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Effective spin chains in frustrated ladders: A study of nanographene-inspired Fermi-Hubbard systems

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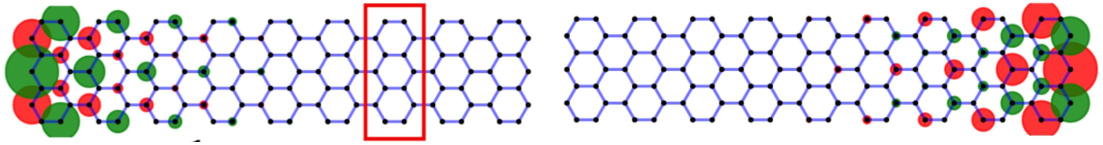
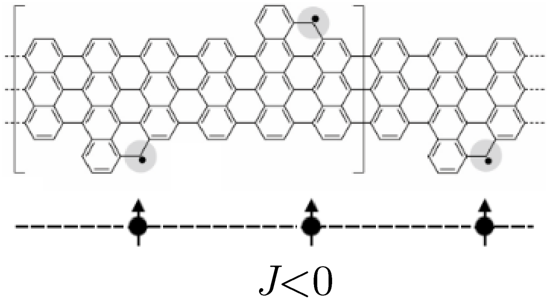
EMMI Workshop: Synthetic Topological Matter
Benasque/Benás, Aug. 31st – Sept. 6th 2025

D. G de Oteyza *et al.*, Carbon-based nanostructures as a versatile platform for tunable π-magnetism. *J. Phys.: Condens. Matter* **34** 443001 (2022)

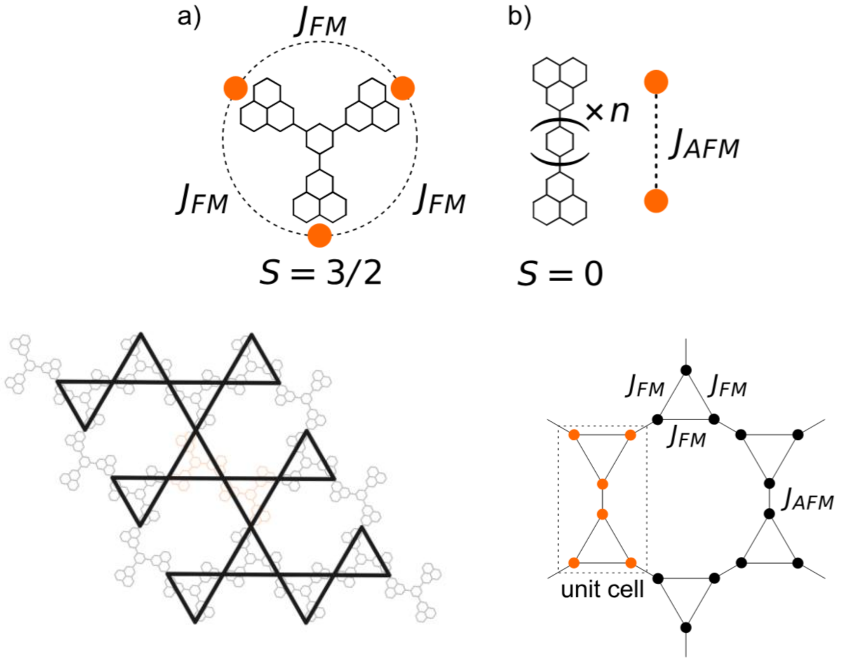
Motivation I



$$\psi_L = \frac{1}{\sqrt{2}}(\psi_B - \psi_{AB}) \qquad \psi_R = \frac{1}{\sqrt{2}}(\psi_B + \psi_{AB})$$

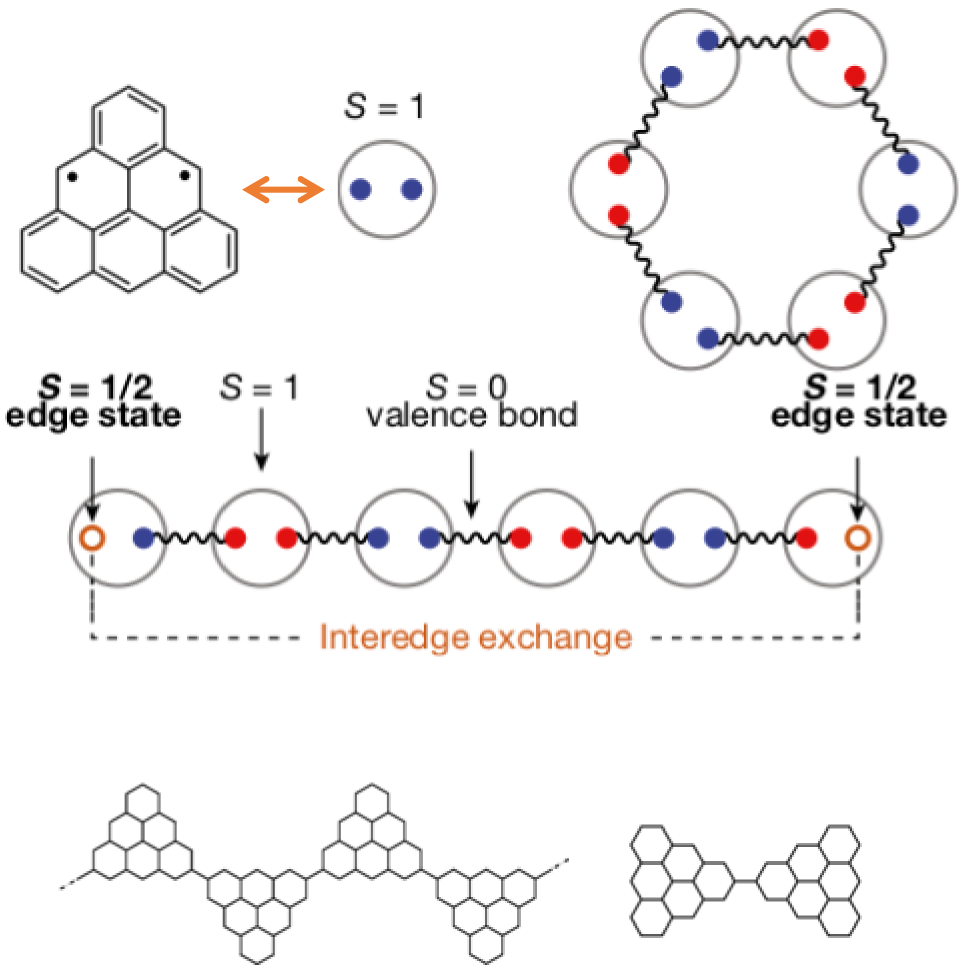


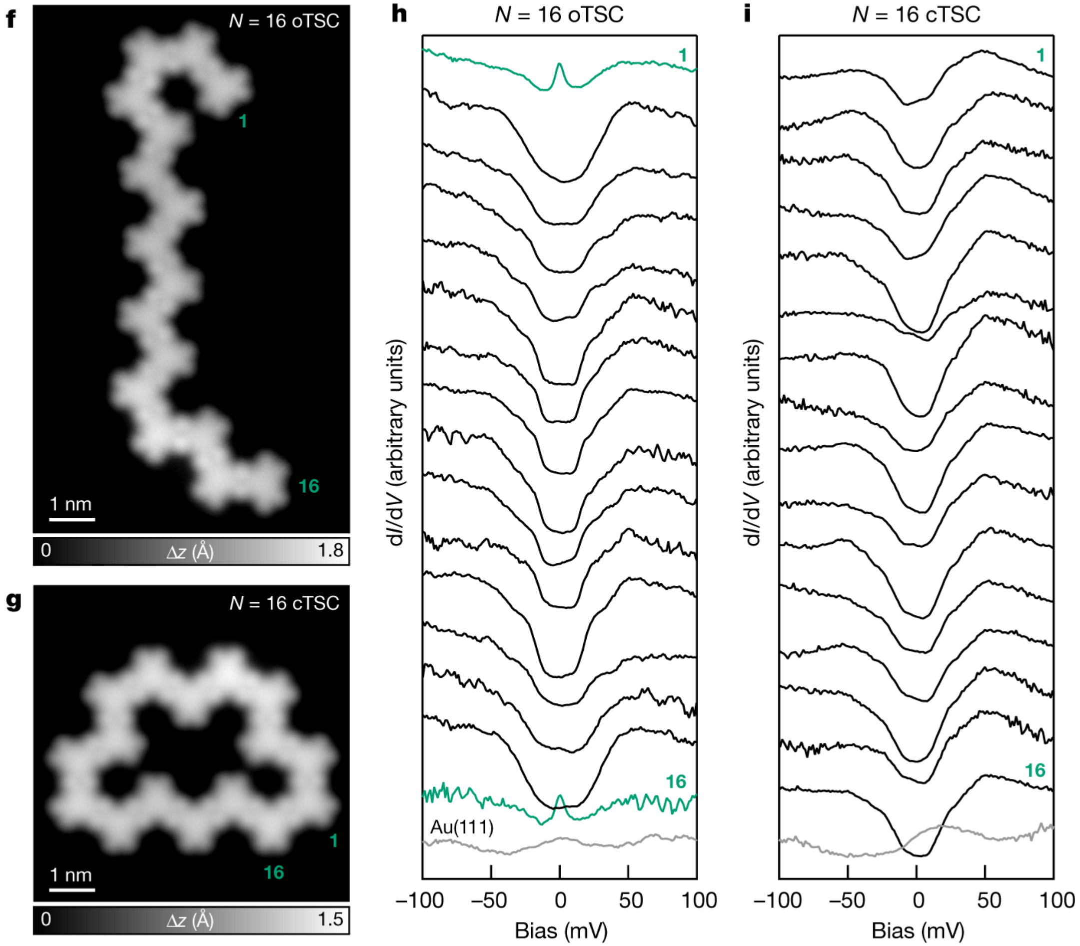
D. J. Rizzo *et al.*, Inducing metallicity in graphene nanoribbons via zero-mode superlattices. *Science* **369**, 1597-1603 (2020)



J. Henriques *et al.*, Designer Spin Models in Tunable Two-Dimensional Nanographene Lattices. *Nano Lett.*, **24**, 3355—3360 (2024)

Motivation II



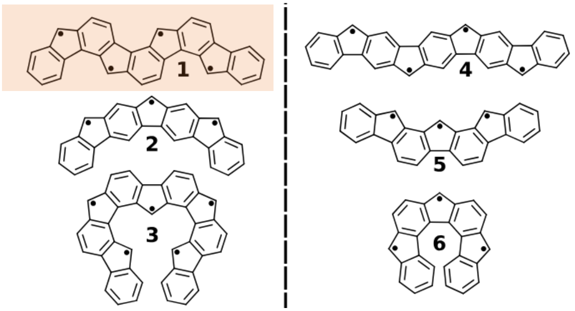


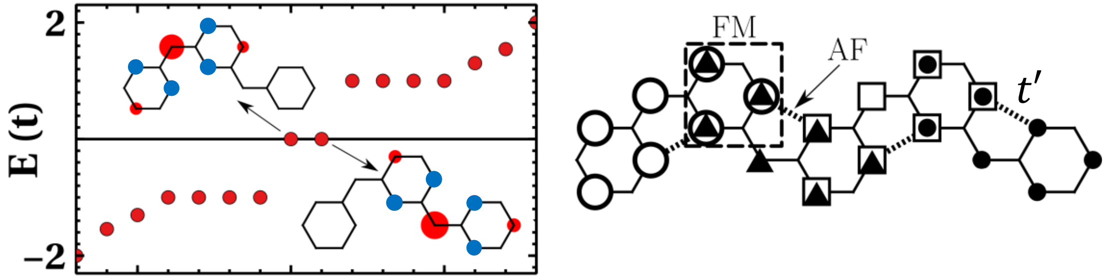
S. Mishra *et al.*, Observation of fractional edge excitations in nanographene spin chains. *Nature* **598**, 287–292 (2021).

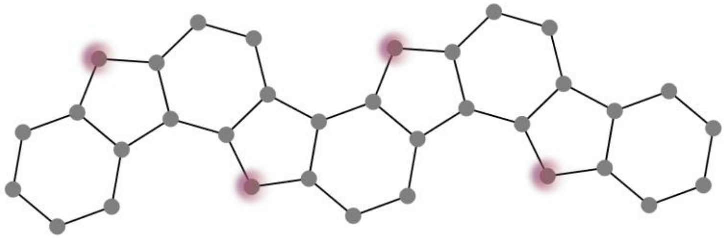
R. Ortiz *et al.* Magnetic frustration and fractionalization in oligo(indenoindenes). *Phys. Rev. B* **107**, L100416 (2023).

Oligo-indenoindenes

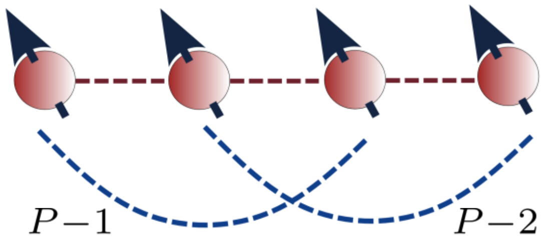
- Oligo-indenoindene (OInIn) molecules are chains of alternating hexagons and pentagons.
- Some variants are predicted to host the potential for studying frustrated spin physics.







$$H = -t \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



$$H' = J_1 \sum_{i=1}^{P-1} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + J_2 \sum_{i=1}^{P-2} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}$$

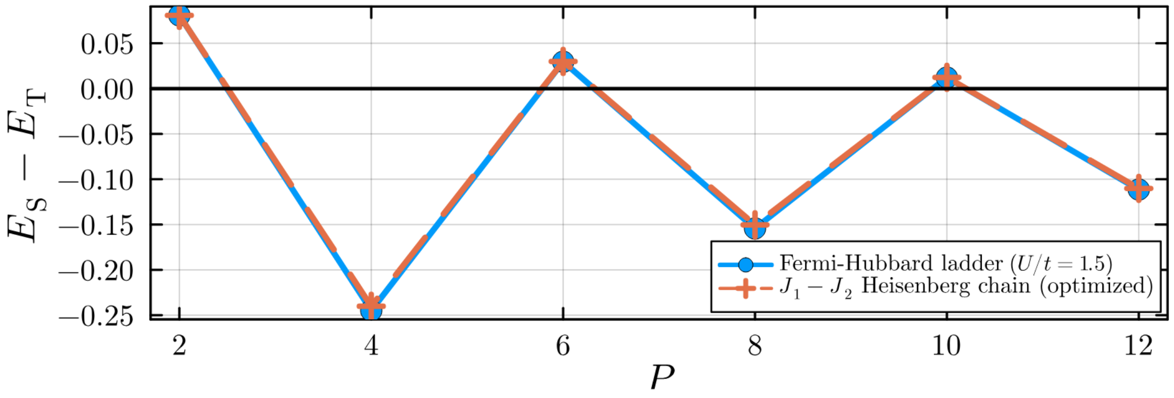
$$J_1 < 0, J_2 > 0; \quad \frac{J_2}{|J_1|} > \frac{1}{4}$$

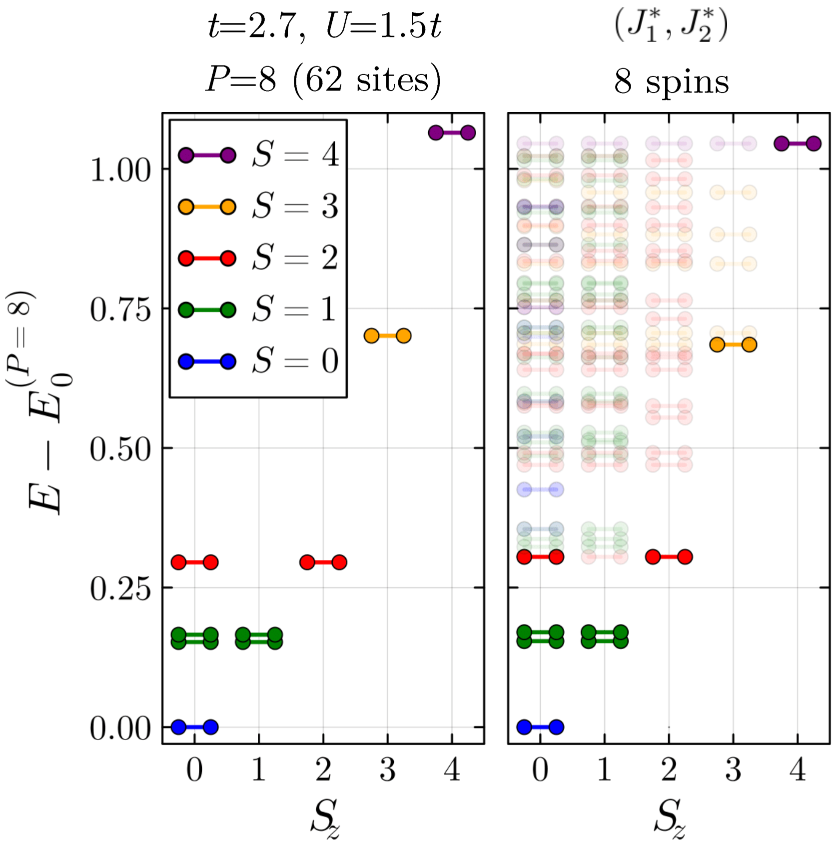
Can we better characterize this mapping with MPS techniques?

*M. Fishman *et al.*, The ITensor Software Library for Tensor Network Calculations, *SciPost Phys. Codebases* **4** (2022).

Matching energy spectra

- Compare the low-energy spectra of the OInIn ladder and J_1-J_2 chain:
  - Obtain first few eigenstates of the half-filled Fermi-Hubbard ladders for various P with DMRG*.
  - Optimize the parameters of the J_1-J_2 chain, such that the difference in the respective energy gaps is minimized.



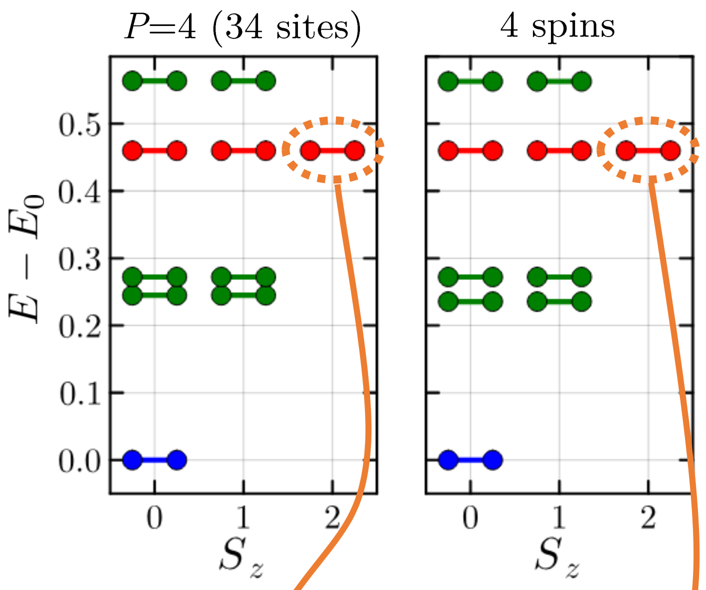


$J_1^* = -0.07$

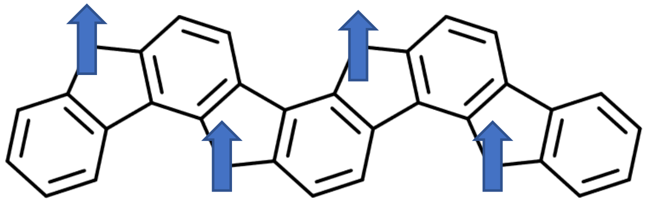
$J_2^* = 0.25$

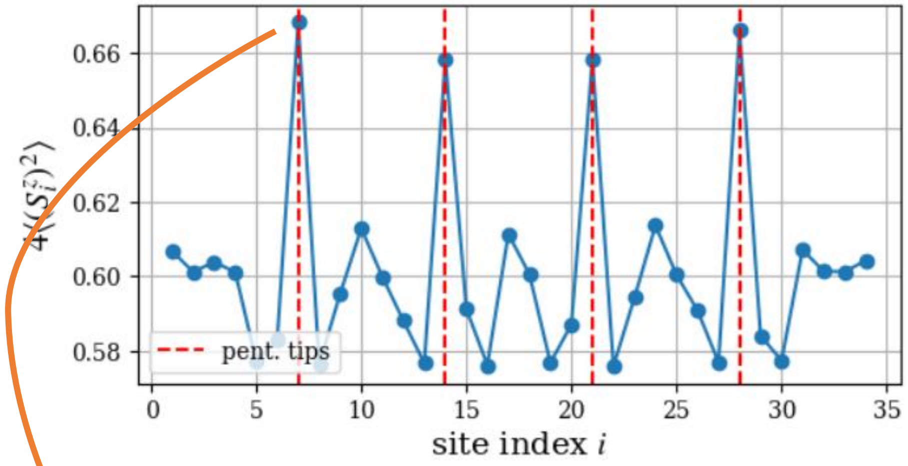
$J_2^*/|J_1^*| > 1/4$

Pentagon tips as spins



$|E_3^{(P=4)}, S=2, S_z=2\rangle \longleftrightarrow |\uparrow\uparrow\uparrow\uparrow\rangle$





pent. tip magnetization:

max possible: 0.33

(ideal: 0.5)

$$\frac{1}{P}\langle \sum_{i\in \text{pent. tips}} S_i^z \rangle \approx 0.21$$

$r = 0.65$

(magnetization approx. ratio)

Better spins

- Spins from delocalized fermionic modes

$$c_{\mathcal{M},\sigma} = \sum_{i\in\mathcal{M}} \alpha_i c_{i,\sigma}$$

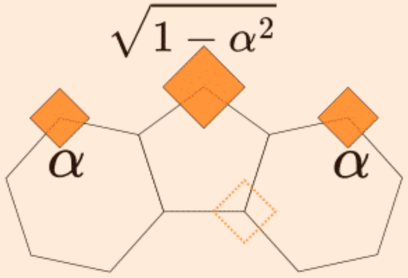
$$(\boldsymbol{\alpha} \in \mathbb{C}^{|\mathcal{M}|}; \sum_i |\alpha_i|^2 = 1)$$

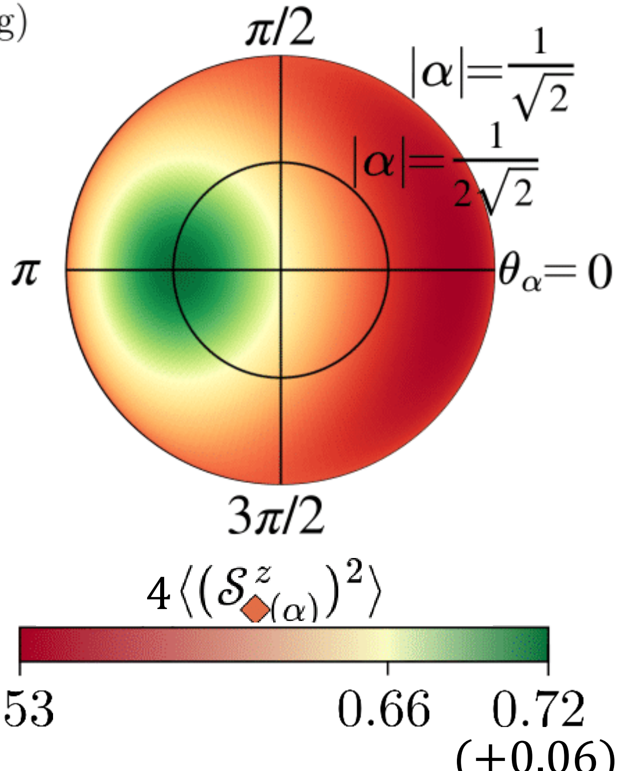
$$\boldsymbol{\mathcal{S}}_{\mathcal{M}} = \sum_{\sigma,\sigma'} \boldsymbol{\tau}_{\sigma,\sigma'} c^\dagger_{\mathcal{M},\sigma} c_{\mathcal{M},\sigma}$$

3-site symmetric modes (non-overlapping)

Optimize: $\boldsymbol{\alpha} = |\alpha| e^{i\theta_\alpha}$

$|\alpha| \in [0, 1/\sqrt{2}]$

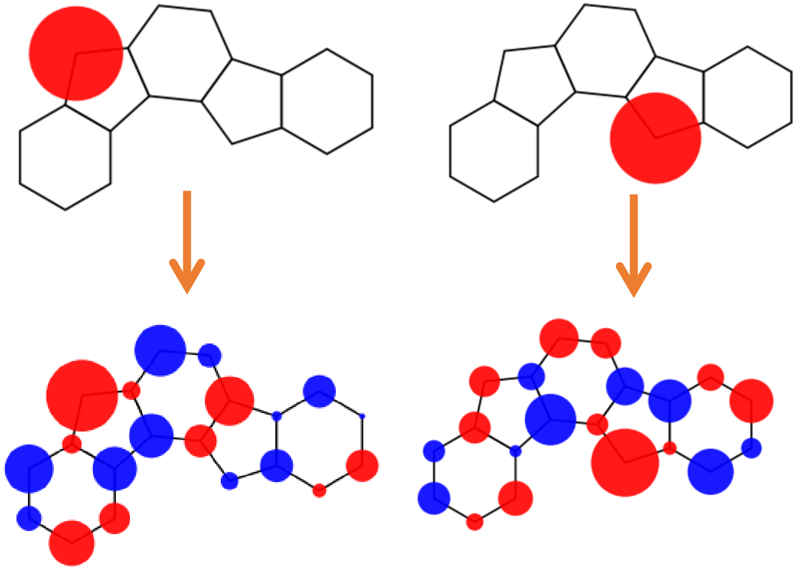




$$\frac{1}{P}\langle\sum_{i=1}^{P} \mathcal{S}^z_i\rangle = 0.31 \rightarrow r = 0.85$$

(+0.20)

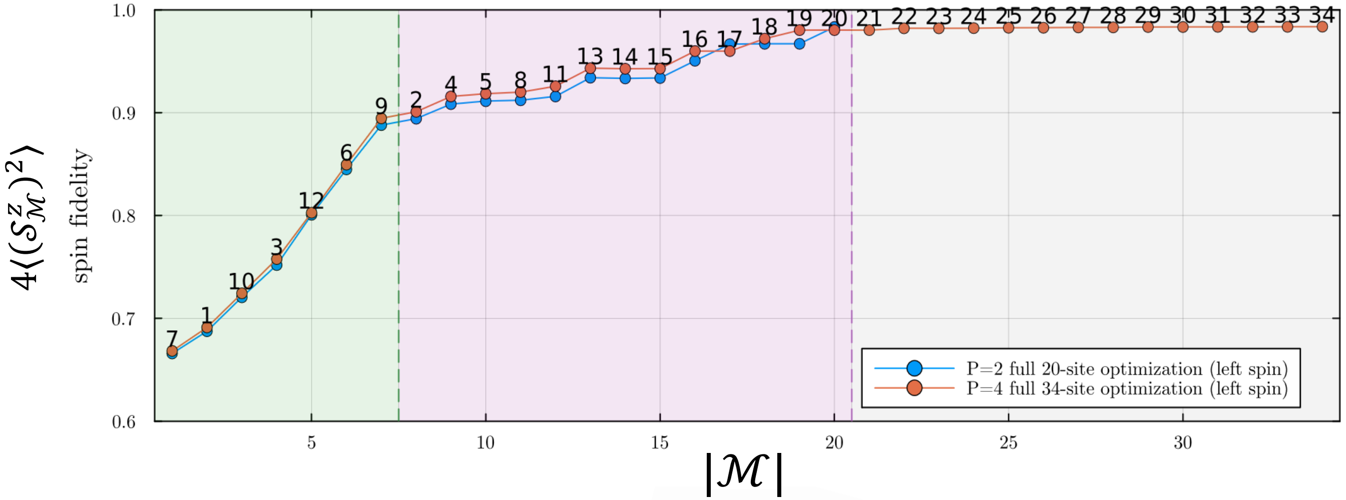
Optimizing all sites



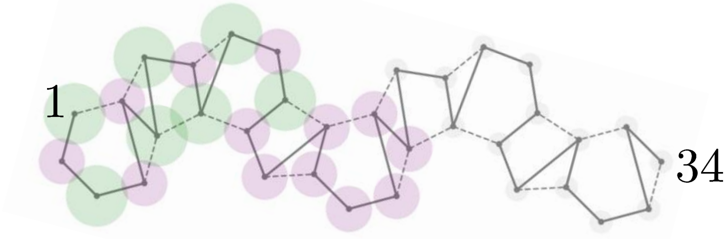
$$4\langle(\mathcal{S}^z_{\mathcal{M}_1})^2\rangle = 0.98$$

$$r = 0.99$$

Very close to a perfectly singly-occupied, perfectly aligned spin!



- We clearly distinguish three kinds of sites by their effect on $4\langle(\mathcal{S}^z_{\mathcal{M}})^2\rangle$:



Highly relevant (pentagon tip and neighboring sites of same sublattice)

Mildly relevant (sites around neighboring pentagons)

Irrelevant (rest of the sites)

- This is consistently observed across different system sizes: optimization cost scales nicely with P.

Transferability of modes

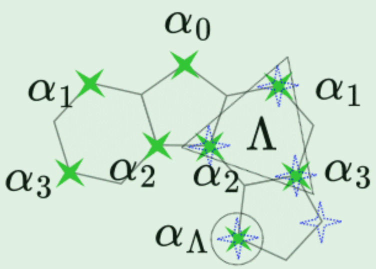
8-site symmetric modes (orthogonal)

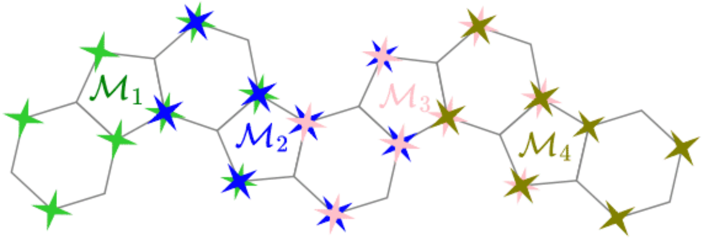
Optimize: $\{\alpha_1, \alpha_2, \alpha_3\}$

$$\alpha_0 \propto \sqrt{1 - 2\sum_{i=1}^{3} \alpha_i}$$

$$\Lambda = \alpha_1^* \alpha_3 + \alpha_2^* \alpha_1 + \alpha_3^* \alpha_2$$

$$\alpha_\Lambda \propto -\Lambda / \alpha_0$$



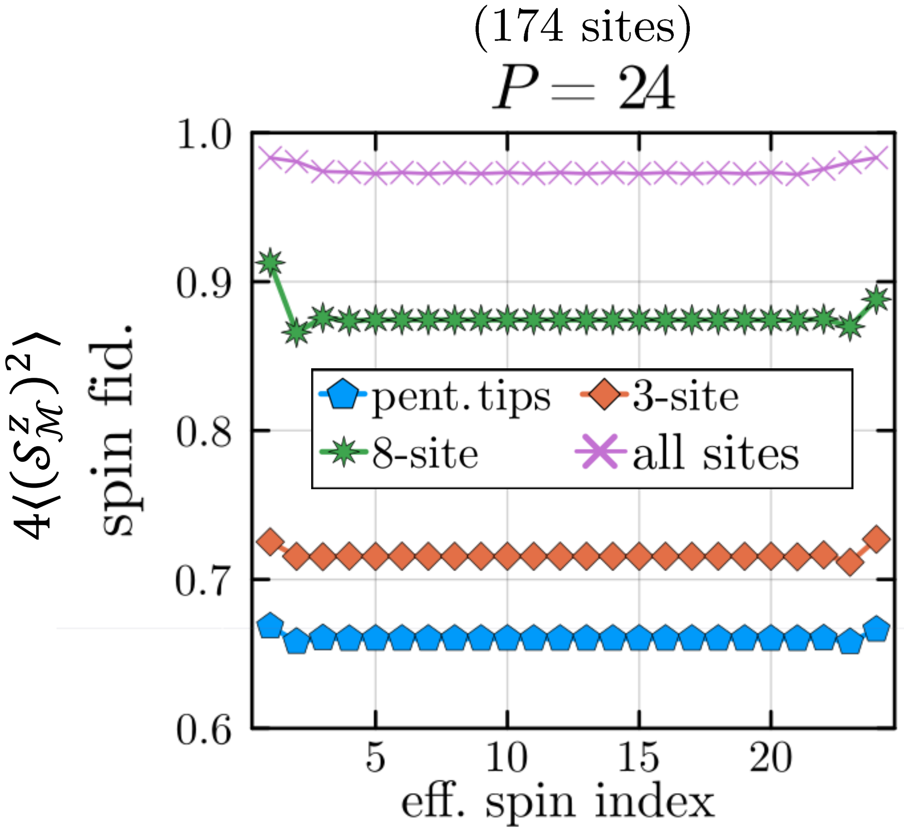


Careful with overlapping modes:

$$\{c^\dagger_{\mathcal{M},\sigma}, c_{\widetilde{\mathcal{M}},\sigma'}\} = \delta_{\sigma,\sigma'} \Lambda$$

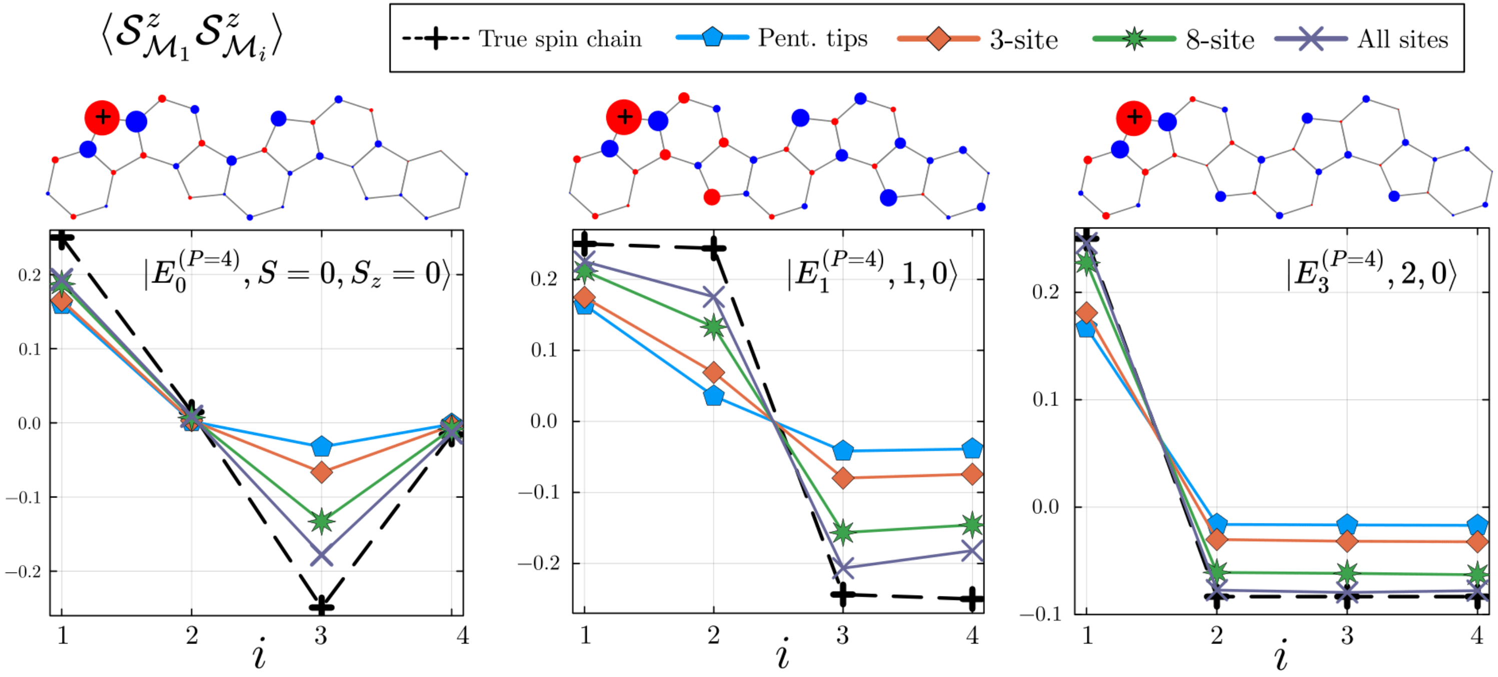
$$\Lambda = \sum_{i \in \mathcal{M} \cap \widetilde{\mathcal{M}}} \alpha_i^* \widetilde{\alpha}_i$$

Different effective spins will not commute if $\Lambda \neq 0$!



Effective spins can be reliably transferred between different system sizes, eigenstates and spin indices!

Correlations and spin flip



- Spin flip

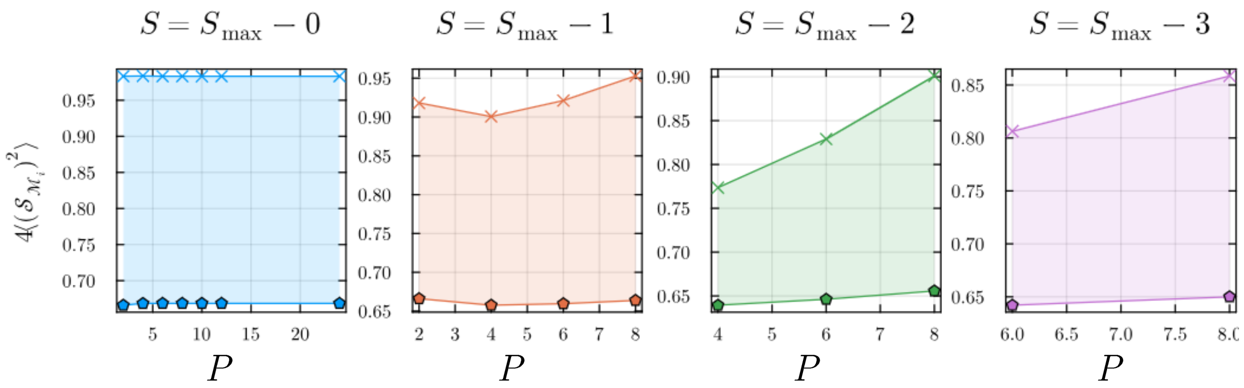
$$|\langle 2,1|\mathcal{S}^-_{\mathcal{M}}|2,2\rangle_{P=4}|^2$$

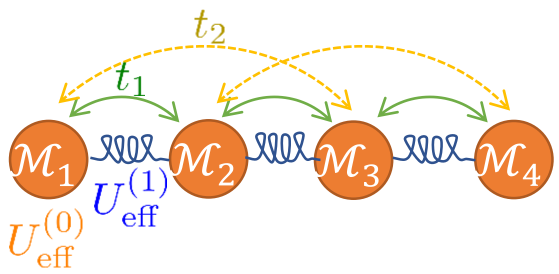
$\mathcal{M}$ **type**	**Overlap sq.**
Pent. only ⬟	0.19
3-site ◆	0.37
8-site ✳	0.72
All sites ×	0.94

Conclusions/outlook

- The ground and excited states of OInIn host effective frustrated spin physics.
- Their energy spectra coincide with J_1-J_2 spin chain in the $J_2/|J_1| > 1/4$ phase with VBS ground-states.
- The effective spins can accurately be extracted via a picture of delocalized fermionic modes.
- The delocalized modes are highly robust and controllable.

- We observe $4\langle(\mathcal{S}^z_{\mathcal{M}})^2\rangle$ is total S dependent:





- This is likely due to singlet formation between eff. modes.
- Propose an "intermediate model" between ladder and spin-chain?

- Study further properties of the systems via effective spin description?

(topology, entanglement entropy, …)

- How to probe the effective modes?