Spatially Modulated Interlayer Exchange Potential in Twisted Bilayer α-$RuCl_3$: Derivation and Analysis

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1 Introduction

Twisted moiré superlattices of α-$RuCl_3$ have emerged as a frontier in condensed matter physics. Unlike graphene, α-$RuCl_3$ is a Mott insulator characterized by bond-dependent Kitaev interactions. When two layers are twisted by an angle θ, the interlayer exchange coupling $J(\mathbf{r})$ becomes spatially periodic. This document derives the harmonic potential $\Phi(x, y)$ that captures the exact scenario of this modulation.

2 Microscopic Foundation

In the continuum limit for small twist angles, the interlayer interaction depends on the local stacking displacement $\mathbf{d}(\mathbf{r})$. For a point $\mathbf{r}$ in Layer 1, the relative shift of Layer 2 is:

$$\mathbf{d}(\mathbf{r}) = \mathcal{R}_\theta \mathbf{r} - \mathbf{r} \approx \theta(\hat{z} \times \mathbf{r}) \tag{1}$$

The interlayer exchange $J(\mathbf{r})$ is periodic over the monolayer reciprocal lattice vectors $\mathbf{G}$. We expand $J(\mathbf{d})$ as a Fourier series:

$$J(\mathbf{r}) = \sum_{\mathbf{G}} J_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{d}(\mathbf{r})} = \sum_{\mathbf{G}} J_{\mathbf{G}} e^{i\theta(\mathbf{G}\times\hat{z})\cdot\mathbf{r}} \tag{2}$$

3 Derivation of the Potential $\Phi(x, y)$

3.1 Symmetry of the α-$RuCl_3$ Honeycomb

The Ruthenium atoms form a honeycomb lattice with lattice constant $a \approx 5.96$ Å. The first shell of reciprocal lattice vectors is:

$$\mathbf{G}_1 = G_0(1, 0), \quad \mathbf{G}_2 = G_0\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \quad \mathbf{G}_3 = G_0\left(-\frac{1}{2}, -\frac{\sqrt{3}}{2}\right) \tag{3}$$

where $G_0 = \frac{4\pi}{\sqrt{3}a}$.

3.2 Construction of Moiré Vectors

The moiré reciprocal lattice vectors $\mathbf{g}_j$ are generated via $\mathbf{g}_j = \theta(\hat{z} \times \mathbf{G}_j)$. Let $\kappa = \theta G_0 = \frac{4\pi\theta}{\sqrt{3}a}$:

$$\mathbf{g}_1 = \theta(0, G_0) = \kappa(0, 1) \tag{4}$$

$$\mathbf{g}_2 = \theta\left(-\frac{\sqrt{3}}{2}G_0, -\frac{1}{2}G_0\right) = \kappa\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \tag{5}$$

$$\mathbf{g}_3 = \theta\left(\frac{\sqrt{3}}{2}G_0, -\frac{1}{2}G_0\right) = \kappa\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \tag{6}$$

3.3 Final Harmonic Form

The potential $\Phi(x, y)$ is the real part of the sum over these three vectors (ensuring C_3 symmetry):

$$\Phi(x, y) = \cos(\mathbf{g}_1 \cdot \mathbf{r}) + \cos(\mathbf{g}_2 \cdot \mathbf{r}) + \cos(\mathbf{g}_3 \cdot \mathbf{r}) \tag{7}$$

Substituting the components of $\mathbf{r} = (x, y)$:

$$\Phi(x, y) = \cos(\kappa y) + \cos\left(-\frac{\sqrt{3}}{2}\kappa x - \frac{1}{2}\kappa y\right) + \cos\left(\frac{\sqrt{3}}{2}\kappa x - \frac{1}{2}\kappa y\right) \tag{8}$$

Using the identity $\cos(A - B) + \cos(A + B) = 2\cos A \cos B$, we arrive at the perfect simplified expression:

$$\boxed{\Phi(x, y) = \cos(\kappa y) + 2\cos\left(\frac{\sqrt{3}}{2}\kappa x\right)\cos\left(\frac{1}{2}\kappa y\right)} \tag{9}$$

4 Physical Discussion: Relevance to α-RuCl$_3$

The interlayer exchange term in the Hamiltonian is expressed as $J_\perp(\mathbf{r}) = J_0 + 2J_1\Phi(x, y)$.

1. **Stacking Regions:**
   - **AA Stacking ($\mathbf{r} = 0$):** $\Phi = 3$. This region exhibits the strongest orbital overlap and maximal $J_\perp$.
   - **AB/BA Stacking:** $\Phi = -1.5$. The interlayer coupling is significantly reduced or can even change sign, suppressing the c-axis magnetic correlation.

2. **Moiré Magnetism:** In α-RuCl$_3$, the spatial modulation of $J_\perp$ acts as a periodic magnetic pressure. This leads to the "moiré zigzag" phase where the direction of the zigzag magnetic order varies between domains.

3. **Twist Angle Tunability:** By varying θ, the moiré period $L_M \approx a/\theta$ changes. At $\theta \approx 2^\circ$, $L_M \approx 170$ Å, creating large magnetic supercells that can host localized Majorana zero modes or exotic magnonic bands.

5 Conclusion

The expression $\Phi(x, y)$ serves as the fundamental building block for the continuum model of twisted α-$RuCl_3$. It maps the geometric interference of two honeycomb lattices directly onto a magnetic energy landscape, providing a blueprint for engineering quantum spin liquids via twistronics.