Rashba Spin–Orbit Coupling Modified Superexchange

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1 Introduction

In Mott insulating systems with strong electron correlations, magnetic exchange interactions arise from virtual hopping processes known as superexchange. When spin–orbit coupling (SOC) is present, these exchange interactions acquire anisotropic and bond-dependent character. In this note, we derive how Rashba SOC, induced by inversion symmetry breaking and an external electric field, modifies the effective exchange parameters J, K, and Γ.

2 Microscopic Model

We start from a half-filled Hubbard model defined on a lattice:

$$H = H_t + H_R + H_U, \tag{1}$$

where

$$H_t = -t \sum_{\langle ij \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right), \tag{2}$$

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{3}$$

Here, t is the nearest-neighbor hopping amplitude and U is the on-site Coulomb repulsion. We consider the strong-coupling limit $U \gg t$.

3 Rashba Spin–Orbit Coupling

When inversion symmetry is broken perpendicular to the plane, an electric field $\hat{z}$ induces Rashba SOC. On the lattice, this appears as a spin-dependent hopping term:

$$H_R = i\lambda_R \sum_{\langle ij \rangle} c_i^\dagger \left[(\hat{\mathbf{z}} \times \hat{\mathbf{d}}_{ij}) \cdot \boldsymbol{\sigma} \right] c_j + \text{h.c.}, \tag{4}$$

where $\hat{\mathbf{d}}_{ij}$ is the unit vector from site j to i and $\boldsymbol{\sigma}$ are the Pauli matrices. The coupling strength λ_R is proportional to the applied electric field.

4 Strong-Coupling Expansion

At half filling and large U, charge fluctuations are suppressed and the low-energy Hilbert space contains one electron per site. The effective Hamiltonian is obtained using second-order perturbation theory:

$$H_{\text{eff}} = -\frac{1}{U} P H_{\text{hop}} H_{\text{hop}} P, \tag{5}$$

where $H_{\text{hop}} = H_t + H_R$ and P projects onto the singly-occupied subspace.

Expanding the product, we obtain three contributions:

$$H_{\text{eff}} = -\frac{1}{U} P \left(H_t H_t + H_t H_R + H_R H_t + H_R H_R \right) P. \tag{6}$$

5 Heisenberg Exchange

The term $H_t H_t$ produces the familiar isotropic Heisenberg interaction:

$$H_J = J_0 \, \mathbf{S}_i \cdot \mathbf{S}_j, \qquad J_0 = \frac{4t^2}{U}. \tag{7}$$

6 Dzyaloshinskii–Moriya Interaction

The cross terms $H_t H_R + H_R H_t$ generate an antisymmetric exchange:

$$H_{\text{DM}} = \mathbf{D}_{ij} \cdot \left(\mathbf{S}_i \times \mathbf{S}_j \right), \tag{8}$$

with

$$\mathbf{D}_{ij} \sim \frac{4t\lambda_R}{U} \left(\hat{\mathbf{z}} \times \hat{\mathbf{d}}_{ij} \right). \tag{9}$$

This interaction is allowed only when inversion symmetry is broken.

7 Symmetric Anisotropic Exchange

The term $H_R H_R$ produces symmetric anisotropic exchange:

$$H_{RR} = \frac{4\lambda_R^2}{U} \left[(\mathbf{n}_{ij} \cdot \mathbf{S}_i)(\mathbf{n}_{ij} \cdot \mathbf{S}_j) - \mathbf{S}_i \cdot \mathbf{S}_j \right], \tag{10}$$

where $\mathbf{n}_{ij} = \hat{\mathbf{z}} \times \hat{\mathbf{d}}_{ij}$.

This can be written as

$$H_{RR} = \sum_{\alpha\beta} \Gamma_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta, \qquad \Gamma_{ij}^{\alpha\beta} = \frac{4\lambda_R^2}{U} n_{ij}^\alpha n_{ij}^\beta. \tag{11}$$

8 Mapping to Kitaev and Γ Interactions

On the honeycomb lattice, each nearest-neighbor bond has a distinct orientation. The vectors $\mathbf{n}_{ij}$ select different spin components on different bonds, leading naturally to Kitaev (K) and off-diagonal (Γ) interactions:

$$K, \Gamma \propto \frac{\lambda_R^2}{U}. \tag{12}$$

Thus Rashba SOC renormalizes the effective exchange parameters as:

$$J_{\text{eff}} = \frac{4t^2}{U} - c_1 \frac{\lambda_R^2}{U}, \tag{13}$$

$$K_{\text{eff}} = K_0 + c_2 \frac{\lambda_R^2}{U}, \tag{14}$$

$$\Gamma_{\text{eff}} = \Gamma_0 + c_3 \frac{\lambda_R^2}{U}, \tag{15}$$

where c_i are geometry-dependent constants.

9 Conclusion

We have shown that Rashba SOC provides a symmetry-allowed and electrically tunable mechanism to modify isotropic and anisotropic exchange interactions in Mott insulators. This offers a microscopic foundation for electric-field control of Kitaev magnets and supports the use of Rashba SOC as a tuning parameter in effective spin models.