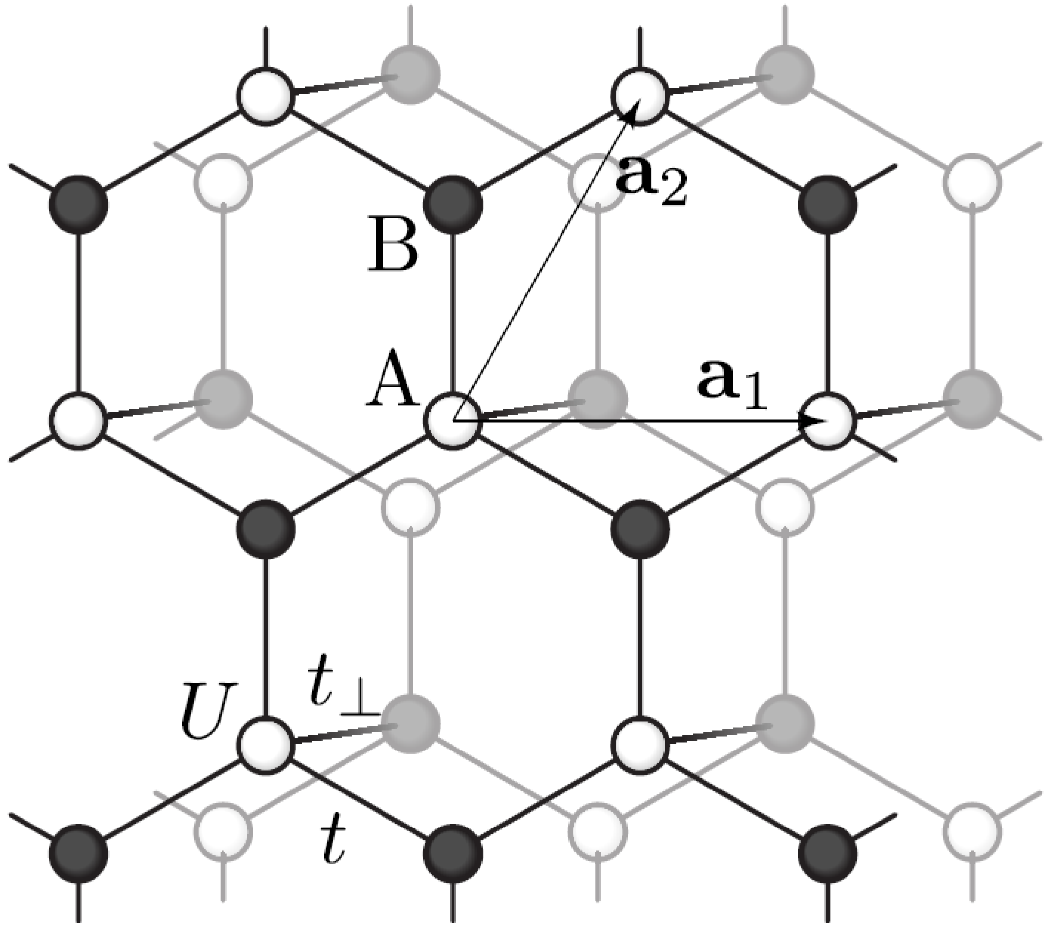
Hubbard model on Graphene bilayer



[Phys. Rev. Lett. 109. 126402 (2012)]

Zi Yang Meng

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LaSigma Journal Club

Motivation & Model

❑ Graphene Bilayer

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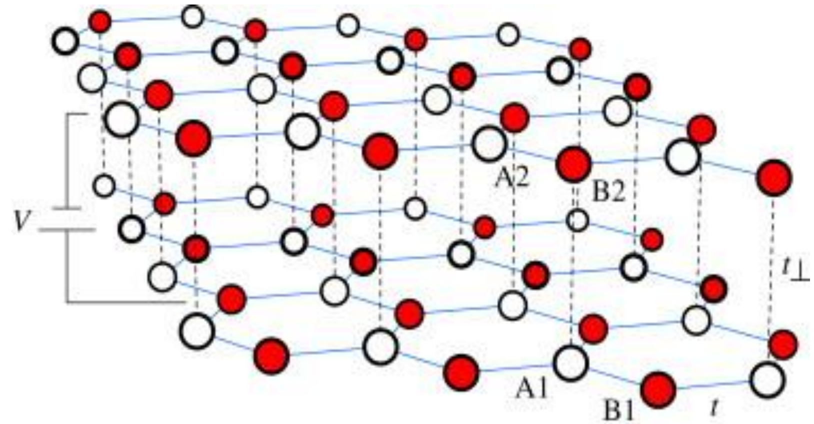


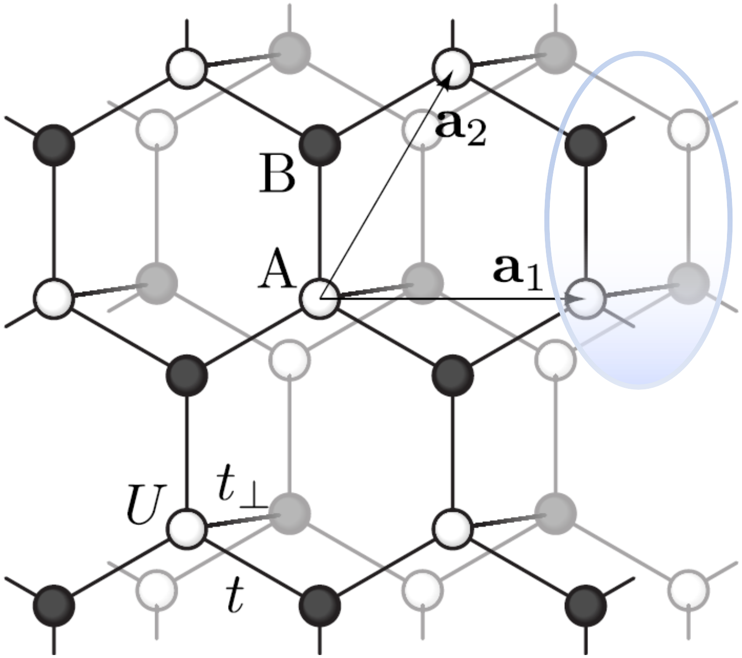
Leading instabilities:
AF, QAH, QSH, SC, Nematic, …

❑ Starts from most basic model

$$H = -t \sum_{\langle i,j \rangle} \vec{c}_i^\dagger \vec{c}_j + \frac{U}{2} \sum_i \left(\vec{c}_i^\dagger \vec{c}_j - 1 \right)^2$$

$$\vec{c}_i^\dagger = \left(c_{i,\uparrow}^\dagger, c_{i,\downarrow}^\dagger \right)$$

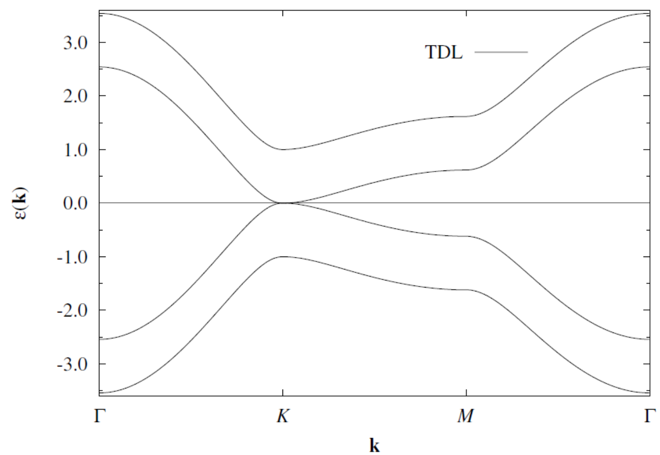
Model

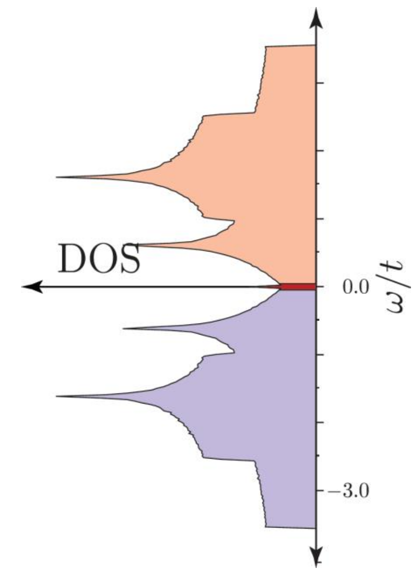


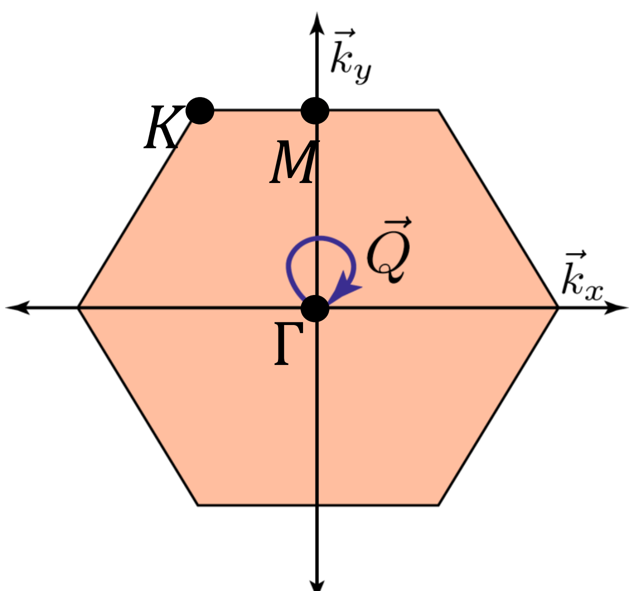
$$H = -t \sum_{\langle i,j \rangle} \vec{c}_i^{\dagger} \vec{c}_j + \frac{U}{2} \sum_i \left(\vec{c}_i^{\dagger} \vec{c}_j - 1 \right)^2$$

four site unit cell

Free dispersion: $t_\perp = t = 1$







Fermi surface instability

$$\chi(\vec{q}) = -\frac{1}{2N} \sum_{\vec{k}} \frac{n_F(\vec{k}+\vec{q}) - n_F(\vec{k})}{\varepsilon(\vec{k}) - \varepsilon(\vec{k}+\vec{q})}$$

Nesting condition

$$\varepsilon(\vec{k} + \vec{Q}) = \varepsilon(\vec{k})$$

Methods

❑ Weak coupling

Mean-field (MF), decouple the interaction $n_{i,\sigma} = \langle n_{i,\sigma} \rangle + (n_{i,\sigma} - \langle n_{i,\sigma} \rangle)$

$$m_i = (\langle n_{i,\uparrow} \rangle - \langle n_{i,\downarrow} \rangle)/2$$

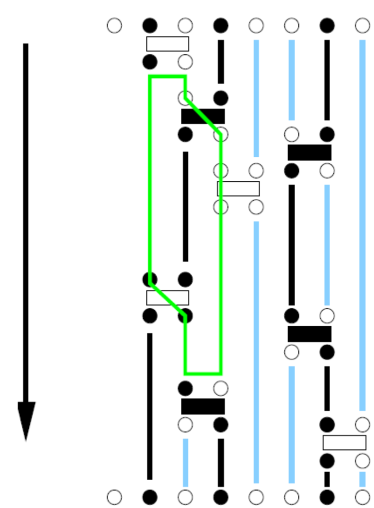
Functional Renormalization group (fRG)

❑ Strong coupling

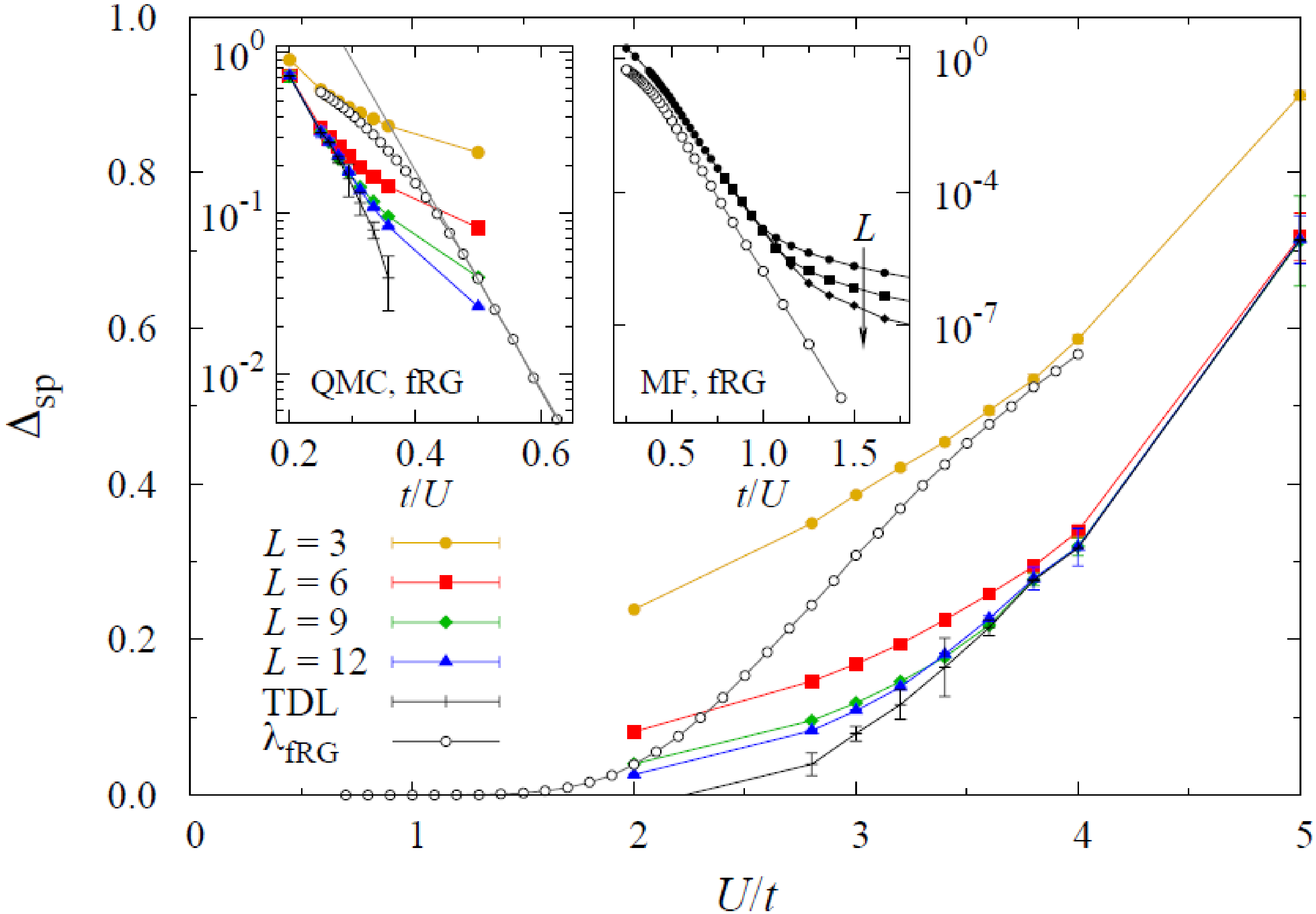
Projective determinantal QMC
fermionic system

$$\frac{\langle \Psi_0 | A | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \lim_{\Theta \to \infty} \frac{\langle \Psi_T | e^{-\Theta H/2} A e^{-\Theta H/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-\Theta H} | \Psi_T \rangle}$$

Stoachastic series expansion QMC
spin system



Results: Metal or Insulator



exponentially opening of the single particle gap

$$\Delta_{sp} \propto \exp(-\alpha \frac{t}{U})$$

QMC and Mf exhibit similar finite size effects.

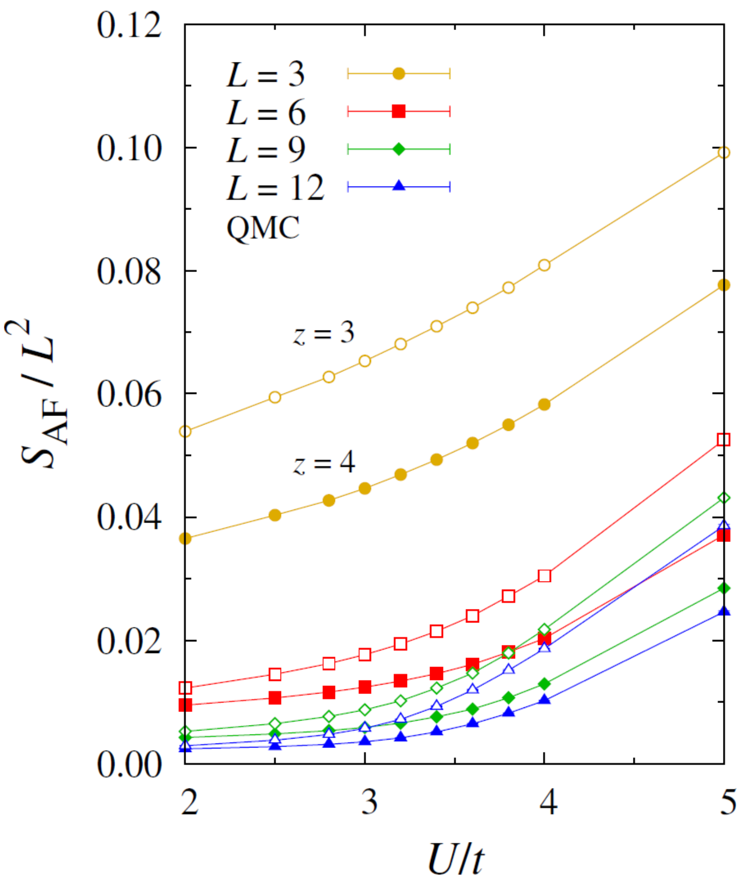
Weak-coupling methods tend to overestimate the onset of order.

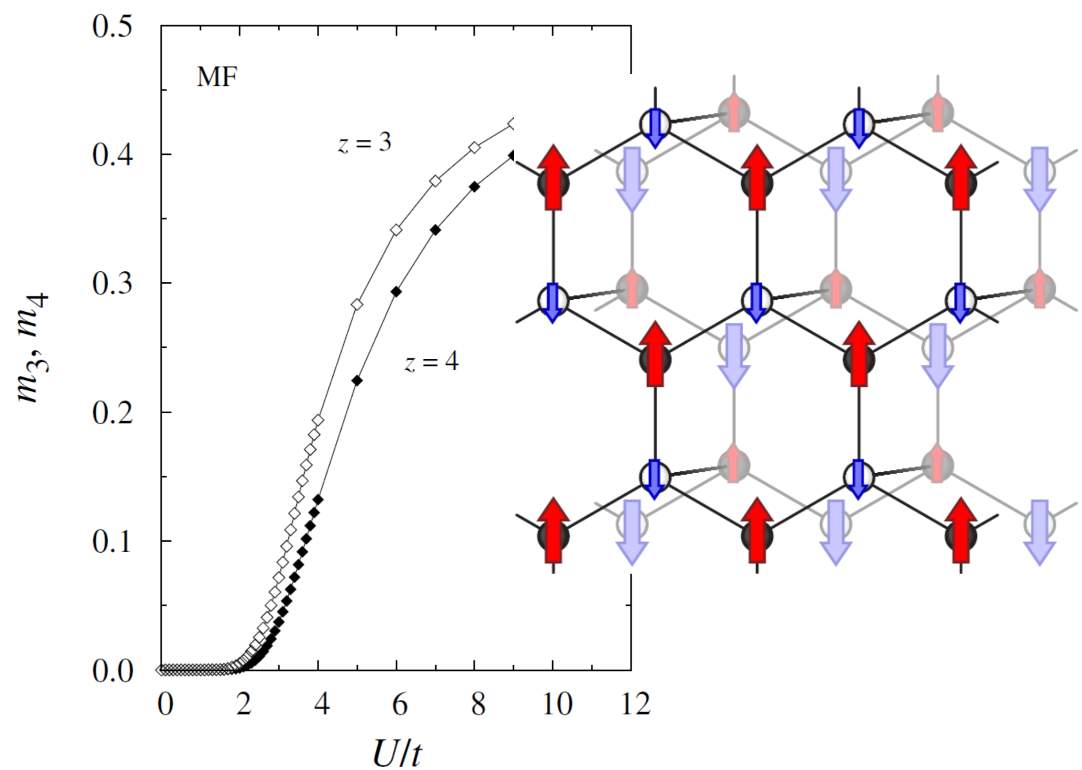
- ❑ continuous opening of the single particle gap.
- ❑ consistent picture of MF, fRG and finite size QMC.

Results: Magnetic order

Antiferromagnetic sublattice-structure factor: $S_{\mathrm{AF},z} = \frac{1}{2L^2} \sum_{i,j|z_i=z_j=z} \epsilon_i \epsilon_j \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ $z = 3{,}4$

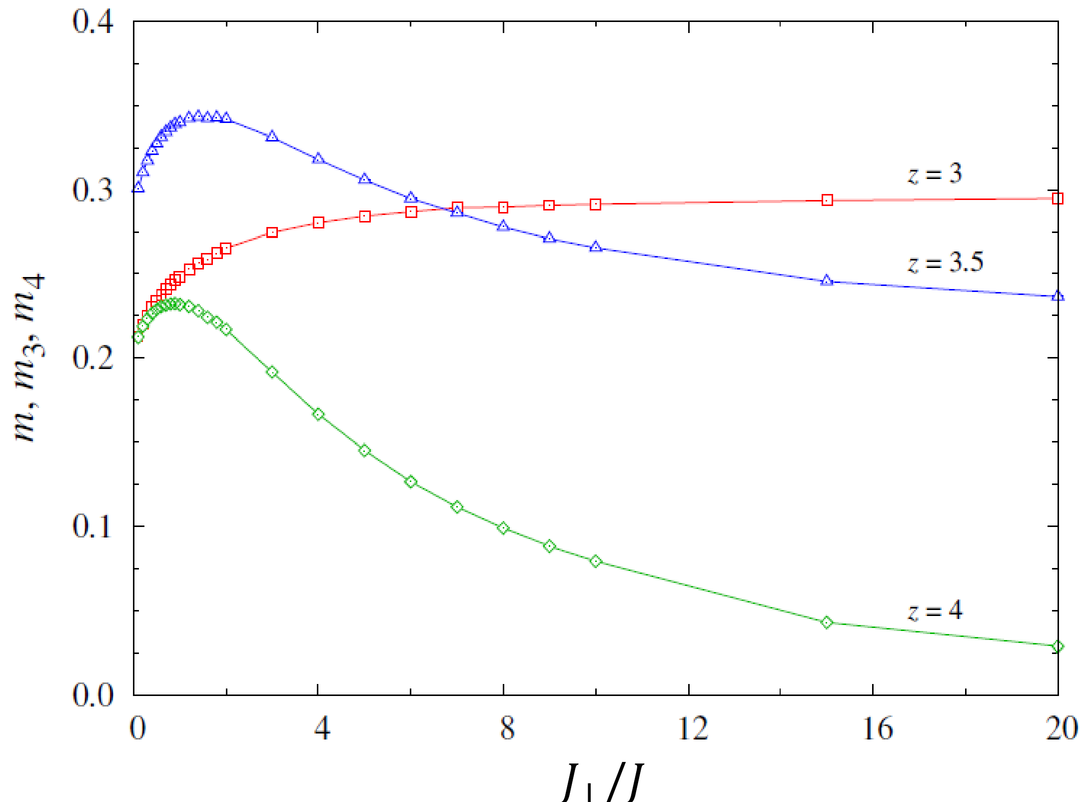
Antiferromagnetic sublattice-order parameter: $m_z = \sqrt{S_{\mathrm{AF},z}/(2L^2)}$

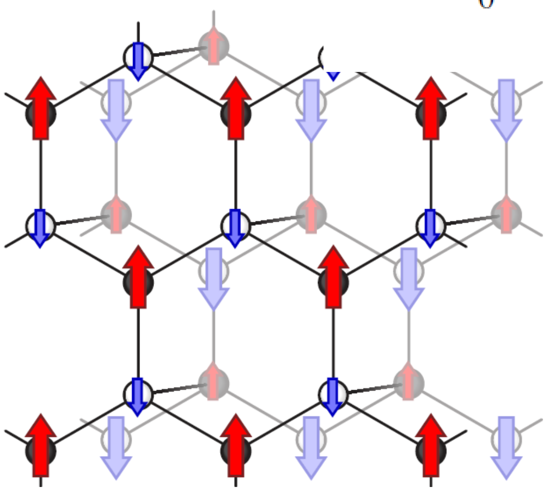




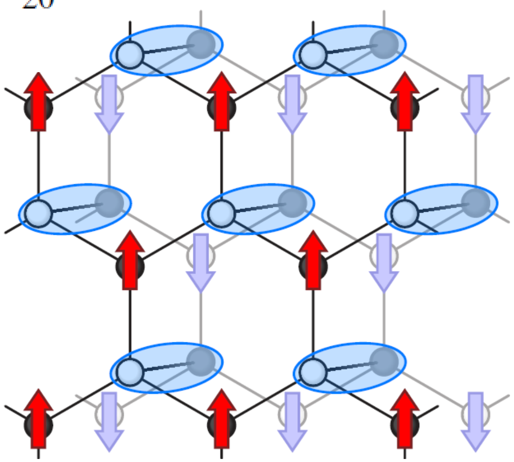
- ❑ exponentially onset of magnetization: $m \propto \Delta_{sp}$, $(U/t)_c = 0^+$
- ❑ different sublattice magnetization for sites with different coordination numbers

AFM instability

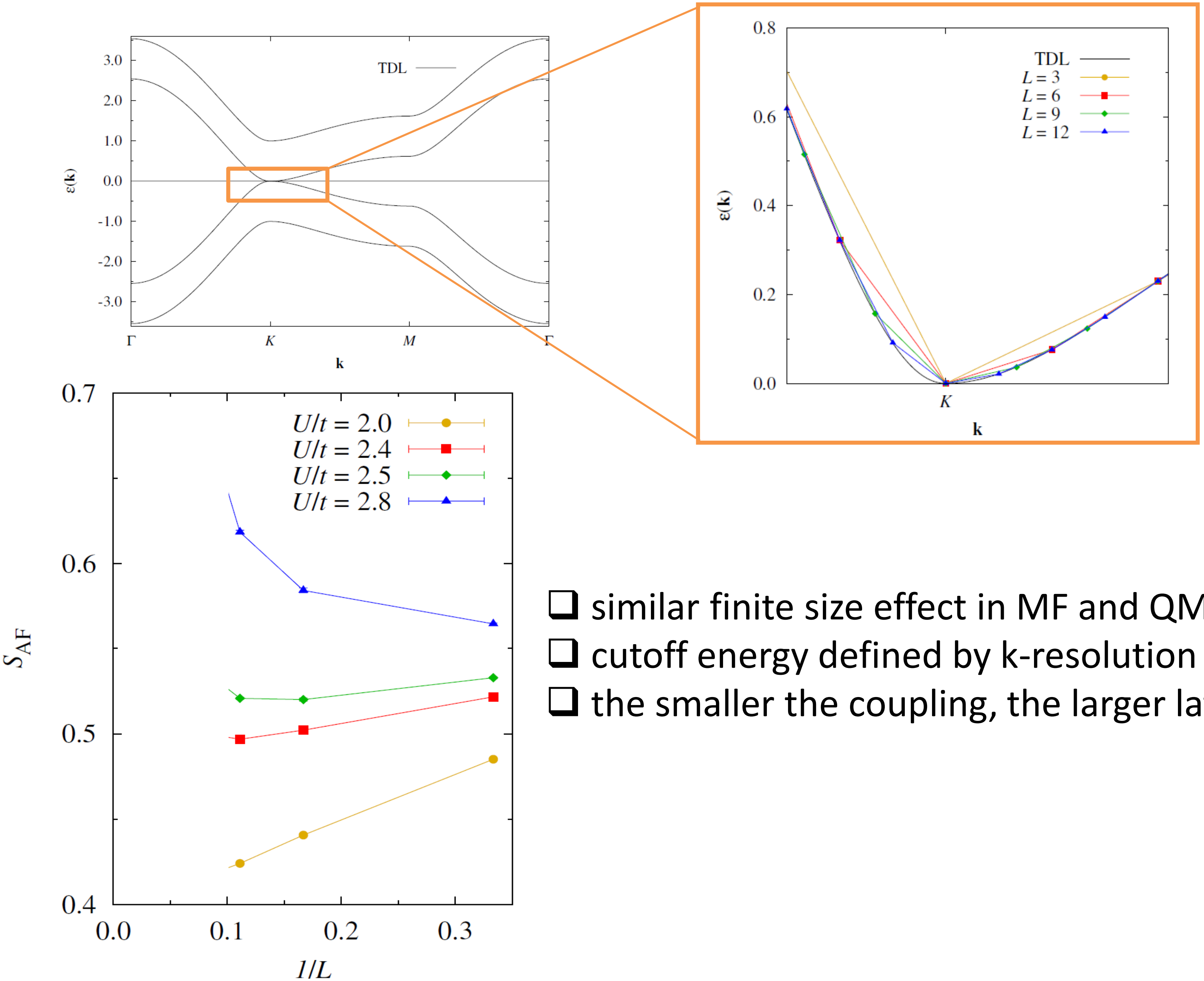




- ❑ Sublattice mag. Z=3 saturates
- ❑ Sublatttice mag. Z=4 suppressed by interlayer singlet formation



Finite size effect

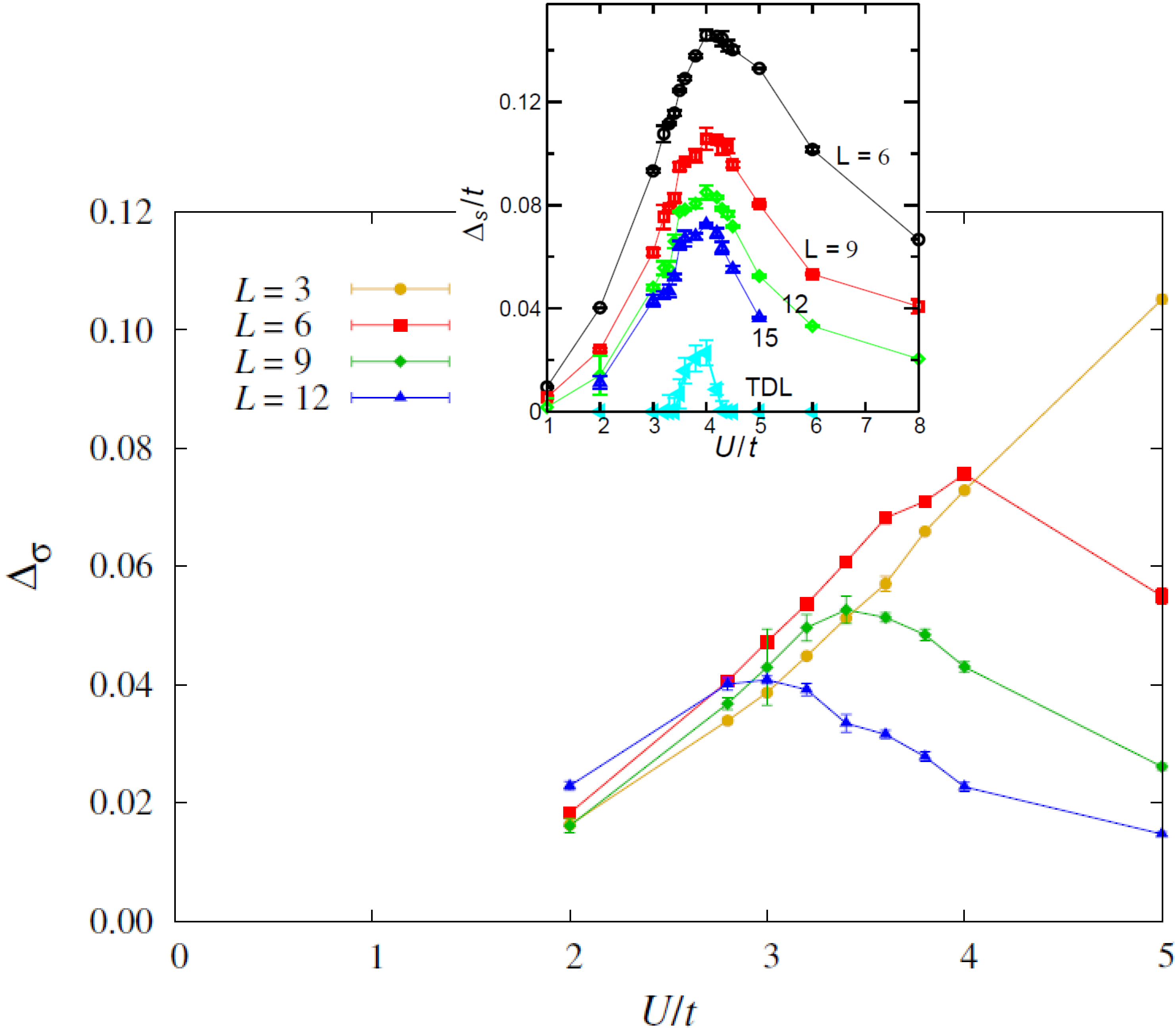


- ❑ similar finite size effect in MF and QMC
- ❑ cutoff energy defined by k-resolution
- ❑ the smaller the coupling, the larger lattice needed

Conclusion

Hubbard model on Graphene bilayer:

- ❑ Fermi surface instability favors AF order.
- ❑ Exponentially opening of single particle gap and AF order parameter.
- ❑ Inhomogeneous participation of the mag. moments in z=3 and 4.
- ❑ Unsual finite size scaling, complimentary methodologies needed.



0.12
0.10
0.08
0.06
0.04
0.02
0.00
0
1
2
3
4
5
U/t
Δ_σ
$L = 3$
$L = 6$
$L = 9$
$L = 12$
Δ_s/t
0.12
0.08
0.04
0
1
2
3
4
5
6
7
8
U/t
L = 6
L = 9
12
15
TDL