Anisotropic Interlayer Exchange in Twisted α-$RuCl_3$: J, K, and Γ Modulation

Theoretical Condensed Matter Physics

December 20, 2025

1 Introduction

In the study of twisted moiré magnets, α-$RuCl_3$ stands out due to its bond-dependent Kitaev interactions. When two layers are twisted by an angle θ, the interlayer coupling is not merely a scalar Heisenberg term but a spatially modulated tensor. This document details the inclusion of the Kitaev ($K_\perp$) and Gamma ($\Gamma_\perp$) terms into the moiré potential framework.

2 The Interlayer Hamiltonian

For a twisted bilayer, the interlayer interaction between site i in Layer 1 and site j in Layer 2 on a bond of type $\gamma \in \{x, y, z\}$ is described by the anisotropic exchange Hamiltonian:

$$H_{\text{inter}}^{(\gamma)} = \sum_{\langle i,j \rangle_\gamma} \left[J_\perp(\mathbf{r}) \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} + K_\perp(\mathbf{r}) S_{1,i}^\gamma S_{2,j}^\gamma + \Gamma_\perp(\mathbf{r}) (S_{1,i}^\alpha S_{2,j}^\beta + S_{1,i}^\beta S_{2,j}^\alpha) \right] \tag{1}$$

where $\mathbf{r} = (x, y)$ is the position vector of the site in the coordinate system of Layer 1, and $\{\gamma, \alpha, \beta\}$ are the three orthogonal spin components.

3 Spatial Modulation and Moiré Potential

3.1 The Geometric Scaling Function

All interlayer terms (J, K, Γ) follow the same spatial periodicity dictated by the moiré interference pattern. The local coupling strength is governed by the symmetry factor $\Phi(x, y)$:

$$\Phi(x, y) = \cos(\kappa y) + 2 \cos\left(\frac{\sqrt{3}}{2} \kappa x \right) \cos\left(\frac{1}{2} \kappa y \right) \tag{2}$$

where $\kappa = \frac{4\pi\theta}{\sqrt{3}a}$ is the moiré wavevector.

3.2 Magnitude Decay Expression

In literature, the exact decay of these interactions as a function of the local displacement $\mathbf{d}(\mathbf{r})$ is often modeled using an exponential fit to *ab initio* data:

$$J_{K,\Gamma}(\mathbf{r}) = J_{K,\Gamma}^{(0)} \frac{\exp\left(-B\frac{\sqrt{C^2+r^2}}{C}\right)}{\exp(-B)} \tag{3}$$

For α-$RuCl_3$, typical parameters are $B \approx 0.049$ and $C \approx 0.029$.

4 Parameters and Physical Significance

4.1 Estimated Interaction Strengths (2025)

As of 2025, the following values are commonly used for the peak coupling (AA stacking regions):

Parameter	Interaction Type	Estimated AA Value (meV)
$J_\perp^{(0)}$	Heisenberg (AFM)	$\approx +0.50$
$K_\perp^{(0)}$	Kitaev (FM)	≈ -0.08
$\Gamma_\perp^{(0)}$	Off-diagonal (AFM)	$\approx +0.03$

4.2 Role of $K_\perp$ and $\Gamma_\perp$

- **Bond Anisotropy:** The inclusion of $K_\perp$ ensures that the interlayer coupling respects the bond-directional symmetry of the honeycomb lattice. This frustrates the standard isotropic zigzag order.
- **Majorana Band Engineering:** In the Kitaev QSL regime, the spatial modulation of $K_\perp$ can induce gaps in the Majorana spectrum, leading to the formation of *Majorana flat bands*.
- **Magnetic Texture:** $\Gamma_\perp$ is crucial for determining the out-of-plane tilt of the spins, which is essential for matching experimental results from magnetic torque and susceptibility measurements.

5 Conclusion

The "perfect" expression for the interlayer physics of α-$RuCl_3$ must treat x and y as the addresses of sites in Layer 1, applying a bond-dependent tensor that oscillates according to $\Phi(x, y)$. This model successfully predicts the complex domain structures and topological transitions observed in twisted van der Waals heterostructures.