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# From Frustrated Ladders to Effective Spin Chains: A Study of Nanographene-Inspired Fermi-Hubbard Systems

Graphene-based systems provide an outstanding platform for the study of emergent physical phenomena and exotic phases of matter. By envisioning certain low-dimensional structures with sublattice imbalances, topological defects or frustration, strongly correlated magnetic ground states with long spin coherence times have been predicted, with a plethora of applications in spintronics, quantum information and quantum simulation [1]. Recently, experimental on-surface synthesis techniques have allowed for the fabrication of such structures, enabling the development of highly controllable spin chains [2, 3]. In this work we employ Density Matrix Renormalization Group (DMRG) to study quasi 1-dimensional structures and their links to effective spin models. We consider chains composed of hexagon/pentagon rings which have previously been analyzed using mean field and complete active space (CAS) based techniques [4]. Our tensor-network approach allows for accurately quantifying this picture, and extending it to low-lying excited states. We propose a formalism that can be used to identify *where* the effective spins in the chain are located via Matrix Product Operators representing delocalized fermionic modes, used to build the effective spin operators with high fidelity. This allows for direct comparison of correlations, magnetizations, entanglement entropies, transition amplitudes and more, between the Fermi-Hubbard ladder and the target system, which gives rise to an accurate and controllable spin model for the low-energy subspace. Our results offer a robust characterization of frustrated carbon-based ladder systems and support their use as tunable, synthetic models for exploring strongly correlated spin physics at the molecular scale.

References

[1] G de Oteyza, D & Frederiksen, T: Carbon-based nanostructures as a versatile platform for tunable $\pi$-magnetism. J. Phys. Condens. Matter 34, 443001 (2022).
[2] Mishra, S et al.: Observation of fractional edge excitations in nanographene spin chains, Nature 598 287-292 (2021).
[3] Zhao, C et al.: Tunable topological phases in nanographene-based spin-1/2 alternating-exchange Heisenberg chains, arXiv:2402.13590 (2024).
[4] Ortiz, R & Giedke, G & Frederiksen, T: Magnetic frustration and fractionalization in oligo(indenoindenes). Phys. Rev. B 107, L100416 (2023).

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