_y$) is the polarization vector and $\lambda_{POL} = 0, \pm 1$ for plane polarized, right handed and left handed circular polarized field respectively. According to the Peierls rule the hopping amplitudes gain a phase $e^{ie\boldsymbol{R}_{ij}\boldsymbol{A}(t)}$ where $\boldsymbol{R}_{ij} = \boldsymbol{R}_i - \boldsymbol{R}_j$, $\boldsymbol{R}_i$ is the position of site i and $\boldsymbol{A}$ is the vector potential $\boldsymbol{A}(t) = \frac{1}{2}(\vec{A}e^{-i\omega t} + \vec{A}^* e^{i\omega t})$, with $\vec{A} = \frac{iE_0}{\omega}\hat{e}$.

Let us define:

$$e\boldsymbol{R}_{ij} \cdot \vec{A} = \alpha_{ij} e^{i\theta_{ij}} \tag{9}$$

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

$$\alpha_{ij} = -\alpha_{ji} \tag{10}$$

$$\theta_{ij} = \theta_{ji} \tag{11}$$

and $\theta_{ij} \in [0, \pi)$. Then we can apply the Jacobi-Anger expansion to Fourier transform the hopping amplitues:

$$e^{ie\boldsymbol{R}_{ij}\cdot\boldsymbol{A}(t)} = \sum_m e^{i(\frac{\pi}{2} - \theta_{ij})m} \mathcal{J}_m(\alpha_{ij}) e^{im\omega t} \tag{12}$$

where $\mathcal{J}_m(x)$ is the mth Bessel function [3], modulating the weight of the mth Fourier mode of the hopping amplitude. Let $\hat{T}_0$ be the hopping part of the hamiltonian, so that $\hat{H}_0 = \hat{T}_0 + \mathrm{U}\hat{D}$. When an electric field is applied, the hopping amplitudes become time dependent so that $\hat{H}(t) = \hat{T}(t) + \mathrm{U}\hat{D}$. Using 12 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. Additionaly we can further decompose the hopping operator into:

$$\hat{T}(t) = \sum_m (\hat{T}_{-1,m} + \hat{T}_{0,m} + \hat{T}_{1,m}) e^{im\omega t} \tag{13}$$

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:

$$\hat{H}'(t) = e^{i\hat{S}(t)}\hat{H}(t)e^{-i\hat{S}(t)} - e^{i\hat{S}(t)} i d_t e^{-i\hat{S}(t)} \tag{14}$$

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 $\hat{S}^{(\nu)}(t) = \sum_m e^{im\omega t}\hat{S}_m^{(\nu)}$. 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:

$$\hat{S}^{(\nu)}(t) = \sum_{d\neq 0}\sum_m \eta^\nu \hat{S}_{d,m}^{(\nu)} e^{im\omega t} \tag{15}$$

where $\hat{S}_{d,m}^{(\nu)}$ changes the double occupancy number by d. From here the procedure is simple but lenghty, we expand 14 in power series of η and determine $\hat{S}^{(\nu)}(t)$ iteratively in ν so that $\hat{H}'^{(\nu)}(t)$ is diagonal in the doublon number. Up to second order we obtain:

$$\hat{H}'(t) \approx \mathrm{U}\hat{D} - \sum_m \hat{T}_{0,m}(t)e^{im\omega t} + \\ + \frac{1}{2}\sum_{mn}\left(\frac{\left[\hat{T}_{1n}, \hat{T}_{-1(m-n)}\right]}{\mathrm{U} + n\omega} - \frac{\left[\hat{T}_{-1n}, \hat{T}_{1(m-n)}\right]}{\mathrm{U} - n\omega}\right)e^{im\omega t} \tag{16}$$

Let $\hat{P}_0$ be the projection operator to the $d = 0$ subspace. Then notice that $\hat{P}_0\hat{H}'^1(t)\hat{P}_0 = 0$, we define $\hat{H}_{\text{eff}}$ to be the time average of $\hat{P}_0\hat{H}'^2(t)\hat{P}_0$. Expressed in terms of creation and anihilation operators we obtain:

$$\hat{H}_{\text{eff}} = -\sum_{i,j,\sigma,\sigma'}\left\{\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}\hat{c}_{j\sigma'}^\dagger \hat{c}_{i\sigma'}\right. \\ \left. t_{ij}^\sigma t_{ji}^{\sigma'}\sum_n \frac{\mathcal{J}_n^2(\alpha_{ij})}{\mathrm{U} + n\omega}\right\} \tag{17}$$

Where t_{ij}^σ are the corresponding amplitudes for the unperturbed Hamiltonian, i.e. $t_{ij}^\sigma = t_1$ for i, j being NN and $t_{ij}^\sigma = t_2 + i\Delta\nu_{ij}\sigma_{\sigma,\sigma}^z$ for i, j being NNN. We can obtain the spin Hamiltonian by using the relations 6 7 and summing over the spin states. The resulting effective spin Hamiltonian is 8 with renormalized coupling constants:

$$J'_{1,ij} = 2t_1^2\frac{\mathcal{J}_n^2(\alpha_{ij})}{\mathrm{U} + n\omega}$$

$$J'_{2,ij} = 2t_2^2\frac{\mathcal{J}_n^2(\alpha_{ij})}{\mathrm{U} + n\omega}$$

$$\boldsymbol{D}'_{2,ij} = -4\nu_{ij}t_2\Delta\hat{e}_z\frac{\mathcal{J}_n^2(\alpha_{ij})}{\mathrm{U} + n\omega}$$

$$\boldsymbol{\Gamma}'_{2,ij} = 2\Delta^2\text{diag}(-1, -1, 1)\frac{\mathcal{J}_n^2(\alpha_{ij})}{\mathrm{U} + n\omega}$$

A similar Hamiltonian including a NN exchange term and a NNN DMI term was first proposed by S. A. Owerre to model honeycome topological magnon insulators [5] [6]. Additionally, experimental results regarding topological properties of spin waves in honeycomb ferromagnet

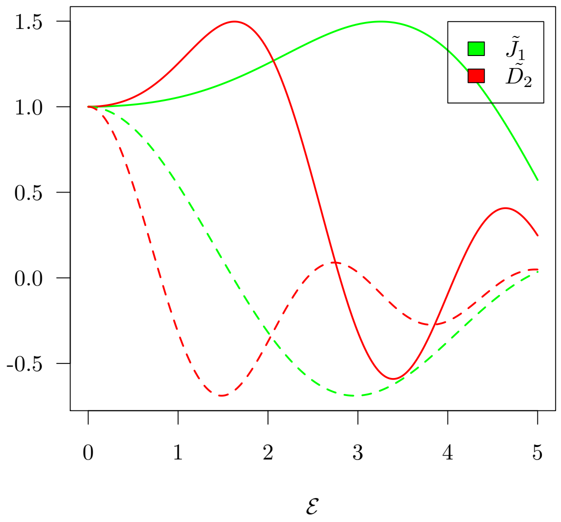

FIG. 2: For circularly polarized light we obtain $\tilde{J}_1 = \frac{J'_{1,ij}}{J_{1,ij}}$ and $\tilde{D}_2 = \frac{D'_{2,ij}}{D_{2,ij}}$ as function of $\mathcal{E} = \frac{eaE_0}{\omega}$, where e is the electron charge and a is the lattice constant. The results are obtain for (units of $\hbar = t_1 = 1$) $t_2 = 0.1$, $\Delta = 0.5$, U $= 10$ and $\omega = 6, 16$. Solid lines are for $\omega = 6$ and dashed lines are for $\omega = 16$. For $\tilde{J}_1$, similar results are obtained by Mentink et Al. [4].

CrI_3 can only be understood by considering this Hamiltonian [7]. This model is also relevant for the study of Spin Hall effects of Weyl magnons [8] [9].

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 [10]. In the presence of DMI alone there will always be SDW in the plane perpendicular to $\boldsymbol{D}$ [11]. In Hamiltonian 8 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. We have shown that we can modulate these parameters thus providing a techique to manipulate the SDW in the ground state.

Disorder

It is possible to introduce the effect of disorder in the model 1 by adding random uncorrelated on-site energies:

$$\hat{H}_0 = -\sum_{\langle i,j\rangle,\sigma} t_1 \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} - \sum_{\langle\langle i,j\rangle\rangle,\sigma} (t_2 - i\Delta\nu_{ij}\sigma^z_{\sigma,\sigma})\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \sum_{i\sigma} \epsilon_i \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma} + \mathrm{U}\hat{D} \tag{18}$$

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

$$\hat{H}^{\mathrm{Dis}}_{\mathrm{eff}} = \sum_{\langle i,j\rangle} J_{1,ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + + \sum_{\langle\langle i,j\rangle\rangle} \{J_{2,ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \boldsymbol{D}_{2,ij} \cdot \boldsymbol{S}_i \times \boldsymbol{S}_j + \boldsymbol{S}_i \boldsymbol{\Gamma}_{ij} \boldsymbol{S}_j\} \tag{19}$$

With:

$$J'_{1,ij} = \frac{2t_1^2\mathrm{U}}{\mathrm{U}^2 - (\epsilon_j - \epsilon_i)^2}$$
$$J'_{2,ij} = \frac{2t_2^2\mathrm{U}}{\mathrm{U}^2 - (\epsilon_j - \epsilon_i)^2}$$
$$\boldsymbol{D}'_{2,ij} = -\frac{4\nu_{ij}t_2\Delta\mathrm{U}}{\mathrm{U}^2 - (\epsilon_j - \epsilon_i)^2}\hat{e}_z$$
$$\boldsymbol{\Gamma}'_{2,ij} = \frac{2\Delta^2\mathrm{U}}{\mathrm{U}^2 - (\epsilon_j - \epsilon_i)^2}\mathrm{diag}(-1,-1,1)$$

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 [12].

Acknowledgments

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