Density Matrix Renormalization Group Studies of Correlated Quantum States Emerging in Moire Materials and Beyond

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U.S. DEPARTMENT OF ENERGY | Office of Science

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Collaborations

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Z. Zhu. et al., arXiv1812.05661 and to be submitted

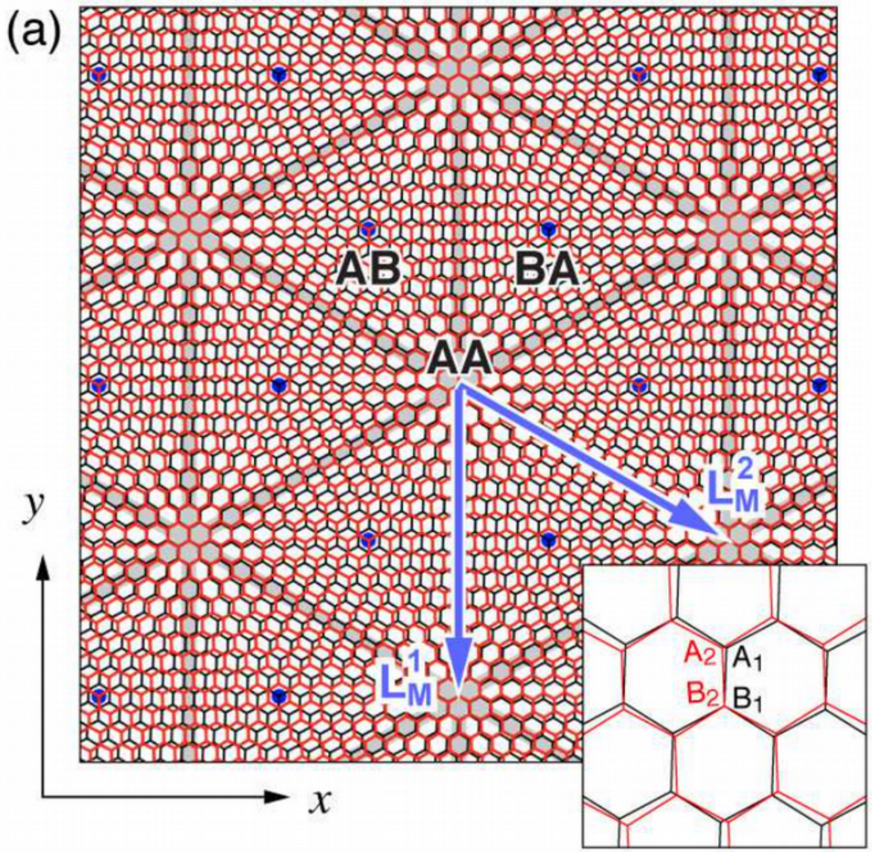
Outline

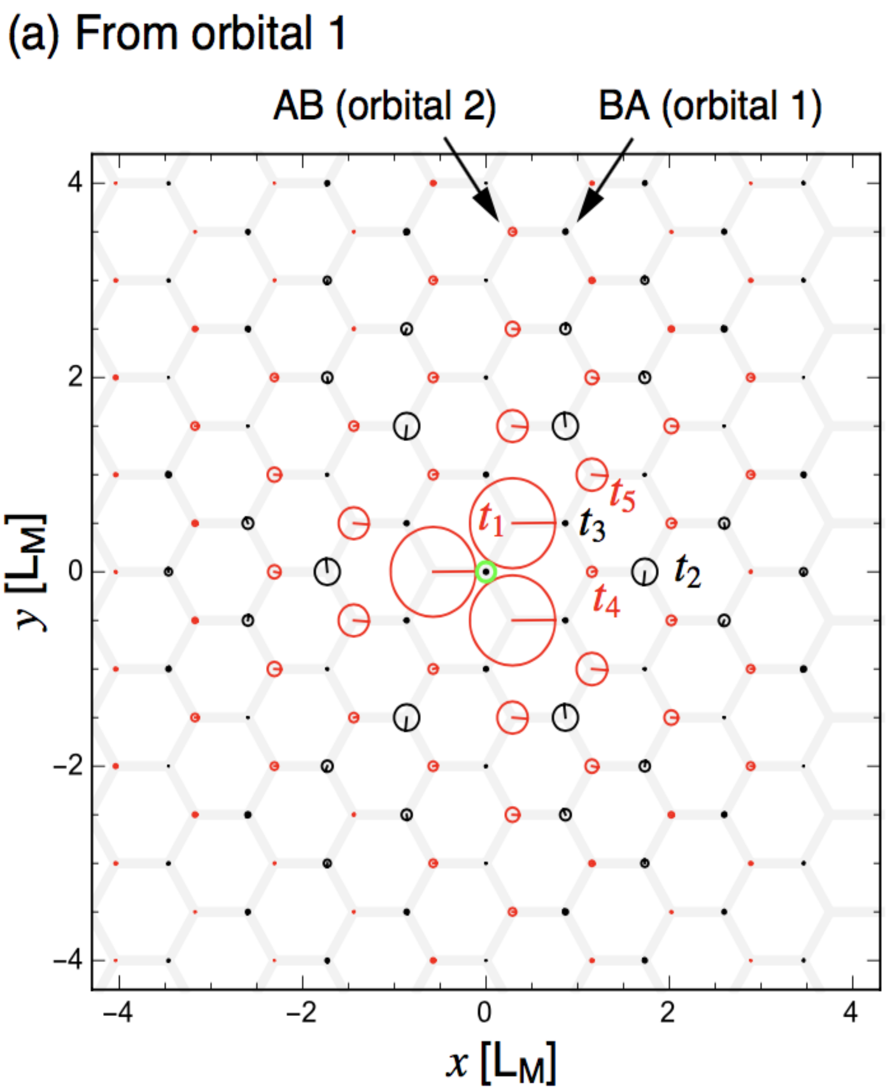
DMRG Studies of Two-Component Hubbard Models for Moire Materials

- Twisted bilayer graphene
- Trilayer graphene-boron nitride with Moire potential

Spin Liquid in Spin-One Kitaev Material

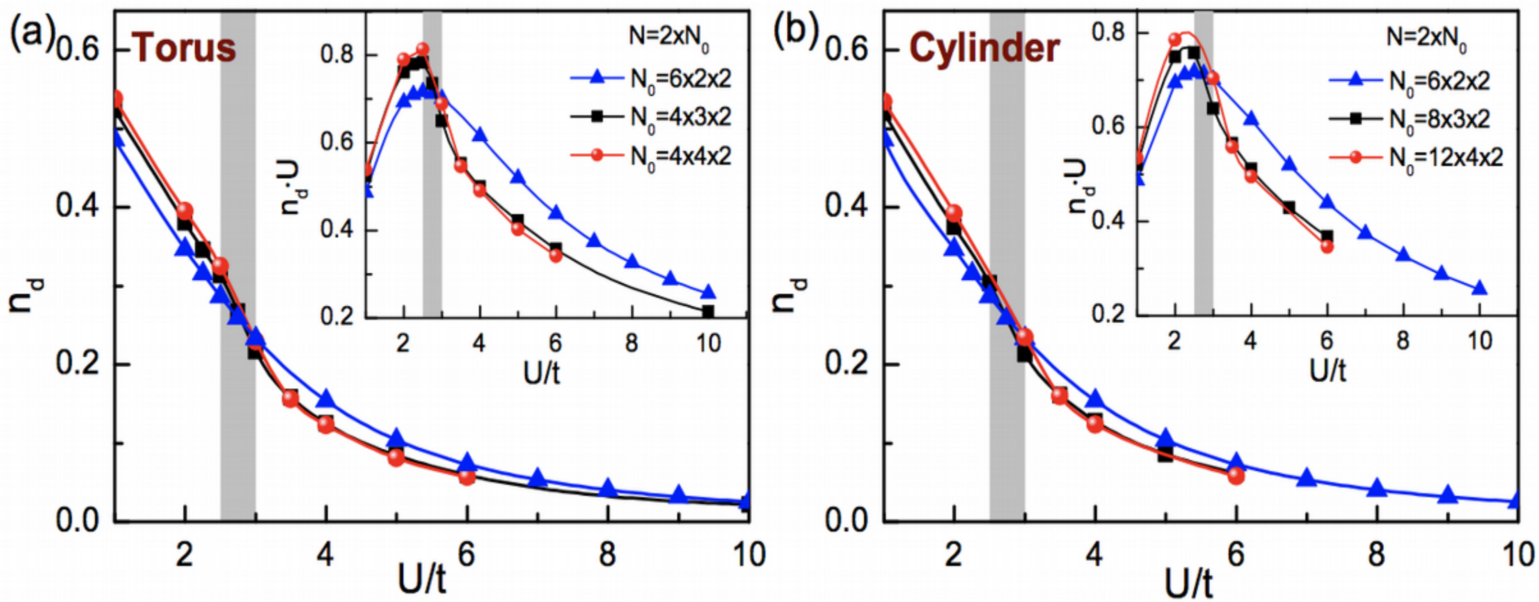
SU4 Hubbard model for twisted graphene





Koshino et al.(18)

Hubbard U driven transition



$$H = H_0 + H_{\rm int},$$

$$H_0 = -t \sum_{\langle i,j\rangle \sigma} \sum_{\alpha=1,2} \left(c^{\dagger}_{i\sigma,\alpha} c_{j\sigma,\alpha} + h.c. \right),$$

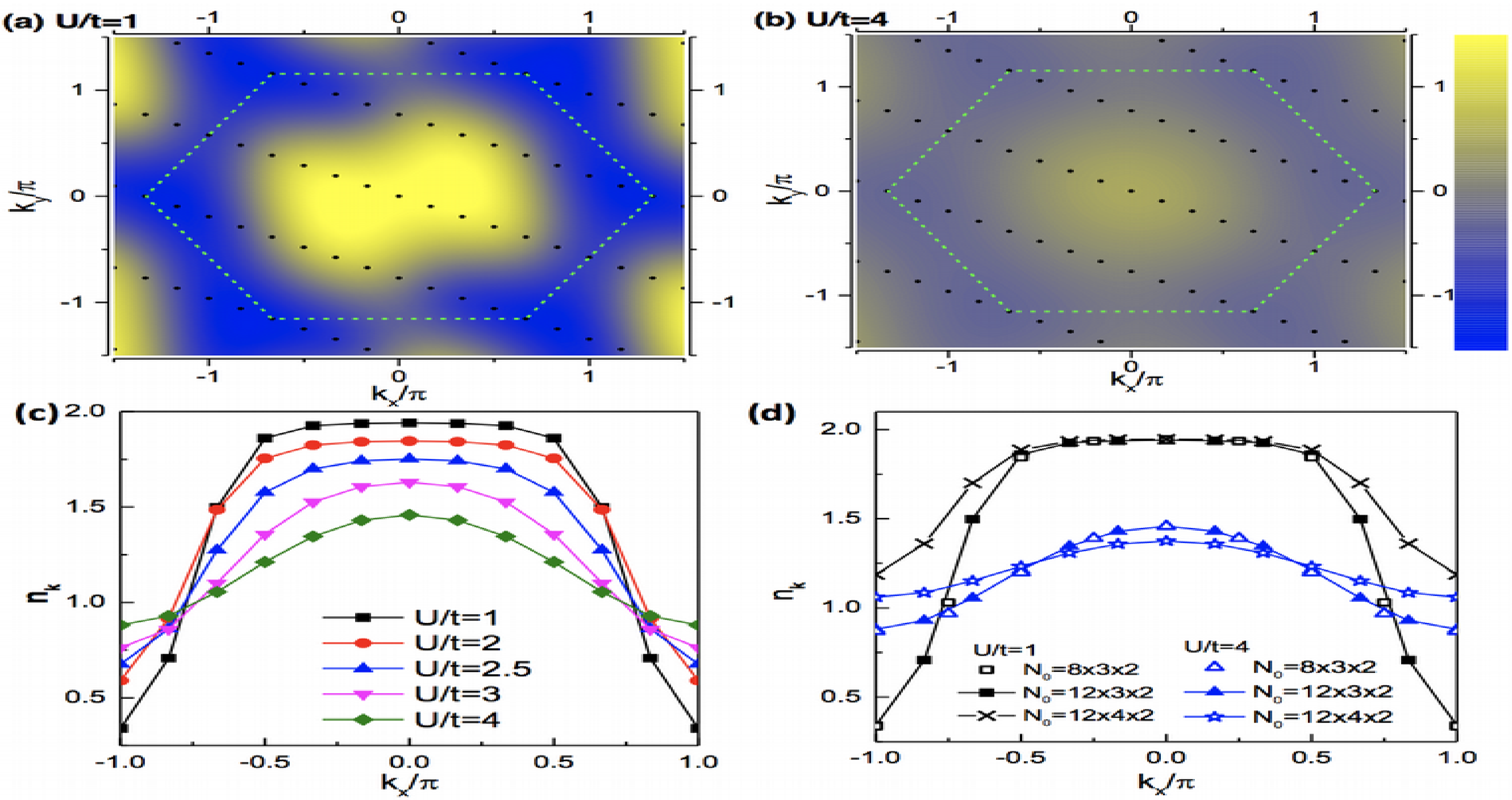
$$H_{\rm int} = U \sum_i \left(\sum_{\sigma,\alpha} n_{i\sigma,\alpha} - 1 \right)^2,$$

Identifying Uc ~3

We consider ¼ filling number
That is one electron per
unit cell

$$n_d = \frac{1}{N_0} \sum_{i=1}^{N_0} \left\langle \left[\sum_{\sigma,\alpha} n_{i\sigma,\alpha} - 1 \right]^2 \right\rangle,$$

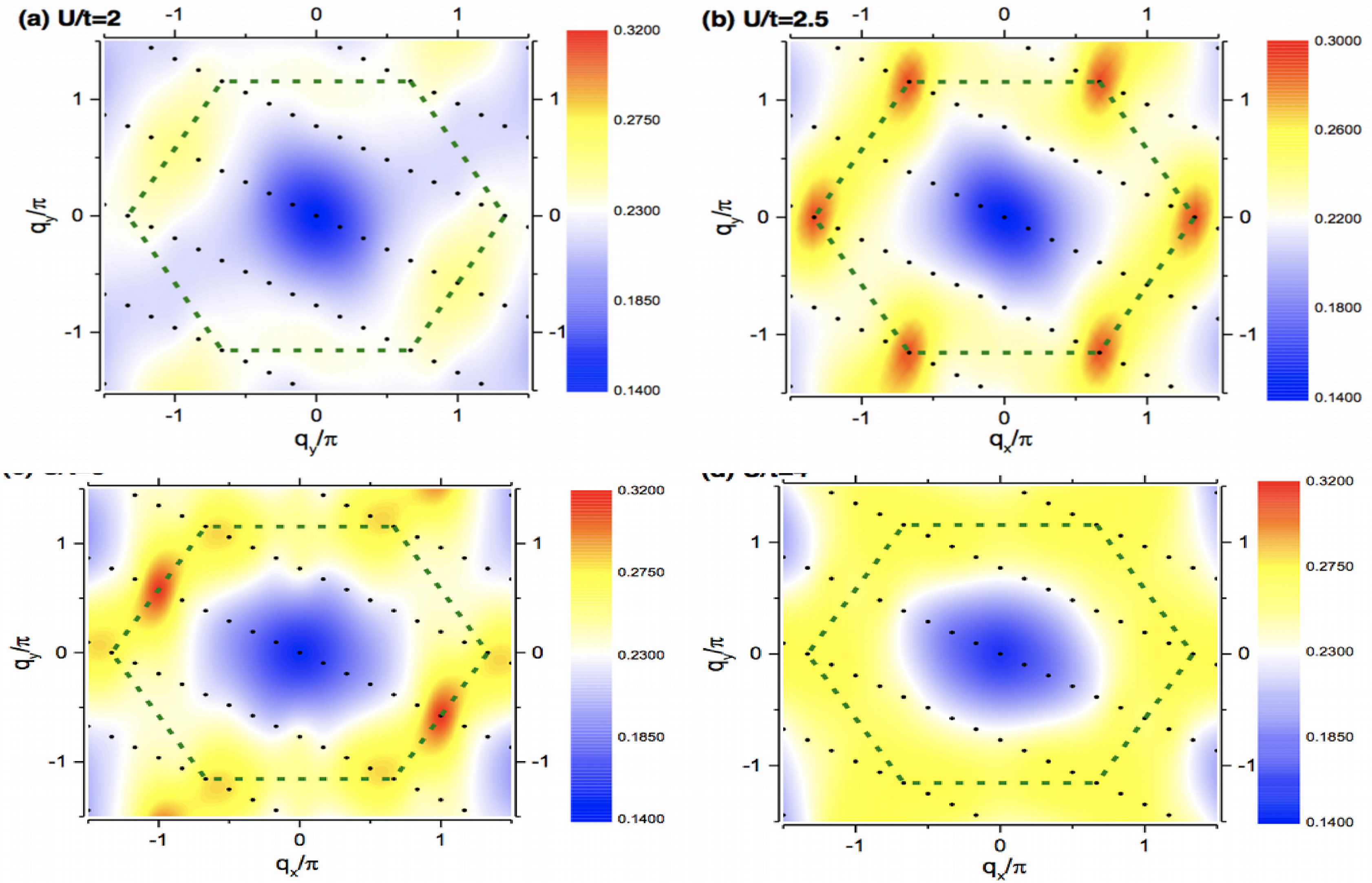
Fermi-surface topology



$$n(\mathbf{k}) = \frac{1}{N_0} \sum_{i,j,\sigma} \left\langle c_{i\sigma}^{\dagger} c_{j\sigma} \right\rangle e^{i\mathbf{k}(\mathbf{r_i}-\mathbf{r_j})}.$$

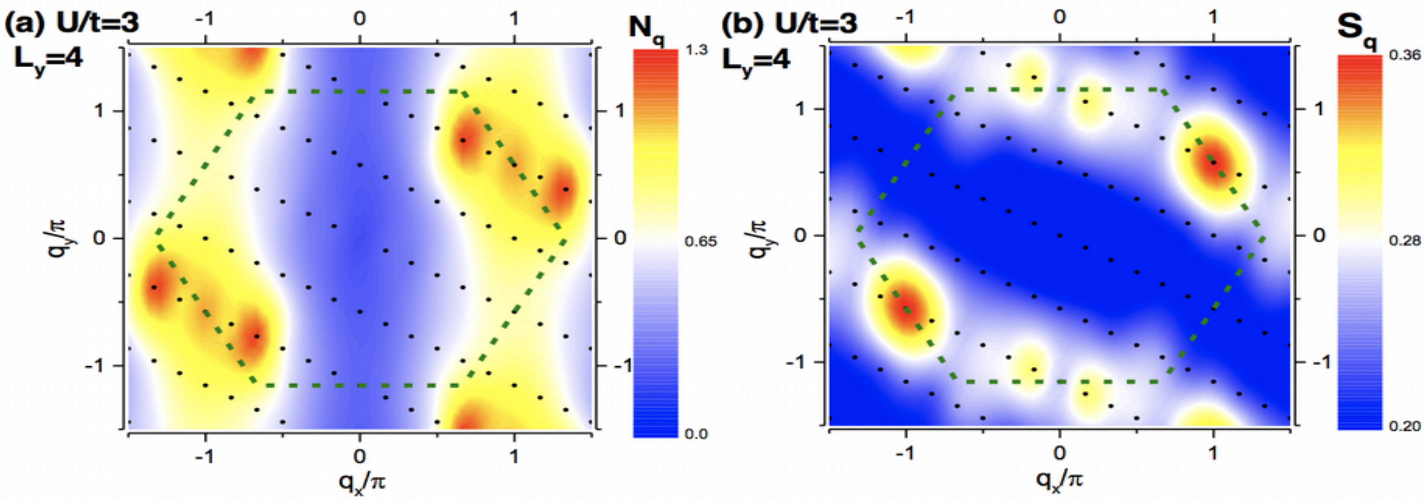
Mott insulator
At U>Uc

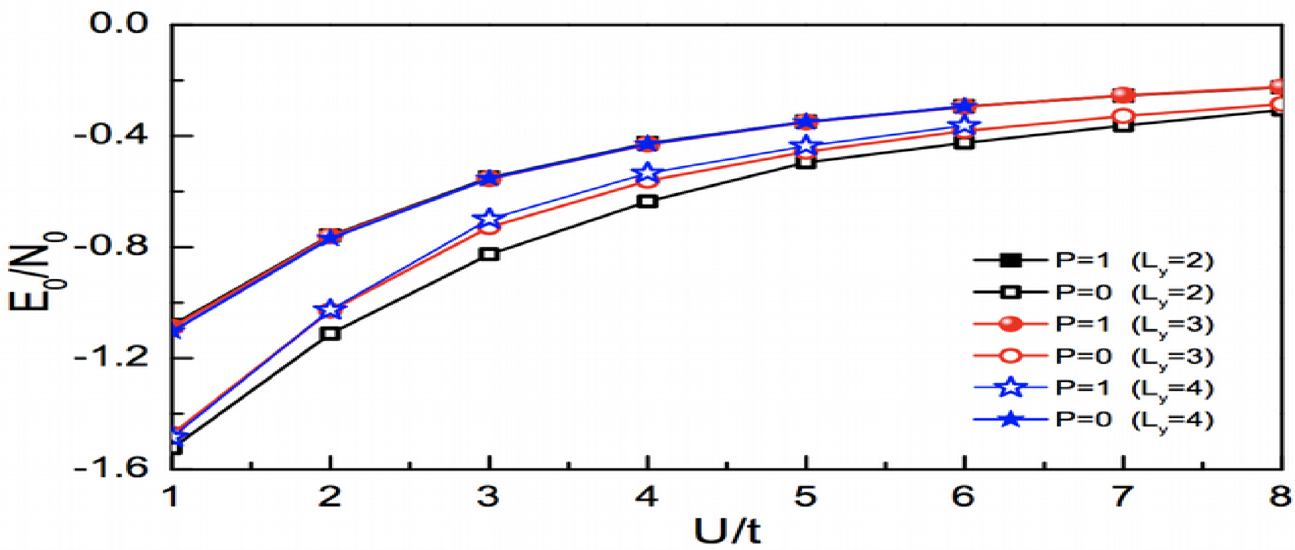
Spin/orbital density structure factor



$$S_{\mathbf{q}} = \frac{1}{N_0} \sum_{i,j} \langle S_i^z S_j^z \rangle e^{i\mathbf{q}(\mathbf{r_i} - \mathbf{r_j})} .$$

Robust spin/orbital peak at larger Ly=4

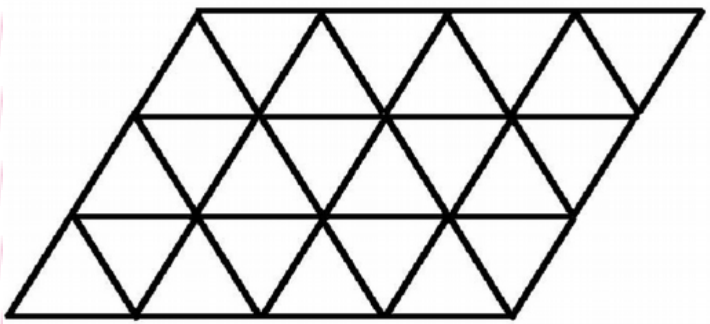


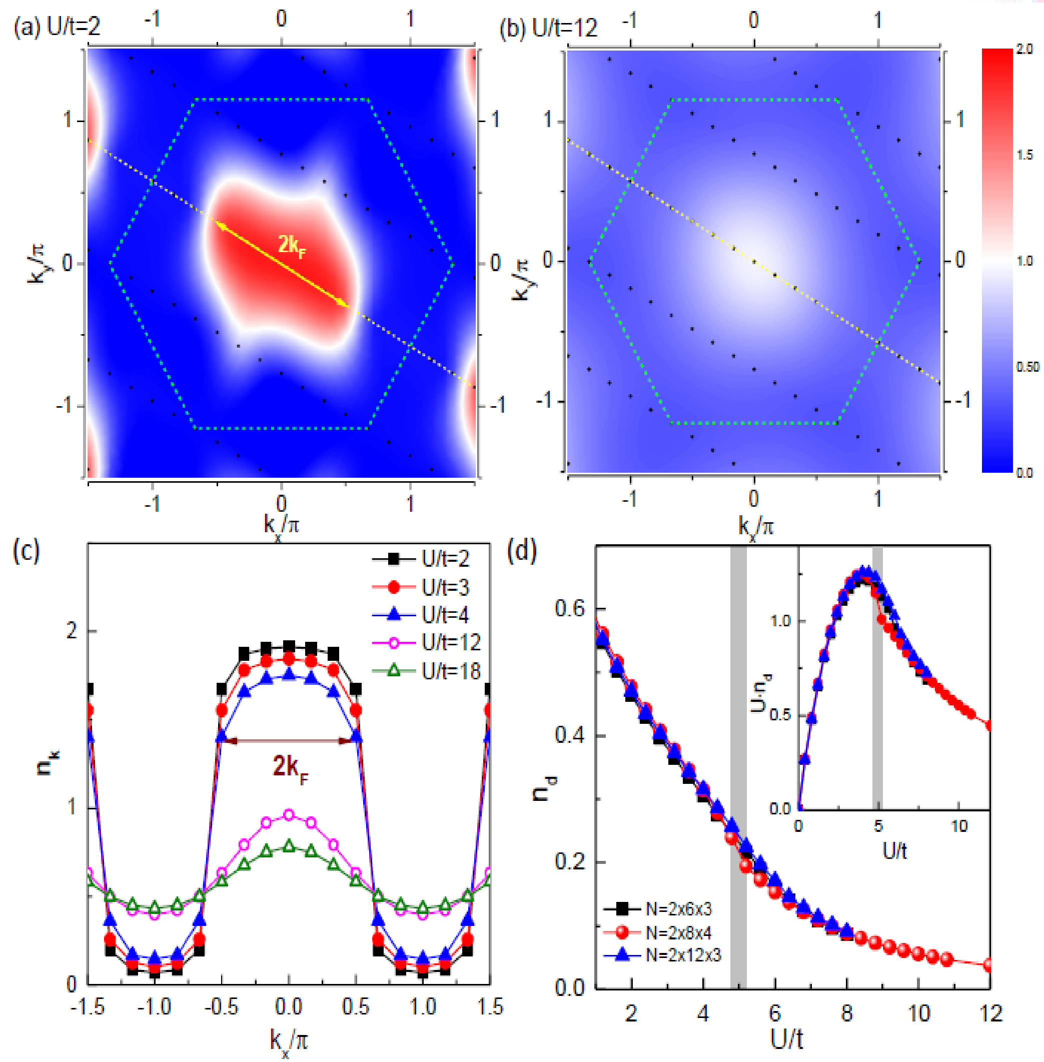


No valley polarization

SU4 Hubbard Model for Trilayer Graphene-Boron Nitride and Twisted Transition Metal Dichalcogenides

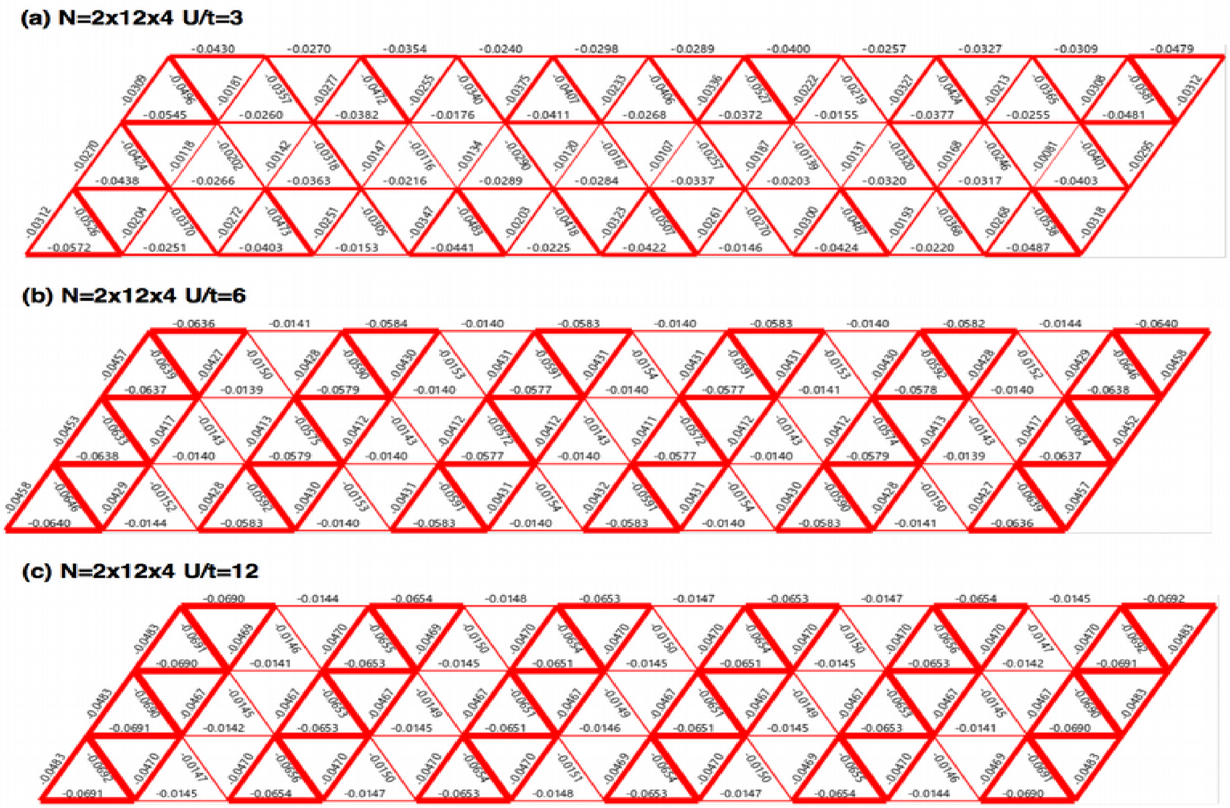
$$H = -t \sum_{\langle i,j\rangle,\sigma\alpha} (c^{\dagger}_{i,\sigma\alpha} c_{j,\sigma\alpha} + h.c.) + U \sum_{i} (\sum_{\sigma\alpha} n_{i,\sigma\alpha} - 1)^2$$





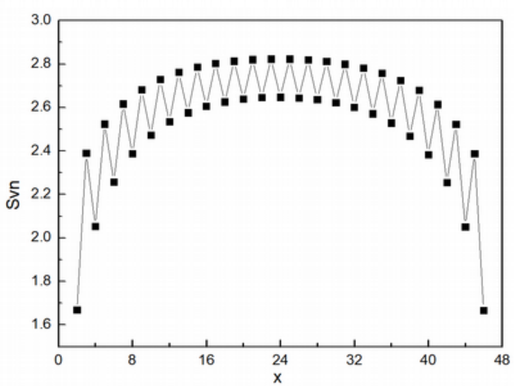
We consider ¼ filling number, one electron per unit cell

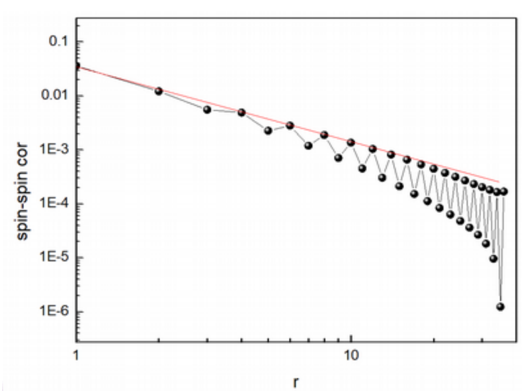
Stripe VBS appears with larger U

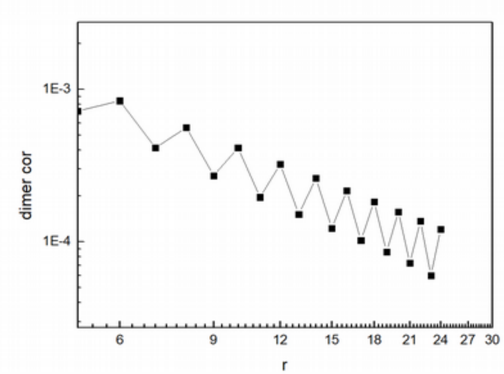


with possible gapless excitations due to half filling of each unit cell

Finite central charge from entanglement entropy

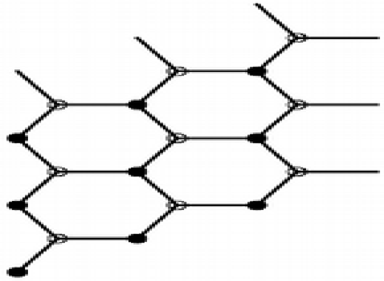






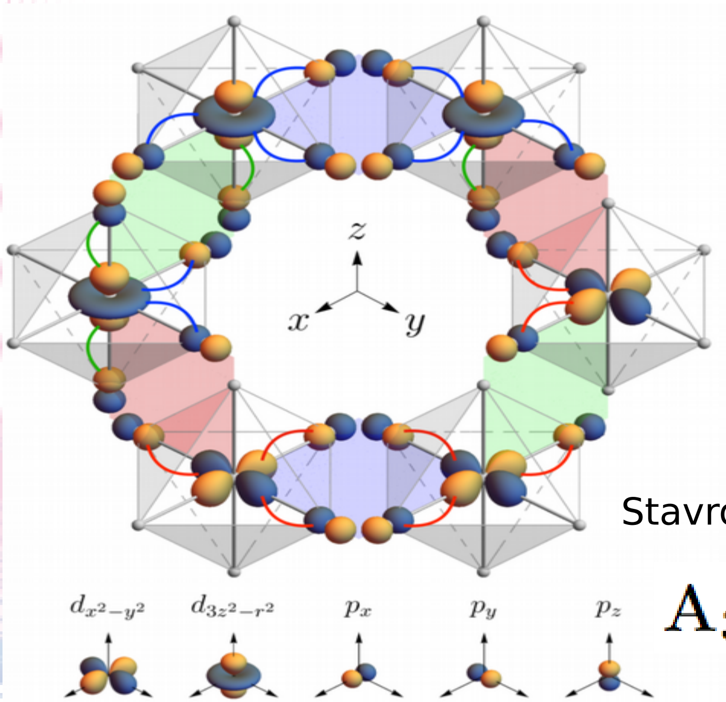
Spin-1 Kitaev-Heisenberg model

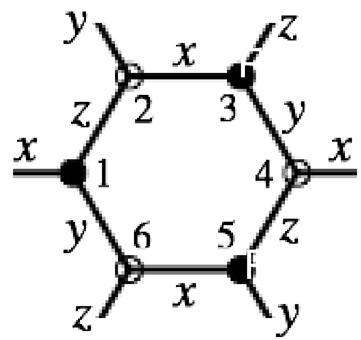
$$\hat{H} = K_x \sum_{\langle i,j \rangle_x} S_i^x S_j^x + K_y \sum_{\langle i,j \rangle_y} S_i^y S_j^y + K_z \sum_{\langle i,j \rangle_z} S_i^z S_j^z + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



$$W_L = e^{i\pi S_1^{\alpha 12}} e^{i\pi S_2^{\alpha 12}} e^{i\pi S_2^{\alpha 23}} e^{i\pi S_3^{\alpha 23}} \ldots e^{i\pi S_{(n-1)}^{\alpha (n-1)n}} e^{i\pi S_n^{\alpha (n-1)n}} e^{i\pi S_n^{\alpha n1}} e^{i\pi S_1^{\alpha n1}}$$

$$W_p = e^{i\pi S_1^z} e^{i\pi S_2^z} e^{i\pi S_2^x} e^{i\pi S_3^x} e^{i\pi S_3^y} e^{i\pi S_4^y} e^{i\pi S_4^z} e^{i\pi S_5^z} e^{i\pi S_5^x} e^{i\pi S_6^x} e^{i\pi S_6^y} e^{i\pi S_1^y}$$





$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

$$W_p = e^{i\pi S_1^x} e^{i\pi S_2^y} e^{i\pi S_3^z} e^{i\pi S_4^x} e^{i\pi S_5^y} e^{i\pi S_6^z}$$

Stavropoulos et al

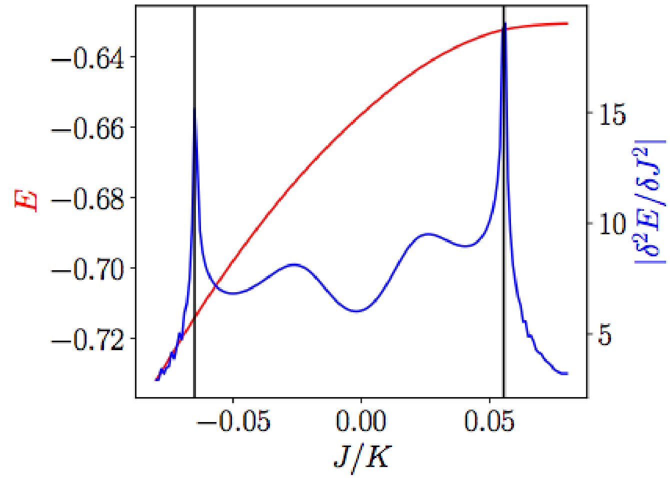
$A_3Ni_2XO_6$

X=Bi, Sb

Conserved Wilson loop operators

Phase diagram

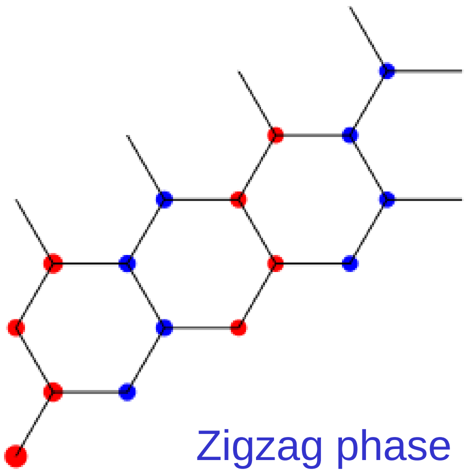
$$\hat{H} = K_x \sum_{\langle i,j \rangle_x} S_i^x S_j^x + K_y \sum_{\langle i,j \rangle_y} S_i^y S_j^y + K_z \sum_{\langle i,j \rangle_z} S_i^z S_j^z + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

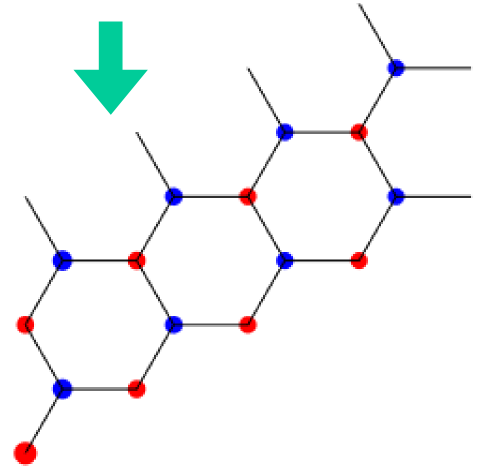


$K = 1.0$

$L_y = 2$

iDMRG





Zigzag phase | Spin liquid | Neel phase

J

-0.0650 0.0555

Summary

Large scale DMRG studies reveal different possible correlated phases for multi-orbital Hubbard models.

These results may be relevant for understanding twisted and trilayer graphene subject to Moire patterns.

Interesting gapless spin liquid is also found for S=1 Kitaev model