# Magnetic Phase Transitions in a Quantum Spin-orbital Liquid

Shi Feng

Department of Physics

The Ohio State University

Collaborators: Niravkumar D. Patel, The Ohio State University
Panjin Kim, National Security Research Institute, Korea
Jung Hoon Han, Sungkyunkwan University, Korea
Nandini Trivedi, The Ohio State University, USA

**arXiv:1912.09516**

DE-FG02-07ER46423

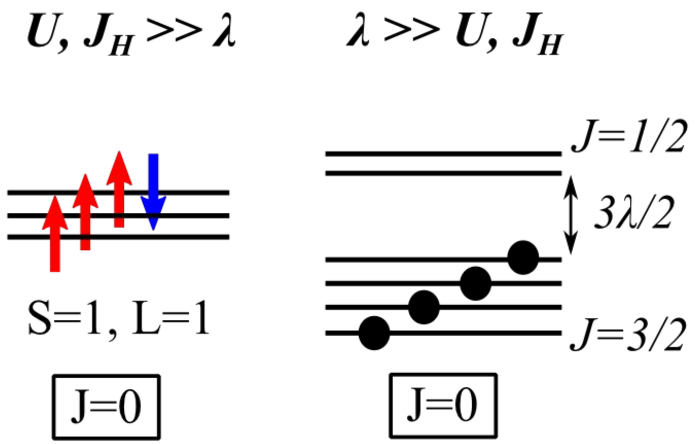
# d4 Materials

## Atomic limit

Weak (left) & Strong (right) Spin-orbital coupling limit

$$H = \sum_i H_{i,U} + \lambda H_{i,SOC}$$

**No atomic moment**



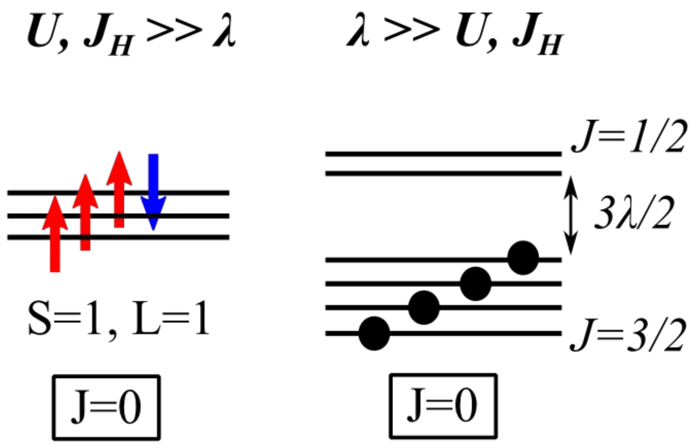
# d4 Materials

## Atomic limit

Weak (left) & Strong (right) Spin-orbital coupling limit

$$H = \sum_i H_{i,U} + \lambda H_{i,SOC}$$

**No atomic moment**




Magnetism in d4 **e.g. Ba2YIrO6, OsCl4**

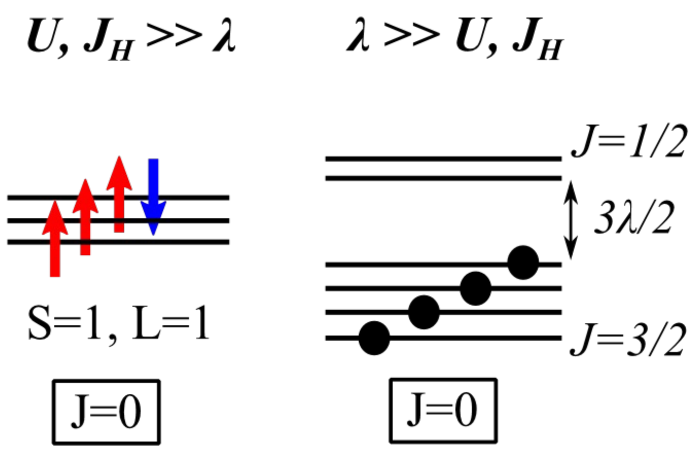
# d4 Materials

## Atomic limit

Weak (left) & Strong (right) Spin-orbital coupling limit

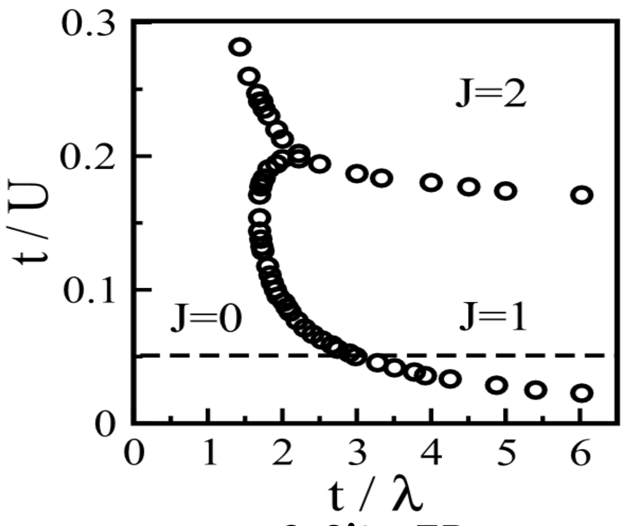
$$H = \sum_i H_{i,U} + \lambda H_{i,SOC}$$

**No atomic moment**




## Magnetism in d4 **e.g. Ba2YIrO6, OsCl4**

$$H = \sum_{\langle ij \rangle} t H_{\langle ij \rangle, hop} + \sum_i H_{i,U} + \lambda H_{i,SOC}$$




2-Site ED

**Effective Hamiltonian:**

$$H_{eff} = -J_{FM} \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$

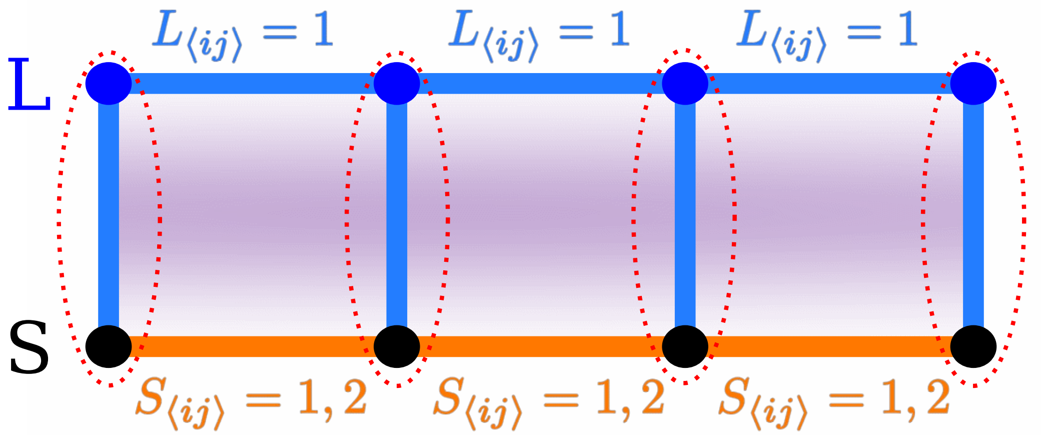
*Meetei, Cole, Randeria, Trivedi, Phys. Rev. B 91, 054412 (2015)*

# 1-D Spin-Orbital Chain

$$H = -J_{FM} \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$

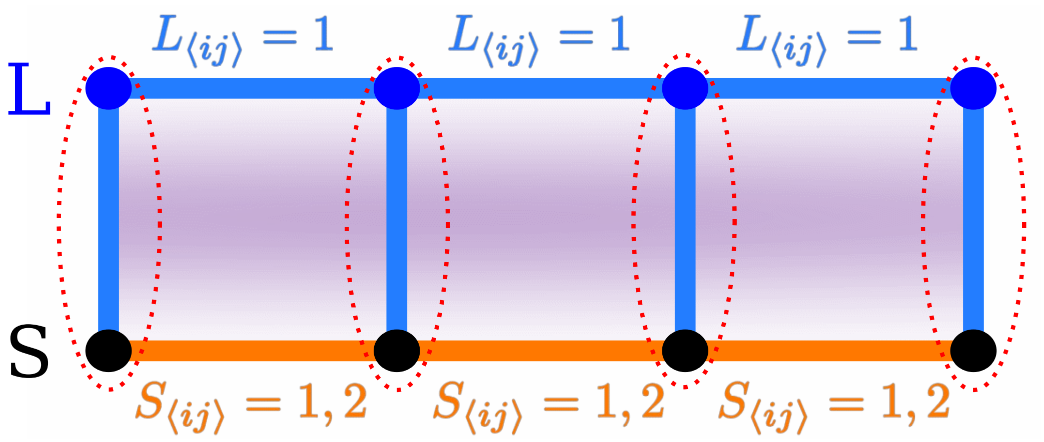
Orbital projection is well-known Uimin-Lai-Sutherland (ULS) interaction

$$h^{ULS}_{\langle ij \rangle} = -P^{(1)}_{\langle ij \rangle} = (\vec{L}_i \cdot \vec{L}_j)^2 + (\vec{L}_i \cdot \vec{L}_j) - 2$$



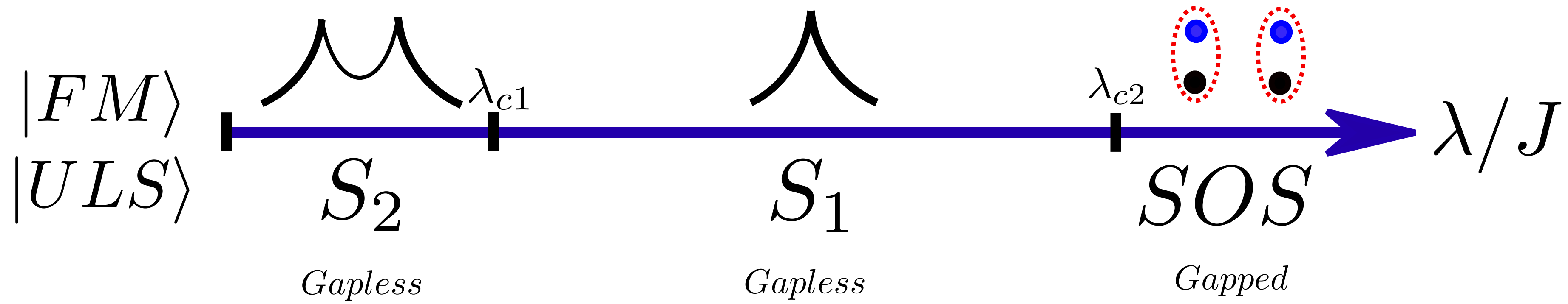
# 1-D Spin-Orbital Chain

$$H = -J_{FM} \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$




Orbital projection is well-known Uimin-Lai-Sutherland (ULS) interaction

$$h^{ULS}_{\langle ij \rangle} = -P^{(1)}_{\langle ij \rangle} = (\vec{L}_i \cdot \vec{L}_j)^2 + (\vec{L}_i \cdot \vec{L}_j) - 2$$

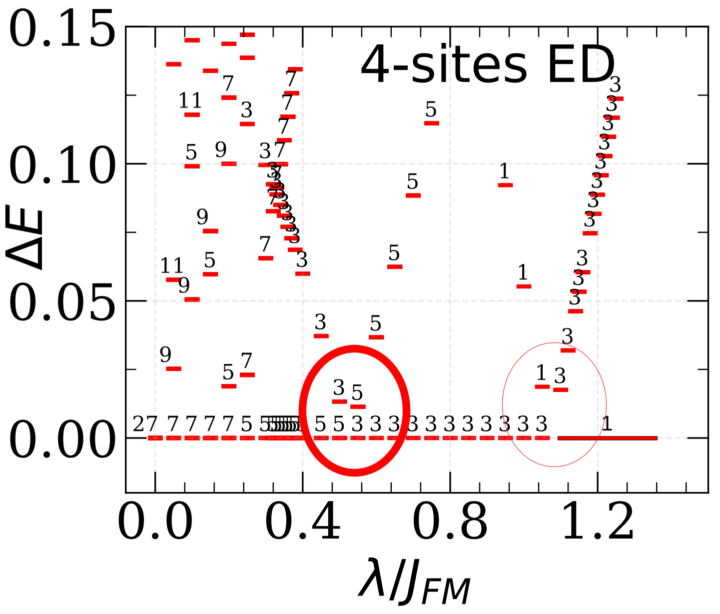


# Phase Diagram

$$H = -J_{FM} \sum_{\langle ij \rangle} \left( \vec{S}_i \cdot \vec{S}_j \right) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$

## 4-site ED

Energy spectrum and degeneracy

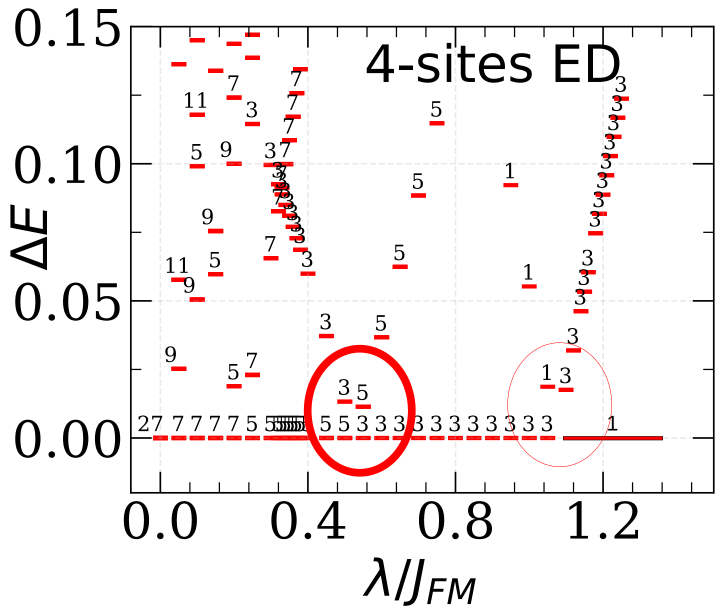


# Phase Diagram

$$H = -J_{FM} \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$

## 4-site ED

Energy spectrum and degeneracy



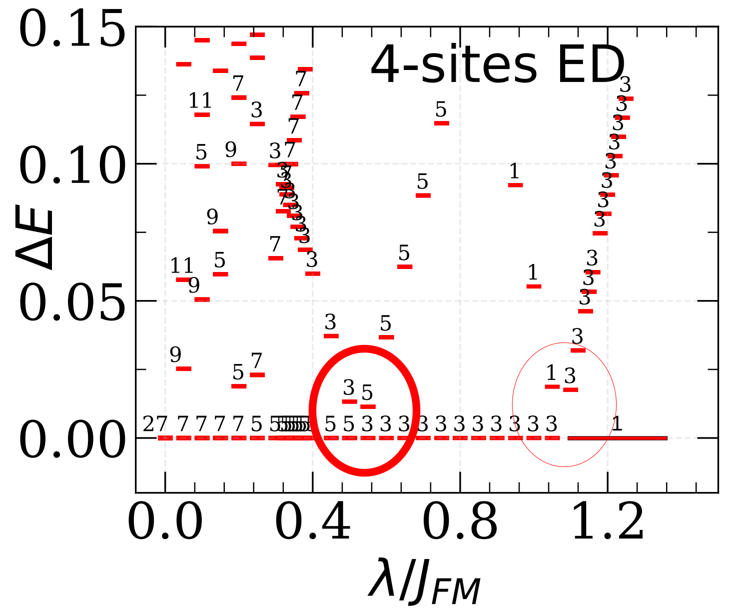

- **Two level crossings near ground state**
- **New intermediate phase**

# Phase Diagram

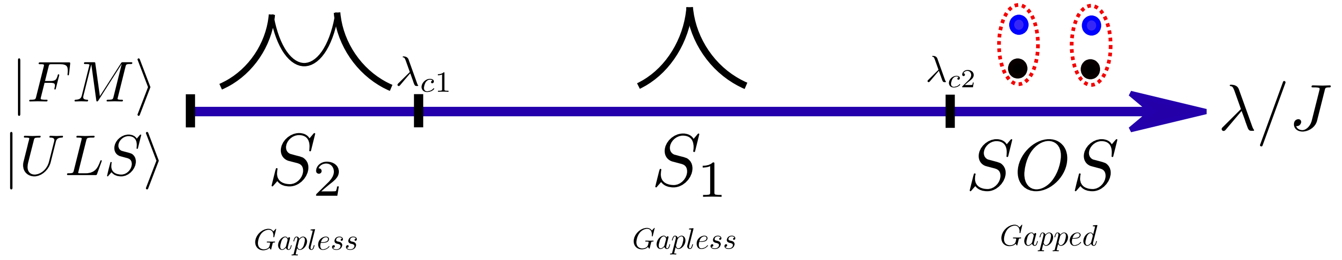
$$H = -J_{FM} \sum_{\langle ij \rangle} \left( \vec{S}_i \cdot \vec{S}_j \right) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$

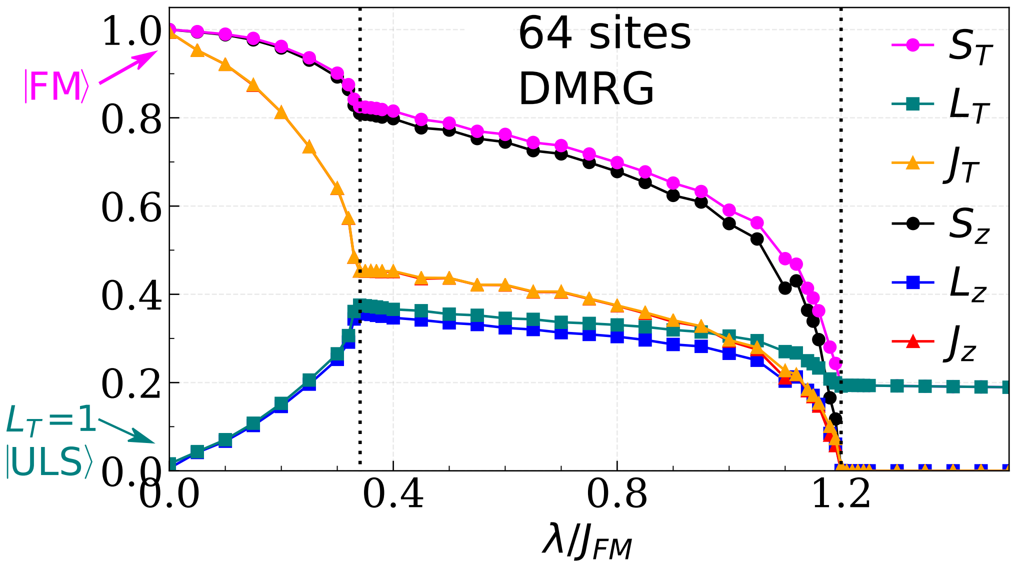
## 4-site ED

Energy spectrum and degeneracy




## 64-site DMRG

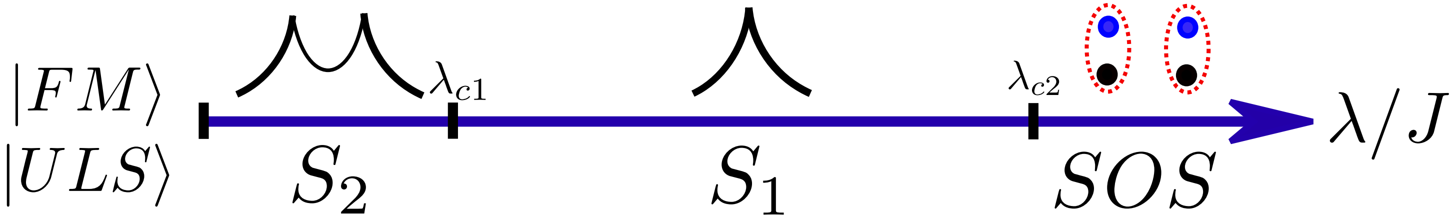



- **Two level crossings near ground state**
- **New intermediate phase**

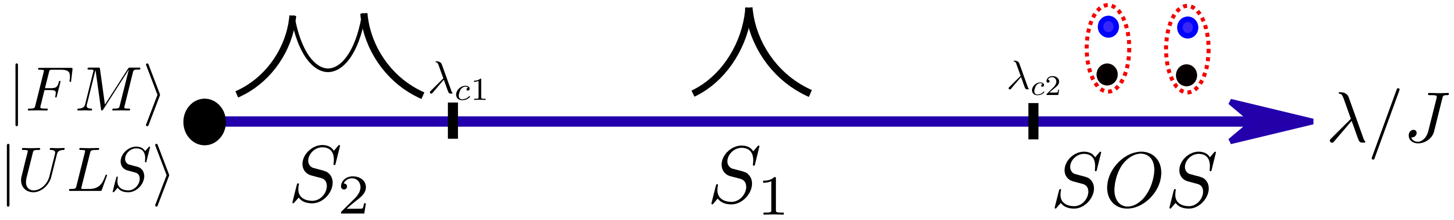
# Real-space Correlation

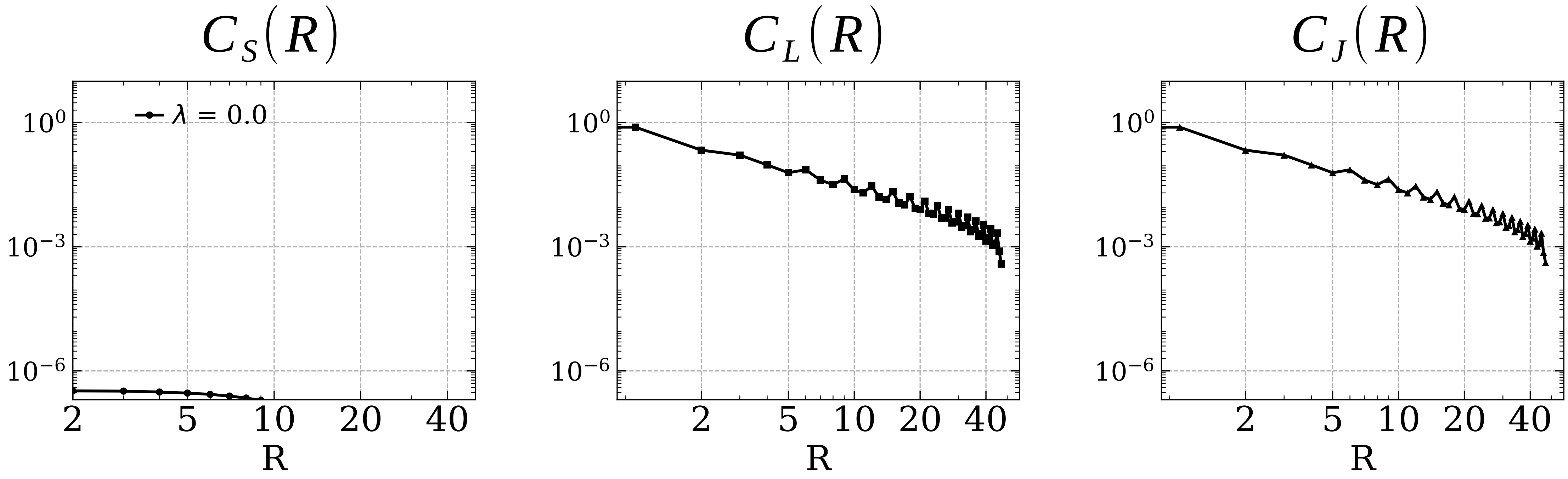
$$C_O(R) = \frac{1}{N_R} \sum_i \langle \delta O_i \cdot \delta O_{i+R} \rangle$$



# Real-space Correlation

$$C_O(R) = \frac{1}{N_R} \sum_i \langle \delta O_i \cdot \delta O_{i+R} \rangle$$

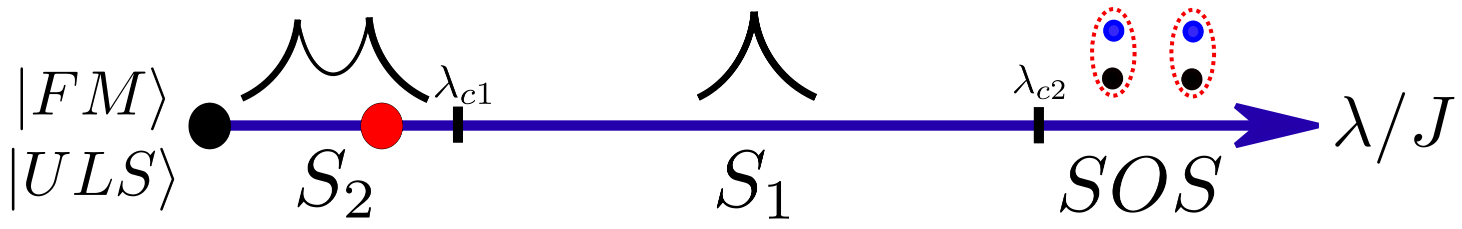


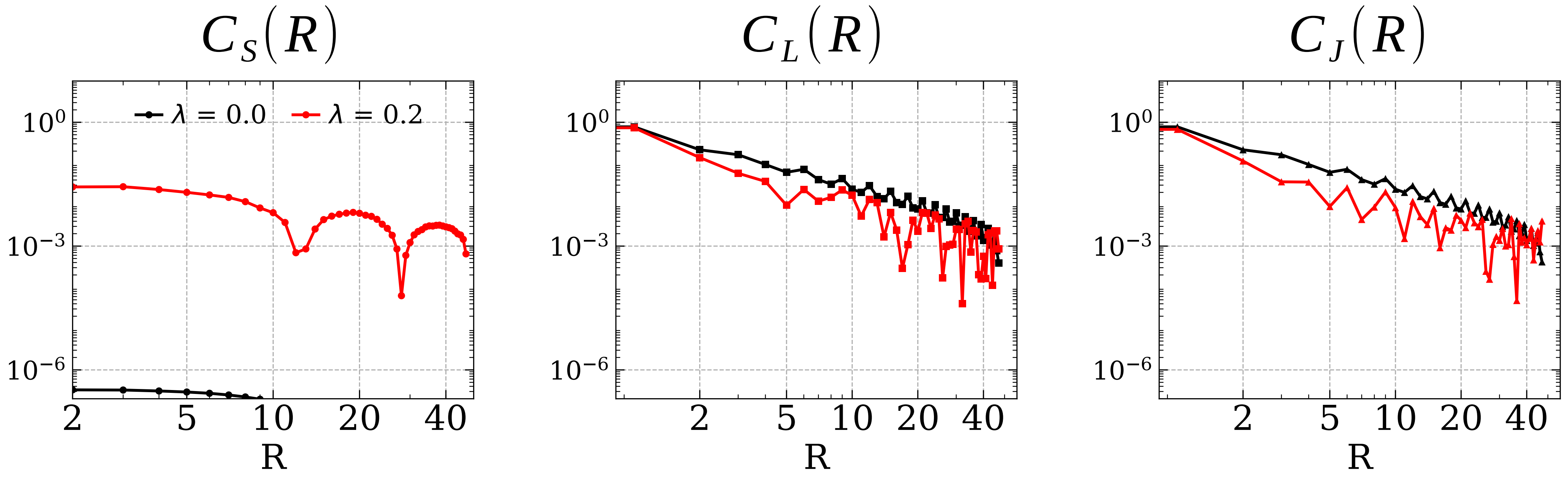




$\log - \log$ scale

# Real-space Correlation

$$C_O(R) = \frac{1}{N_R} \sum_i \langle \delta O_i \cdot \delta O_{i+R} \rangle$$

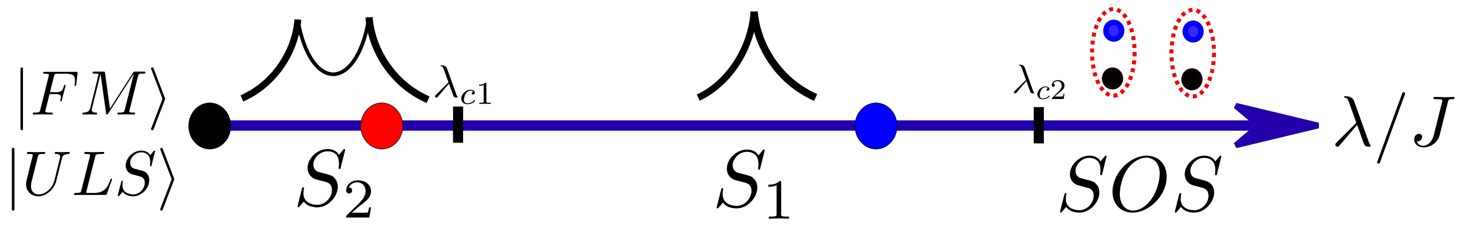


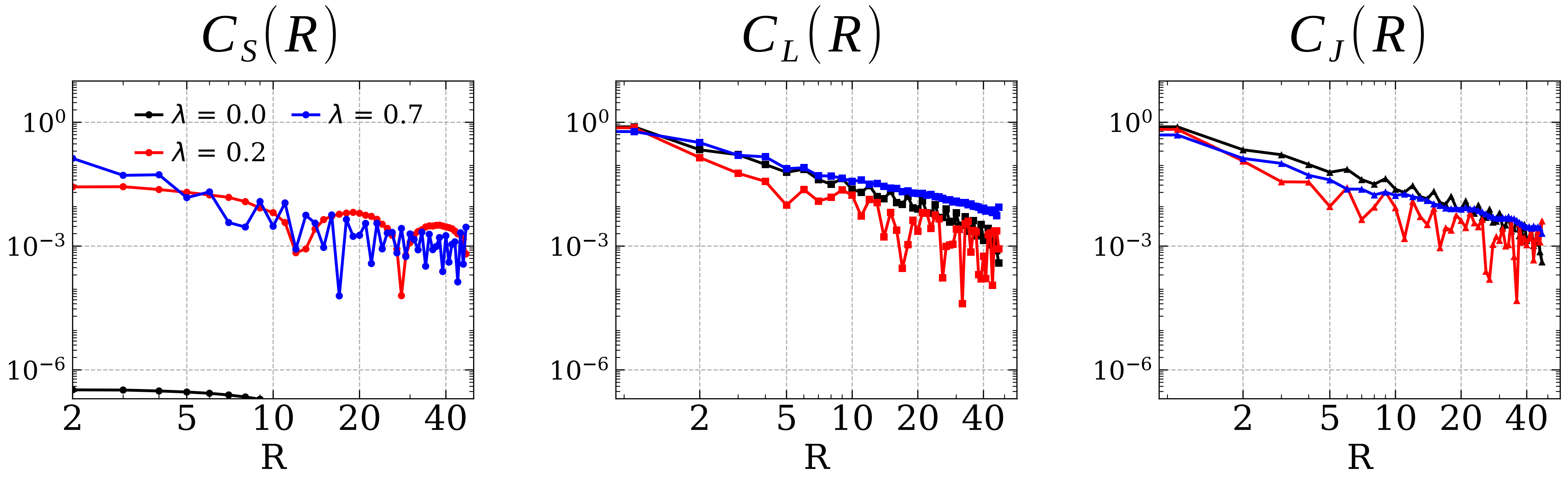




log − log scale

# Real-space Correlation

$$C_O(R) = \frac{1}{N_R}\sum_i \langle \delta O_i \cdot \delta O_{i+R} \rangle$$

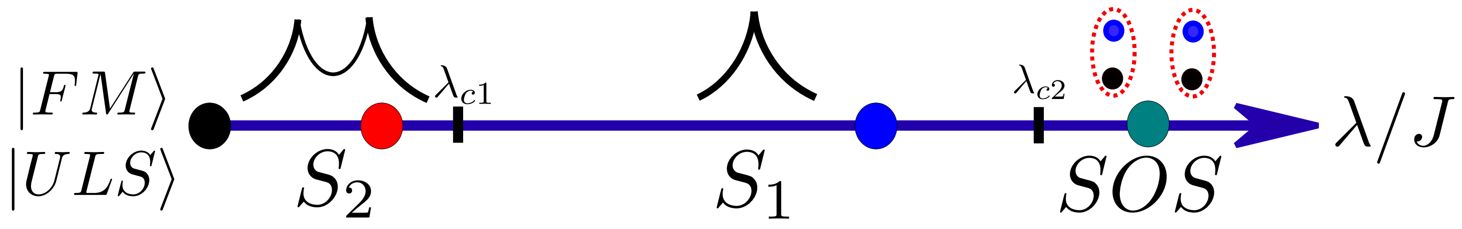


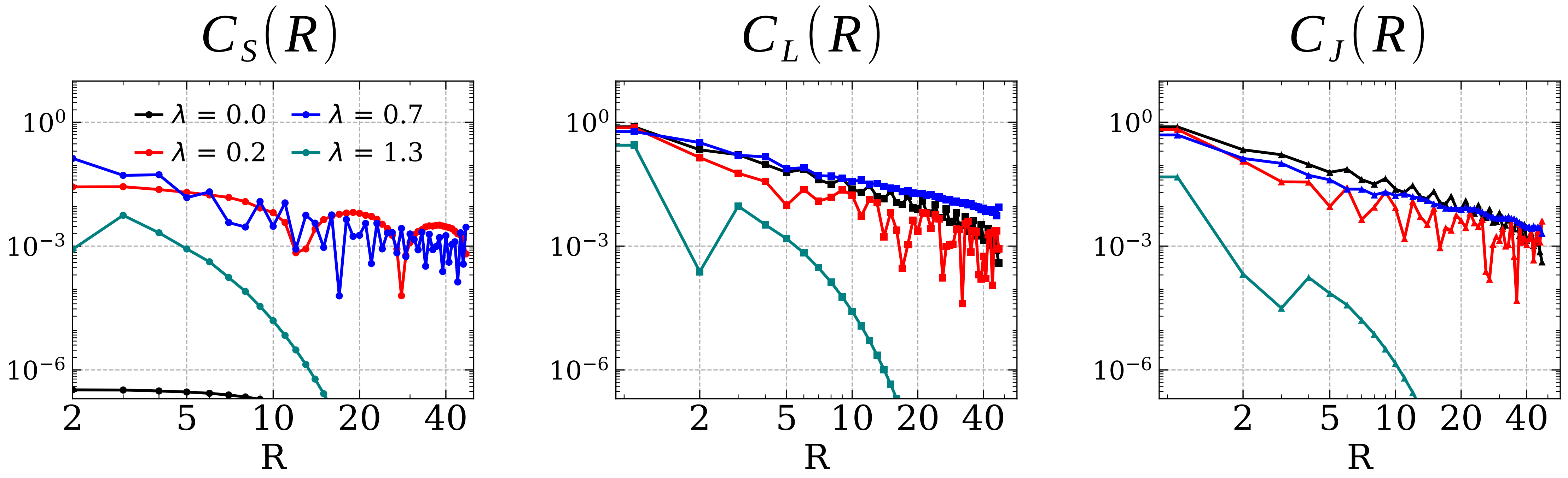




log − log scale

# Real-space Correlation

$$C_O(R) = \frac{1}{N_R} \sum_i \langle \delta O_i \cdot \delta O_{i+R} \rangle$$

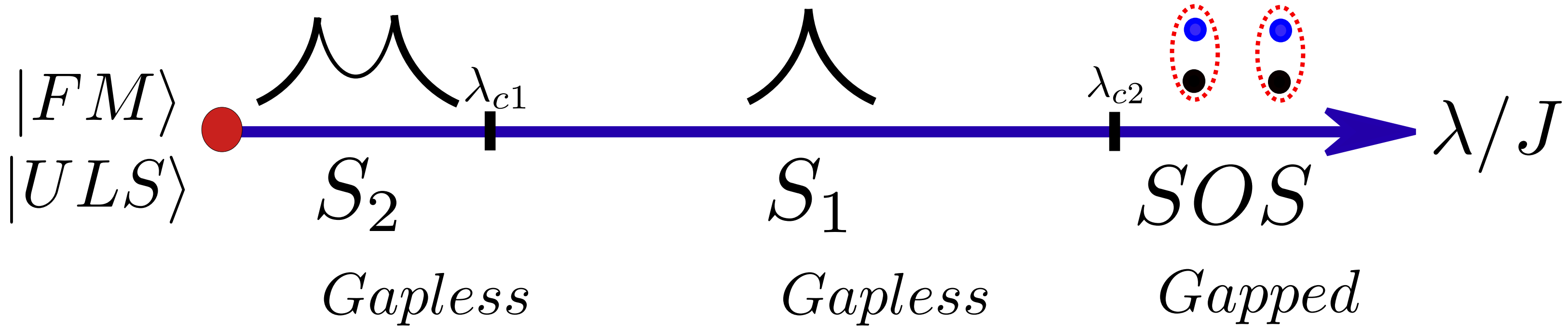


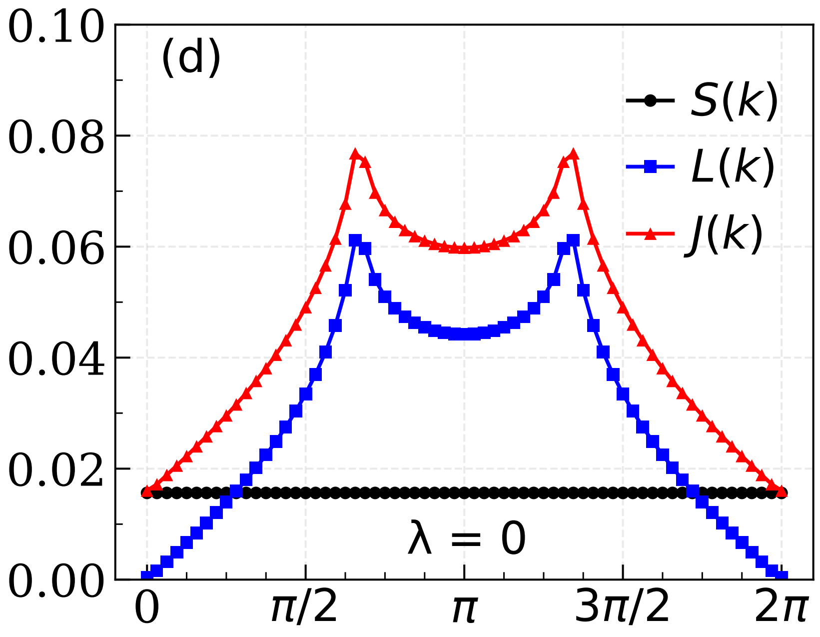




log − log scale

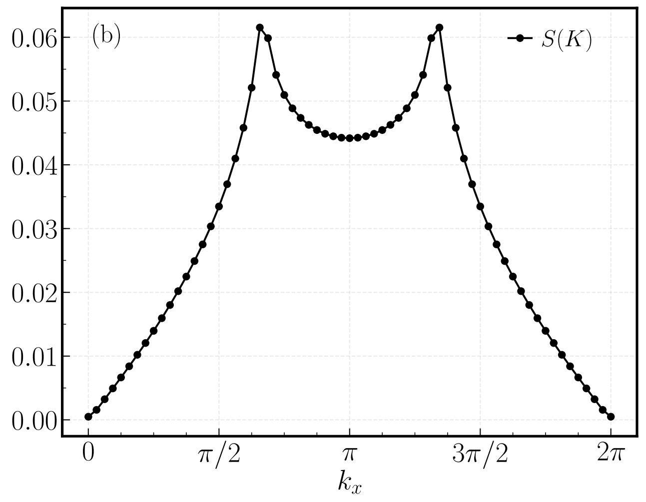
# Static Structure Factor

$$O(k) = \frac{1}{N^2} \sum_{i,j} e^{ik(r_i - r_j)} \langle \delta O_i \cdot \delta O_j \rangle$$




$$H_{ULS} = \sum_{\langle ij \rangle} \left( -P^{(1)}_{\langle ij \rangle} \right)$$



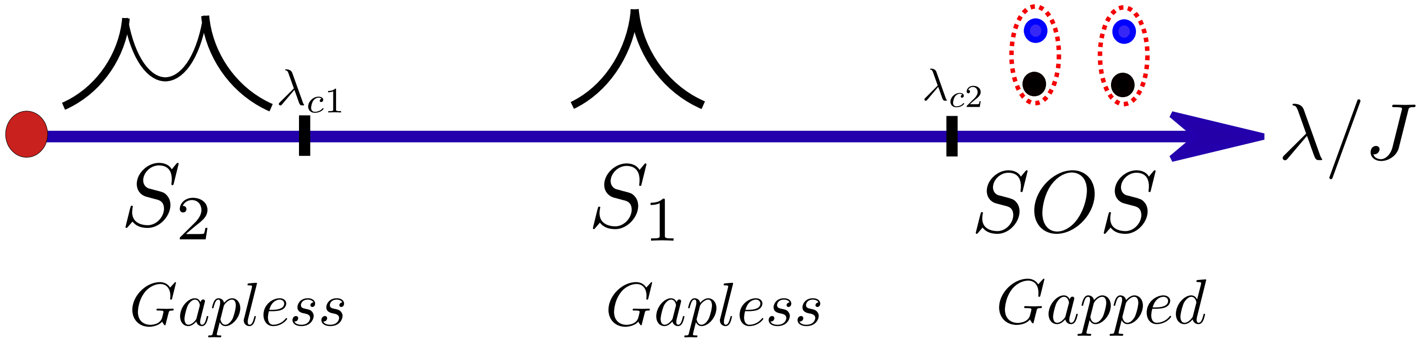

**spin-orbital separation at zero on-site SOC**

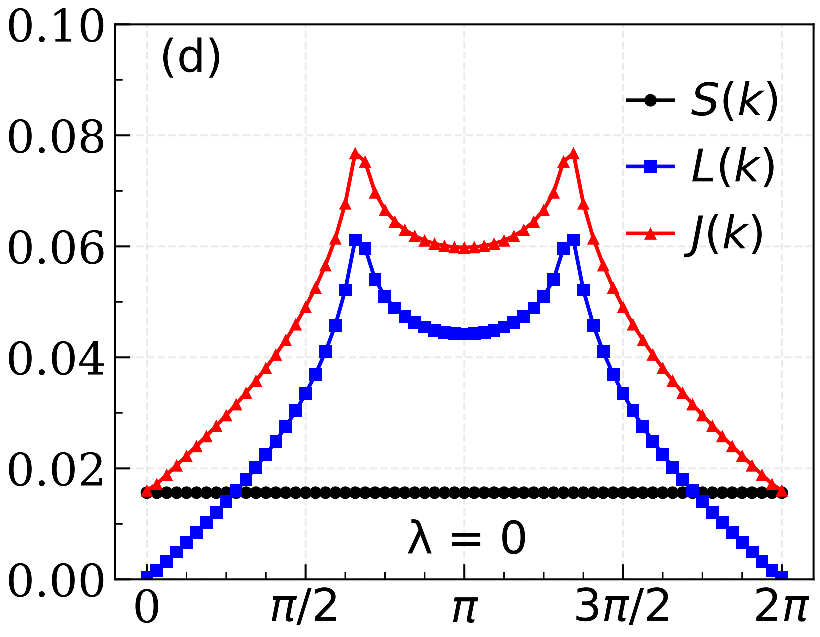
$$|\psi_{\lambda \to 0}\rangle \simeq |FM\rangle \otimes |ULS\rangle$$

# Static Structure Factor

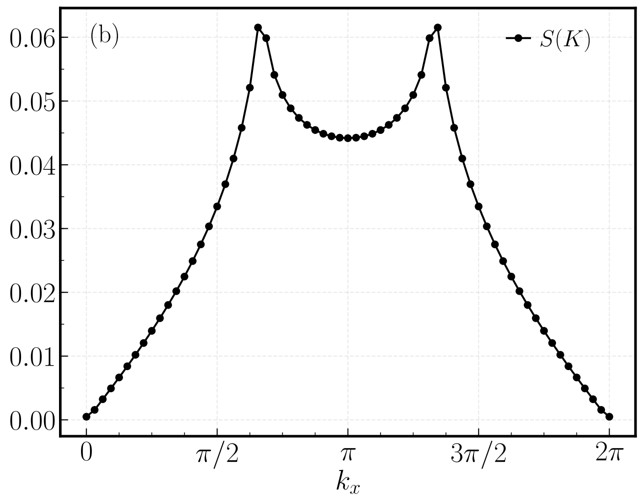
$$O(k)=\frac{1}{N^2}\sum_{i,j} e^{ik(r_i-r_j)}\langle \delta O_i \cdot \delta O_j \rangle$$

$|FM\rangle$
$|ULS\rangle$



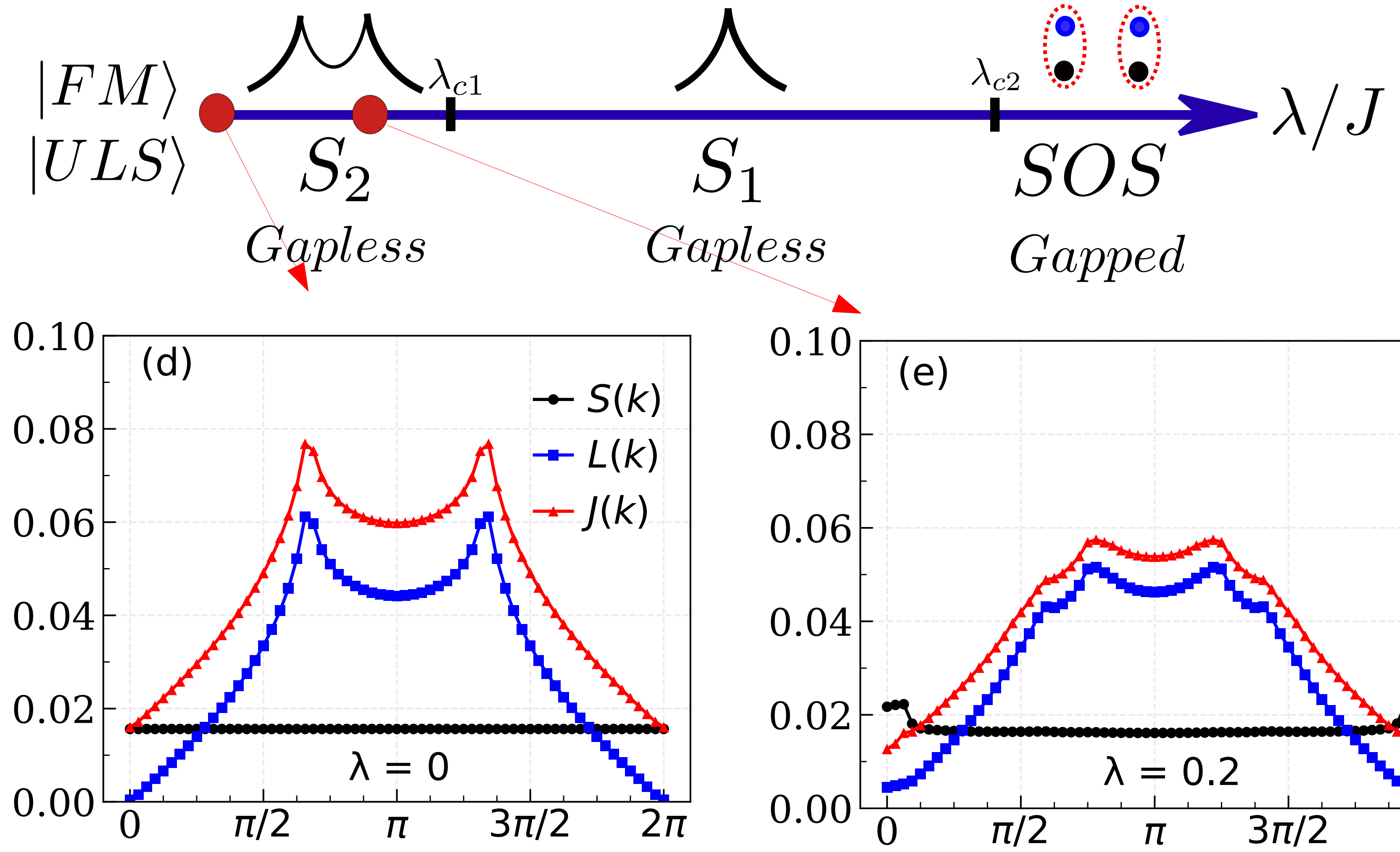

$$H_{ULS}=\sum_{\langle ij\rangle}\left(-P^{(1)}_{\langle ij\rangle}\right)$$



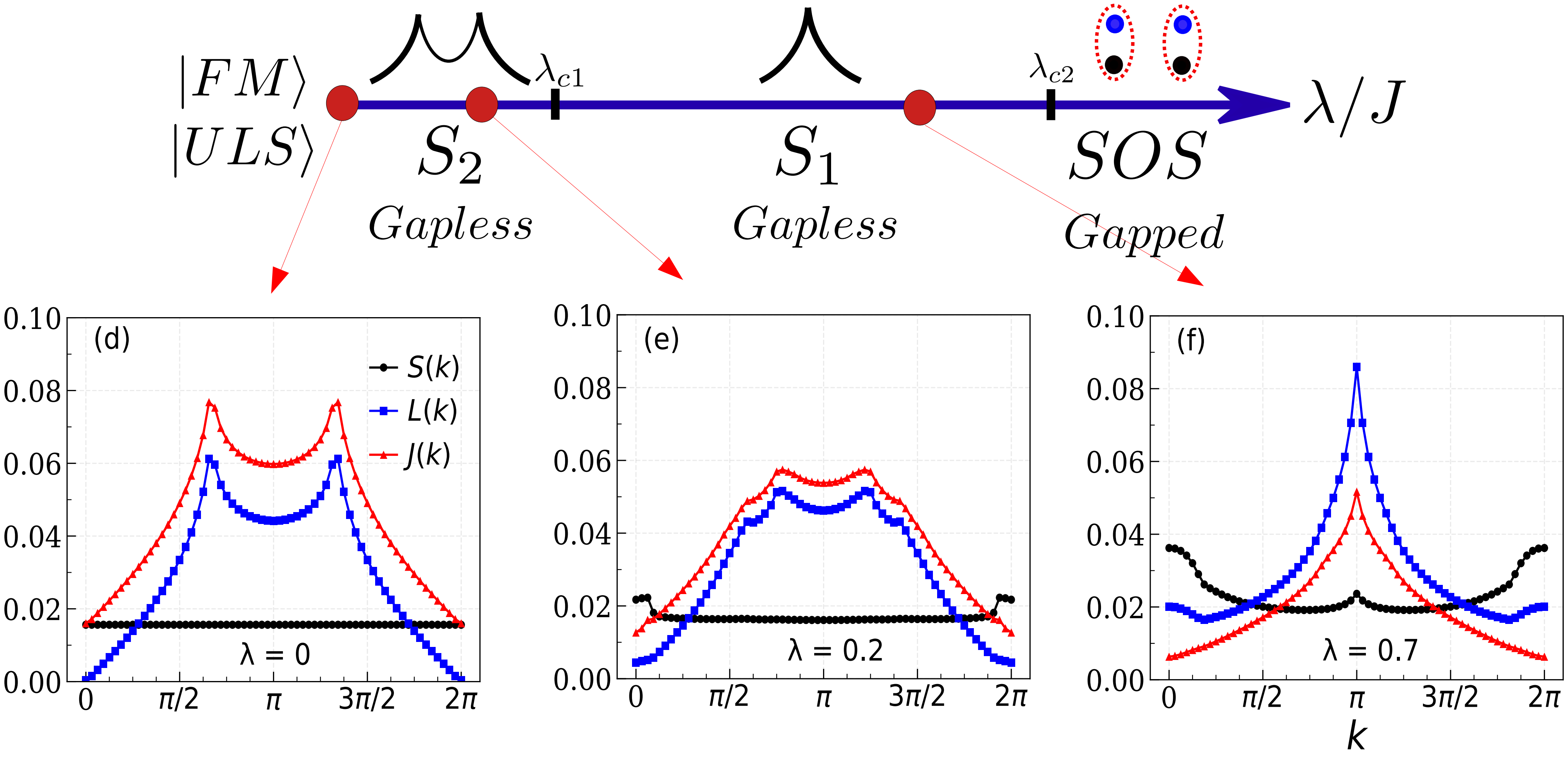

**spin-orbital separation at zero on-site SOC**

$$|\psi_{\lambda\to 0}\rangle \simeq |FM\rangle \otimes |ULS\rangle$$

# Static Structure Factor



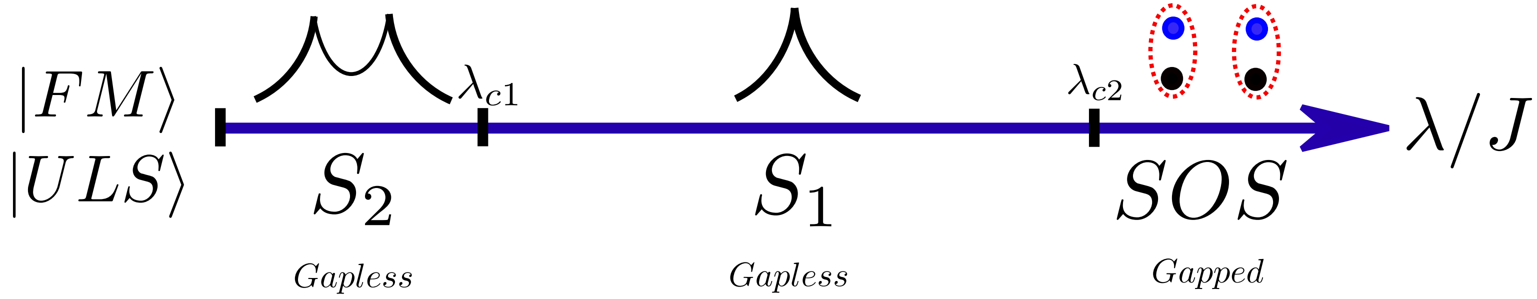
# Static Structure Factor



# Summary

In the 1d SOC model, we found 3 phases:

- Gapless S2 phase
- Gapless S1 phase
- Gapped SOS phase

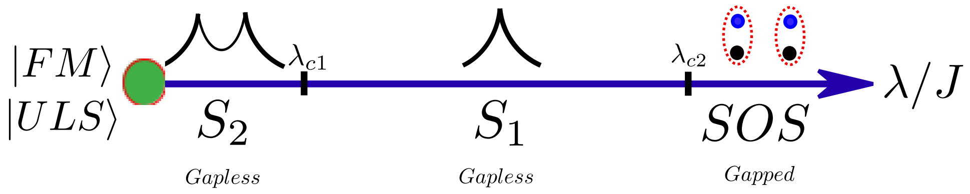



- Real-space correlation decay
- Static structure factor

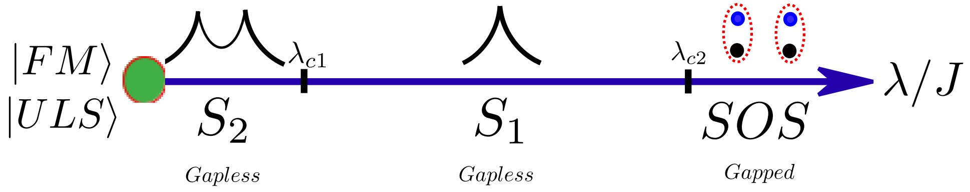
arXiv:1912.0951

# Spin-Orbital Separation

Zero on-site SOC limit $\lambda = 0$

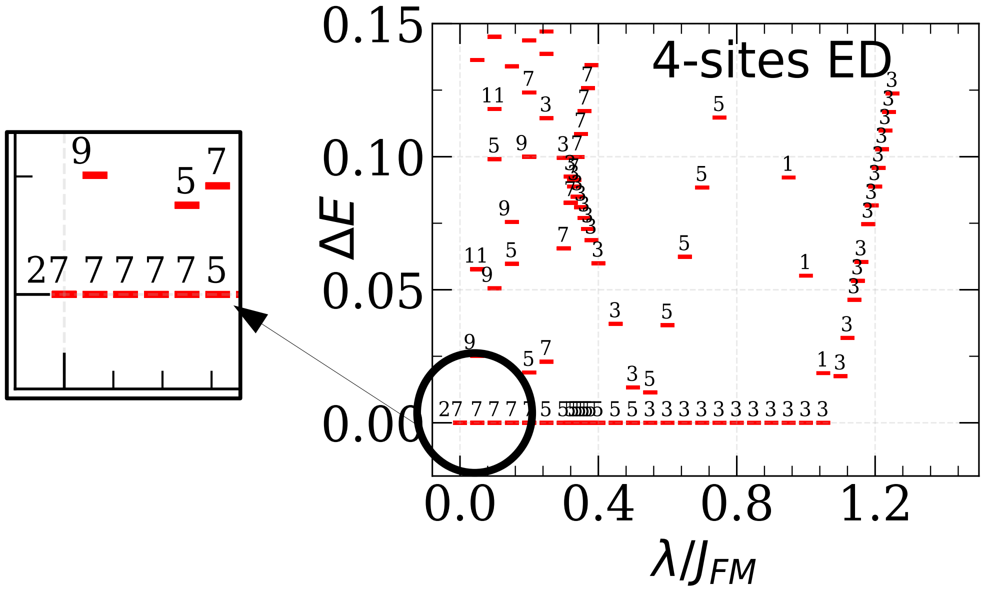


# Spin-Orbital Separation



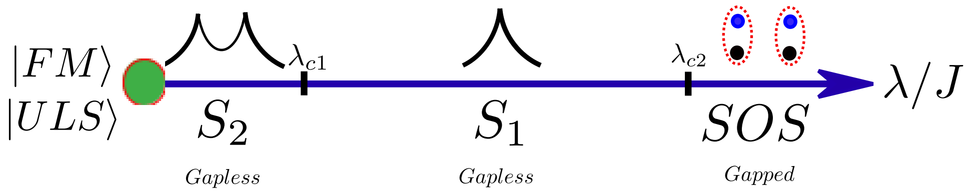

## Zero on-site SOC limit $\lambda = 0$

- **27-fold degeneracy** in ground stat (g.s.) obtained using 4-site ED with PBC



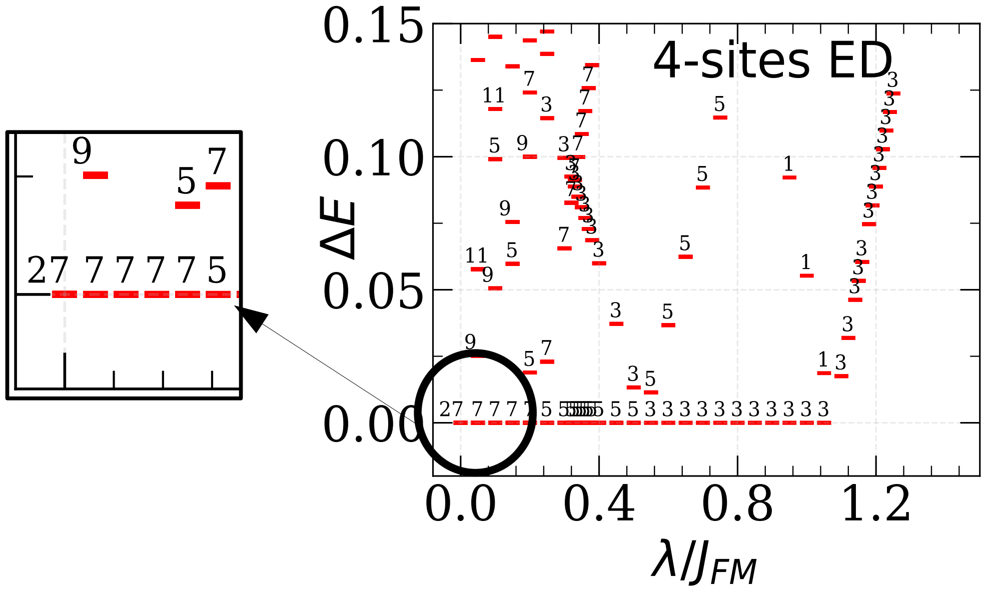

Energy spectrum and degeneracy

# Spin-Orbital Separation



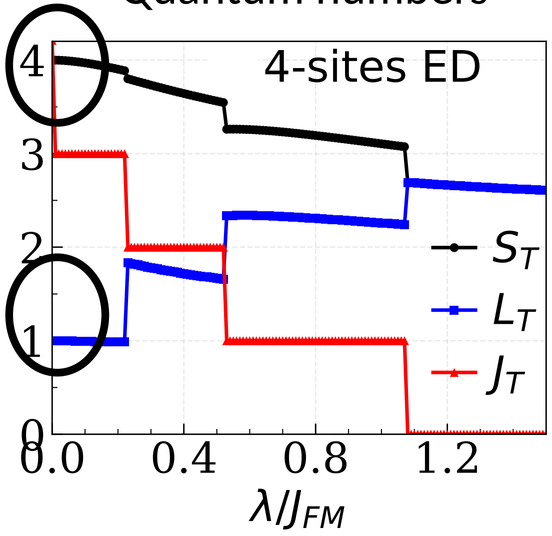

## Zero on-site SOC limit $\lambda = 0$

- **27-fold degeneracy** in ground stat (g.s.) obtained using 4-site ED with PBC




Energy spectrum and degeneracy

Quantum numbers




$[S_T^2, H] = 0$

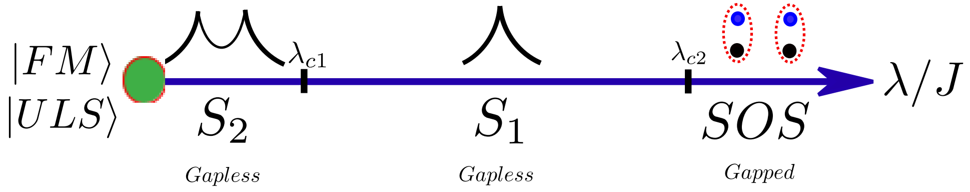
$[L_T^2, H] = 0$

$S_T = 4 \Rightarrow 2S_T + 1 = 9$ fold spin degeneracy

$L_T = 1 \Rightarrow 2L_T + 1 = 3$ fold orbital degeneracy

**27 fold**
**total degeneracy**

# spin-orbital separation

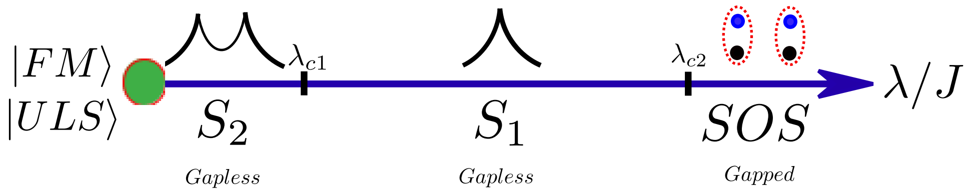



## Zero on-site SOC limit $\lambda = 0$

$S_T = 4 \Rightarrow 2S_T + 1 = 9$ fold spin degeneracy $\quad |S_T = N\rangle = |FM\rangle$

$L_T = 1 \Rightarrow 2L_T + 1 = 3$ fold orbital degeneracy $\quad |L_T = 1\rangle = |ULS\rangle$

# spin-orbital separation




Zero on-site SOC limit $\lambda = 0$

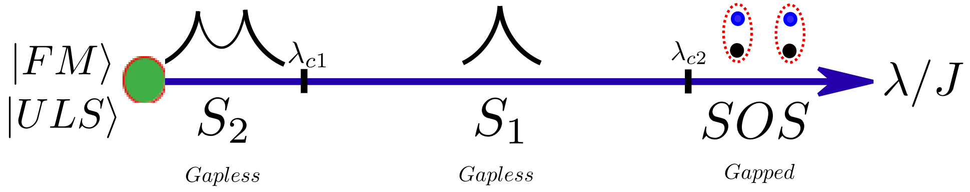
$S_T = 4 \Rightarrow 2S_T + 1 = 9$ fold spin degeneracy

$L_T = 1 \Rightarrow 2L_T + 1 = 3$ fold orbital degeneracy

$$\left.\begin{array}{l} |S_T = N\rangle = |FM\rangle \\ \\ |L_T = 1\rangle = |ULS\rangle \end{array}\right\} \quad |\psi_{\lambda\to 0}\rangle \simeq |FM\rangle \otimes |ULS\rangle$$

# spin-orbital separation

Zero on-site SOC limit $\lambda = 0$




$S_T = 4 \Rightarrow 2S_T + 1 = 9$ fold spin degeneracy

$L_T = 1 \Rightarrow 2L_T + 1 = 3$ fold orbital degeneracy

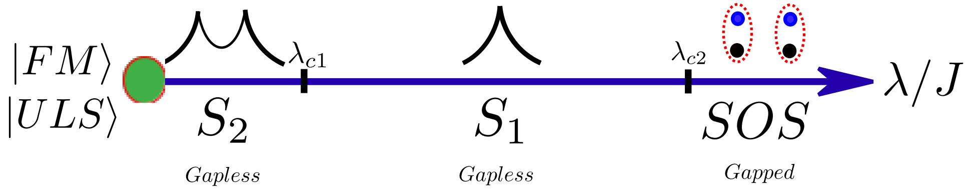
$$\left.\begin{aligned} |S_T = N\rangle &= |FM\rangle \\ |L_T = 1\rangle &= |ULS\rangle \end{aligned}\right\} \quad |\psi_{\lambda\to 0}\rangle \simeq |FM\rangle \otimes |ULS\rangle$$

$$H = J\sum_{\langle ij\rangle} (\overbrace{\vec{S}_i \cdot \vec{S}_j}^{-H_{FM}})(\overbrace{-P^{(1)}_{\langle ij\rangle}}^{H_{ULS}}) \longrightarrow H_{\lambda\to 0} \simeq \left(-J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j\right) \otimes \left(\sum_{\langle ij\rangle} h^{ULS}_{\langle ij\rangle}\right)$$

***spin-orbital separation in SOC system***

# spin-orbital separation

Zero on-site SOC limit $\lambda = 0$



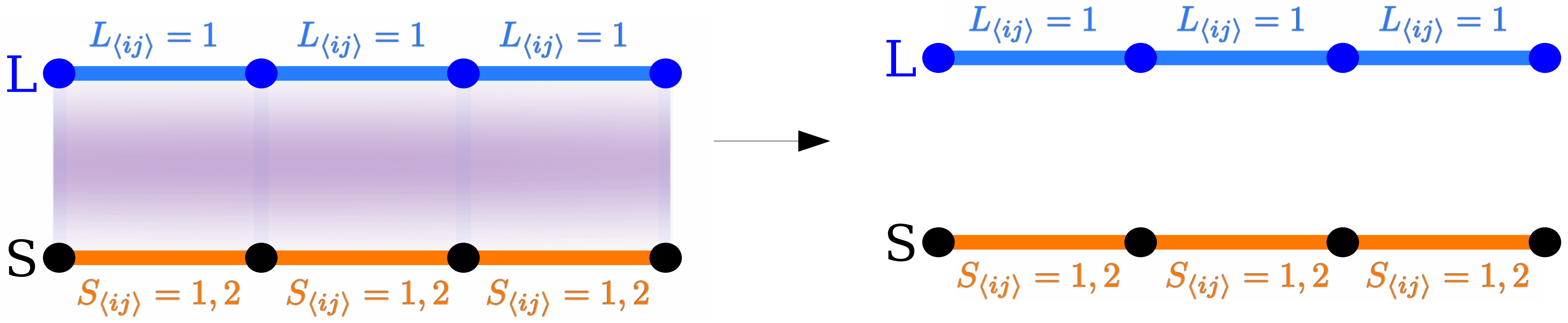

$S_T = 4 \Rightarrow 2S_T + 1 = 9$ fold spin degeneracy

$L_T = 1 \Rightarrow 2L_T + 1 = 3$ fold orbital degeneracy

$$|S_T = N\rangle = |FM\rangle, \quad |L_T = 1\rangle = |ULS\rangle \quad \Big\} \quad |\psi_{\lambda\to 0}\rangle \simeq |FM\rangle \otimes |ULS\rangle$$

$$H = J \sum_{\langle ij\rangle} \overbrace{(\vec{S}_i \cdot \vec{S}_j)}^{-H_{FM}} \overbrace{(-P^{(1)}_{\langle ij\rangle})}^{H_{ULS}} \longrightarrow H_{\lambda\to 0} \simeq \left(-J \sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j\right) \otimes \left(\sum_{\langle ij\rangle} h^{ULS}_{\langle ij\rangle}\right)$$

***spin-orbital separation in SOC system***



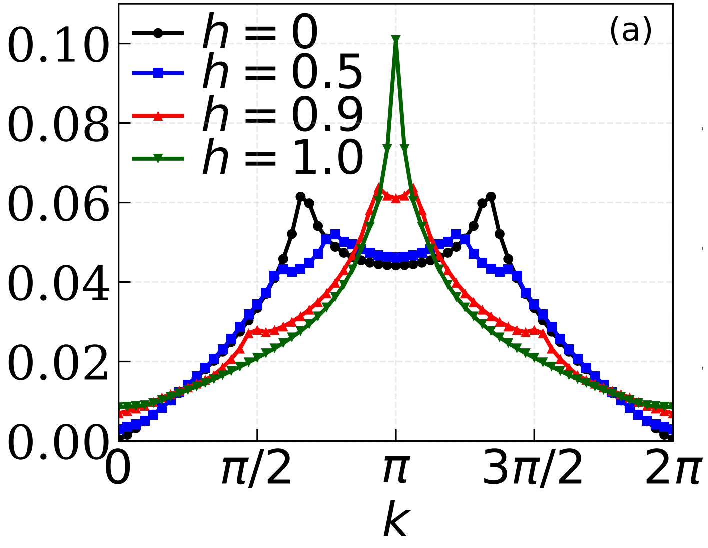
# ULS – Hz Approximation

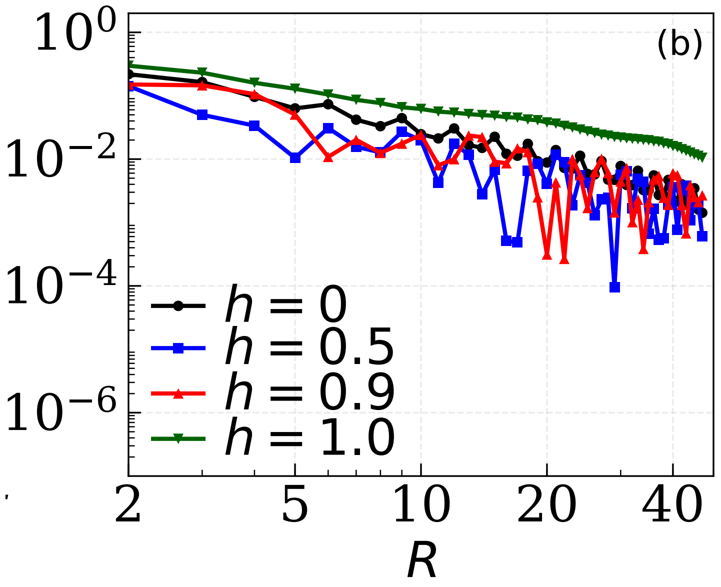
$$H = -J_{FM} \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$

- Factorize Hamiltonian into spin and orbital sectors

- Mean field approximation in Ising FM limit

$$H_{eff} = J_{eff} \sum_{\langle ij \rangle} (-P^{(1)}_{\langle ij \rangle}) + h_{eff} \sum_i L^z_i$$



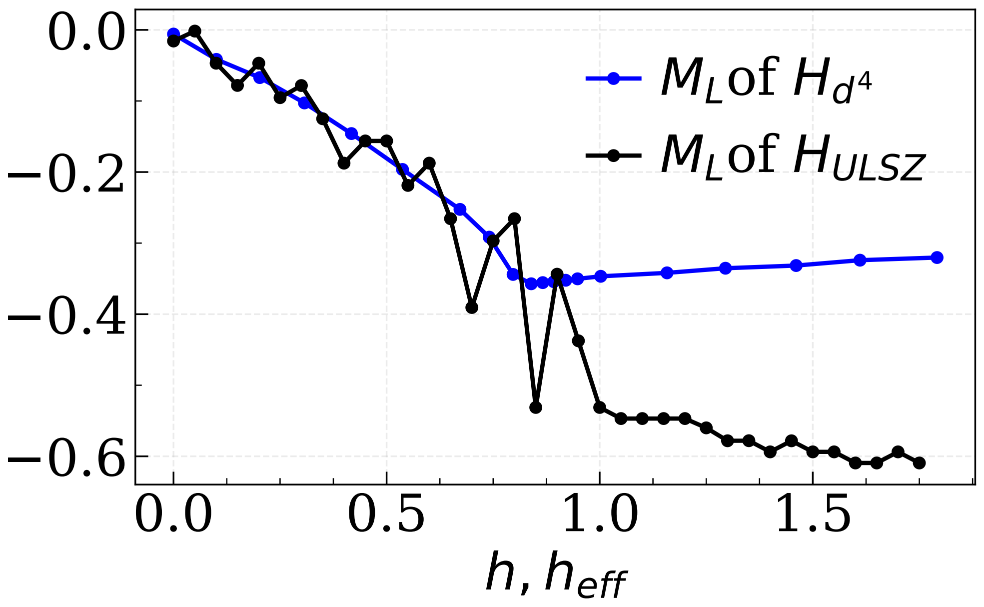



# ULS – Hz Approximation

$$H = -J_{FM} \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) P^{(1)}_{\langle ij \rangle} + \lambda \sum_i \vec{S}_i \cdot \vec{L}_i$$

- Factorize Hamiltonian into spin and orbital sectors

- Mean field approximation in Ising FM limit




$$H_{eff} = J_{eff} \sum_{\langle ij \rangle} (-P^{(1)}_{\langle ij \rangle}) + h_{eff} \sum_i L_i^z$$

approximation breaks down for strong coupling