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Quantum geometry induced magnetic order in the flat-band dice lattice*

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Introduction

- Quantum geometry plays an important role in flat-band systems.
- A dice-lattice flat band has been realized experimentally in the layered electride YCl recently [1].
- How the quantum geometry of the dice lattice modifies the magnetic response and stabilizes magnetically ordered state.

Model and Method

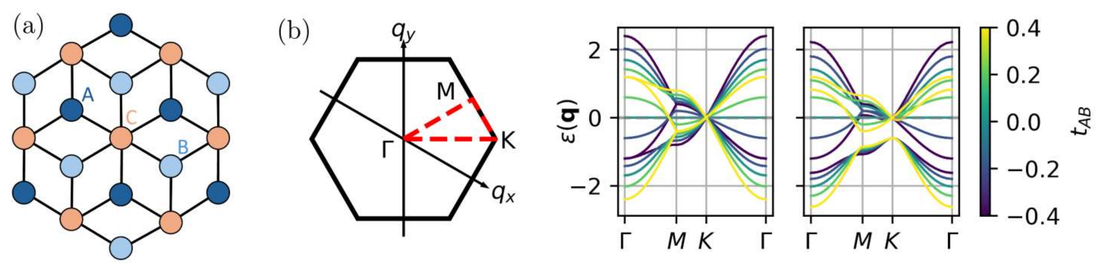

Figure: Schematic diagrams of the dice lattice and the first Brillouin zone and the band structures

The Hubbard model Hamiltonian:

$$H = -\sum_{\langle i,j\rangle,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + \text{h.c.}) + \epsilon_C n_C + U\sum_i n_{i\uparrow}n_{i\downarrow} + \mu\sum_i n_i.$$

Equations for the generalized magnetic susceptibility (GMS) [2]:

$$\delta\left\langle \hat{S}^z(\mathbf{r})\right\rangle = -\chi_s(0)h(\mathbf{r}) + \frac{1}{2}\lim_{\mathbf{q}\to 0}\partial_{q_\mu}\partial_{q_\nu}\chi_s(\mathbf{q})\partial_{r_\mu}\partial_{r_\nu}h(\mathbf{r}),$$
$$= -\chi_s(0)h(\mathbf{r}) - \partial_{r_\mu}\left(\frac{1}{2}\lim_{\mathbf{q}\to 0}\partial_{q_\mu}\partial_{q_\nu}\chi_s(\mathbf{q})B_\nu(\mathbf{r})\right),$$

$$\chi^0(\mathbf{q}, i\Omega_n) = \sum_{nm}\frac{1}{N_\mathbf{k}}\sum_\mathbf{k}\frac{f(\epsilon_n(\mathbf{k}+\mathbf{q})) - f(\epsilon_m(\mathbf{k}))}{\epsilon_m(\mathbf{k}) - \epsilon_n(\mathbf{k}+\mathbf{q}) + i\Omega_n} |\langle u_n(\mathbf{k}+\mathbf{q})|u_m(\mathbf{k})\rangle|^2$$

$$\chi^0_{\text{band}}(\mathbf{q}, i\Omega_n) = \sum_{nm}\frac{1}{N_\mathbf{k}}\sum_\mathbf{k}\frac{f(\epsilon_n(\mathbf{k}+\mathbf{q})) - f(\epsilon_m(\mathbf{k}))}{\epsilon_m(\mathbf{k}) - \epsilon_n(\mathbf{k}+\mathbf{q}) + i\Omega_n}.$$

The key point of the difference between χ^0 and χ^0_{band} is that if the information of the eigenstates (quantum geometry) from the Hamiltonian is considered.

Ferromagnetic fluctuation: $\lim_{\mathbf{q}\to 0}\partial_{q_\mu}\partial_{q_\nu}\chi_s(\mathbf{q}) < 0$

Antiferromagnetic fluctuation: $\lim_{\mathbf{q}\to 0}\partial_{q_\mu}\partial_{q_\nu}\chi_s(\mathbf{q}) > 0$

Implementation:

- Hartree–Fock (HF) approximation
- Two-particle response functions
- TRIQS–TPRF toolbox [3]

Results

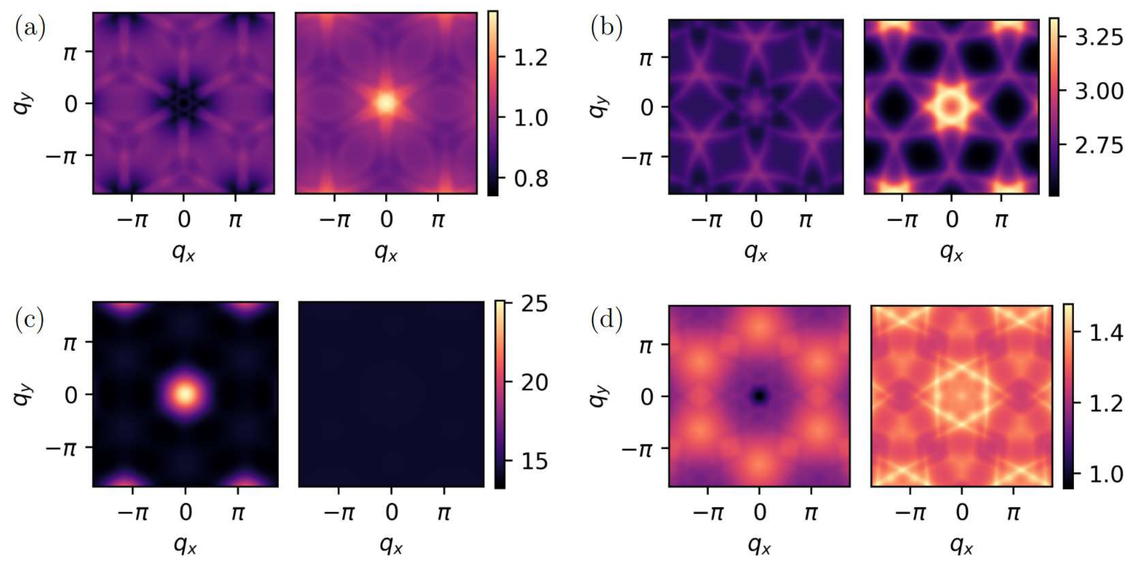

Figure: The bare spin susceptibility of the dice lattice model at the Fermi surface with (a): $t_{AB} = -0.4$, (b): $t_{AB} = -0.08$, (c): $t_{AB} = 0.0$, and (d): $t_{AB} = 0.4$. For each figure, left panel: $\chi^0_s(\mathbf{q})$; right panel: $\chi^0_{s:\text{band}}(\mathbf{q})$.

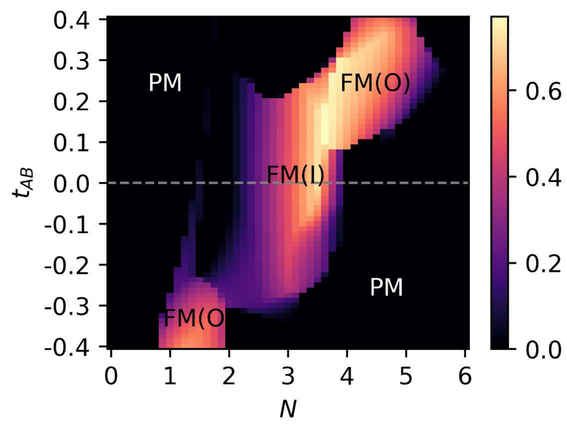

Figure: Phase diagram of the dice lattice model solved by Hartree-Fock approximation with U = 1.52 versus electron filling N and the hopping parameter t_{AB}.

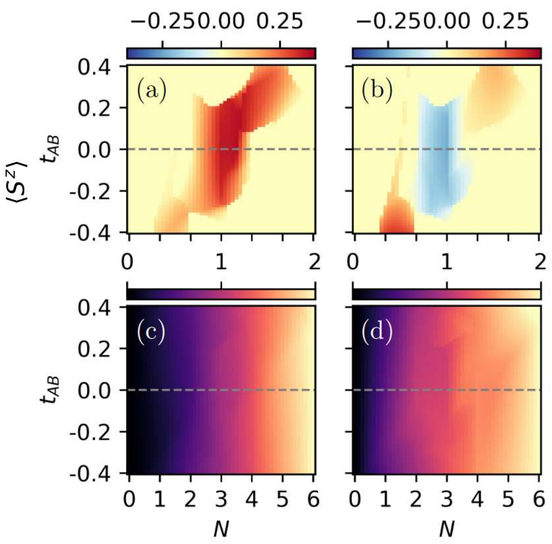

Figure: The spin polarization ⟨Sz⟩ as a function of total filling number N and hopping parameter t_{AB} (a): at site A, and (b): at site C. (c) and (d) present the filling number at site A and C as functions of t_{AB} and N, respectively.

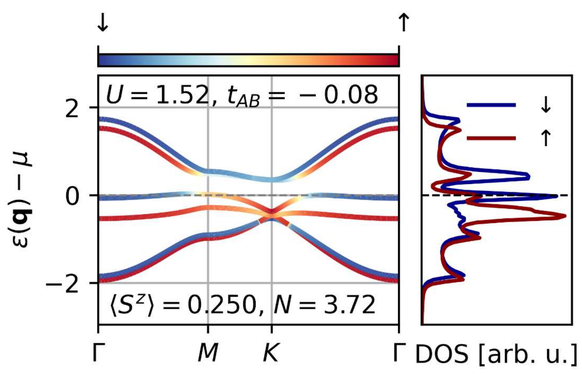

Figure: Band structure of the effective three-orbital Hubbard model on YCl solved by Hartree-Fock approximation.

Discussions

- Dice-lattice Hubbard model provides a concrete platform of research in quantum geometry and magnetic order.
- Quantum-geometry contribution is crucial in GMS that determines the magnetic order in this model.

References

[1] S. Geng, et al., arXiv:2508.21311.
[2] T. Kitamura, et al., Phys. Rev. Lett. 132, 036001 (2024).
[3] H. U. R. Strand, https://triqs.github.io/tprf/latest/ (2025).
*This is an unpublished work.