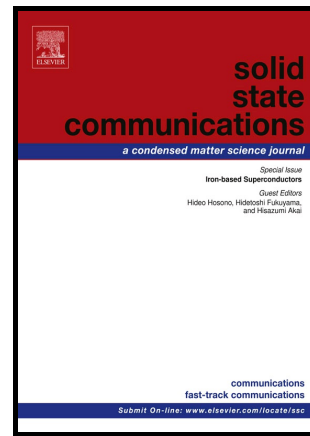


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Magnetism and thermodynamics of the anisotropic frustrated spin-1

Heisenberg antiferromagnet on a body-centered cubic lattice

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Abstract

The magnetic and thermodynamic properties of anisotropic frustrated spin-1 Heisenberg antiferromagnet on a body-centered cubic lattice for Néel phase (the region of weak frustration) are systematically investigated by use of the double-time Green's function method within the random phase approximation and the Anderson and Callen's decoupling. The zero-temperature sublattice magnetization and Néel temperature increase with spin anisotropy strength and single-ion anisotropy strength, and decrease with frustration strength. This indicates that quantum fluctuation is suppressed by spin anisotropy and single-ion anisotropy, by contrast, is strengthened by frustration. It is possible to tune the quantum fluctuations by the competition of anisotropy strength and frustration strength to change the ground state properties of magnetic materials. Although we find that both the spin anisotropy and the single-ion anisotropy suppress the quantum fluctuations, but their respective effects on the thermodynamic quantities, especially the internal energy and free energy, are different at zero temperature and finite temperature. Furthermore, when these two kinds of anisotropic coexist, the effect of the spin anisotropy on the sublattice magnetization and internal energy is larger than that of the single-ion anisotropy.

Keywords: A. Frustrated spin-1 Heisenberg antiferromagnet; D. Thermodynamic properties; C. Spin anisotropy and single-ion anisotropy; E. Double-time Green's function method.

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