FINITE-TEMPERATURE QUANTUM TRANSFER-MATRIX SIMULATIONS OF THE FRUSTRATED SPIN 1/2 CHAINS

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9.7 cm

Thermodynamical properties of the one-dimensional $S = 1/2$ Heisenberg model with nearest and next-nearest neighbour interactions are studied by the numerically exact quantum transfer-matrix method and the results are applied to the quasi-one-dimensional magnetic systems $CuGeO_3$ and $Pb[Cu(SO_4)(OH)_2]$.
The Suzuki-Trotter formula is used to obtain a classical system with spin $\sigma = 3/2$ and effective interactions between nearest neigbours only [1]. The magnetic susceptibility curve is calculated and compared with experimental results performed in a wide temperature range, revealing the presence of frustration in the model proposed for $CuGeO_3$ and $Pb[Cu(SO_4)(OH)_2]$. For the pure $CuGeO_3$, temperature dependence of the dimerization parameter below the spin-Peierls transition point is also estimated. The technique is extended for the finite-chain segments and applied to the diluted $CuGeO_3$ obtained by the neutron beam with three different intensities. The corresponding sizes of segments are also estimated for all the samples.

[1] G. Kamieniarz, M. Bieliński and J.P. Renard, *Phys. Rev. B* **60**, 14521 (1999)

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