

1D spin-crossover molecular chain with degenerate states

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A. Gudyma¹  and Iu. Gudyma^{2,a)} 

AFFILIATIONS

¹Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany

²Physical, Technical and Computer Sciences Institute of Yuriy Fedkovich Chernivtsi National University, 58012 Chernivtsi, Ukraine

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a) Author to whom correspondence should be addressed: yugudyma@gmail.com

ABSTRACT

A study of the one-dimensional molecular chain (MC) with two single-particle degenerate states is presented. We establish connection of the MC with the Ising model with phononic interactions and investigate properties of the model using a transfer-matrix method. The transfer-matrix method offers a promising pathway for simulating such materials properties. The role of degeneracy of states and phononic interaction is made explicit. We analyze regimes of the system and parameters of the occurring crossover. Here, we present exact results for the magnetization per spin, the correlation function, and the effective volume of the system. We demonstrate the possibility of the existence of two peaks in the specific heat capacity thermal behavior.

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