Magnetic properties of triangulene spin-1 chains

Emha Riyadhul Jinan Alhadi[1], Yasser Saleem[2], Weronika Pasek[1], Pawel Potasz[1]

[1]Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland
[2]Institut für Physikalische Chemie, Universität Hamburg, Hamburg, Germany

Spin chains can be physically realized in a variety of ways, for example using a scanning tunneling microscope (STM) on solid surfaces to manipulate molecules with atomic precision, or by creating chains of connected molecules [1]. Recent observation of edge states in triangulene chains revealed the existence of the Haldane phase related to antiferromagnetic spin S = 1 chain physics in these nanostructures [2]. Edge states in a finite system are characteristic features that reveal symmetry protected topological order with a gapped excitation spectrum in an infinite system [3]. A single triangulene molecule has a ground state with total spin S=1, and neighboring triangulene are antiferromagnetically coupled due to Lieb's theorem on a Hubbard model [4].

In this work, we start with a fermionic Hamiltonian with realistic Coulomb interaction parameters for extended Hubbard model and investigate the electronic and magnetic properties of coupled triangulenes froming a chain. Combining tight-binding, Hartree-Fock, and exact diagonalization methods (TB+HF+ED) [5], we investigate the role of different scattering elements in the many-body Hamiltonian and determine the terms responsible for the antiferromagnetic exchange between neighboring triangulenes. We derive simplified effective model describing, recently predicted [6], superexchange mechanism playing a crucial role here.

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