

The Geometric Frustration Effects in Nanostructured Magnetic Systems

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We numerically investigate the geometric frustration effects in finite ring-shaped antiferromagnetic $S = 1/2$ Heisenberg models with an odd number spins in a ring. It is shown that, in a single ring, the lattices always display heterogeneous distortions for an arbitrarily large spring constant. However for any nonzero antiferromagnetic interring coupling in a finite two-leg spin ladder structure, a second order magnetoelastic transition (not the thermodynamic transition) takes place from the heterogeneous lattice distortion phase to the uniform phase (without lattice distortion) when the spring constant is increased. For ferromagnetic inter-ring coupling, there exists a critical coupling strength J_{\perp}^c , for $J_{\perp} > J_{\perp}^c$ a first order magnetoelastic transition is present.

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I. INTRODUCTION

Single molecular magnets (SMMs), which are nanostructured spin systems and formed by a finite number of exchange-coupled transition-metal ions, have become extensively investigated topics in condensed matter physics [1–11]. On the one hand, the SMMs can be regarded as the bridge to explore the crossover from microscopic magnetism to collective effects in macroscopic structure. On the other hand, the unique properties in these systems, such as giant magnetostriction [1], resonant tunneling of the magnetization [2, 3] and geometric phase effects [4] promise to open new frontiers in technology and fundamental research. In experiments, plenty of SMMs, especially with high-symmetry ring-shaped structures [5–9], have been synthesized and intensively studied. Recently, in the Cu₈ ring, the ⁶³Cu NQR (nuclear quadrupole resonance) spectrum shows four structurally nonequivalent Cu ions [9], which is perhaps related to the appearance of lattice dimerization. The lattice dimerization is a magnetoelastic (ME) instability, which may originate from the spin-phonon interaction. This phenomenon was first predicted to occur in the infinite $S = 1/2$ Heisenberg antiferromagnetic (AF) chain [12], and afterward, was observed experimentally in the quasi-one-dimensional $S = 1/2$ compound CuGeO₃ [13]. Due to the size effects, in finite spin systems, the spin-phonon interaction becomes stronger, and the lattice distortion behavior is evidently different from that in thermodynamic limit [14–16].

In spin systems, the geometric frustrations have strong effects on the ground state properties. For example, for a square Heisenberg antiferromagnet (HAF), the ground state