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A Quantum Monte Carlo Study on Mixed-Spin Chains of 1/2-1/2-1-1 and 3/2-3/2-1-1XU Zhao-Xin,¹ ZHANG Jun,² and YING He-Ping^{1,3}

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Abstract: The ground-state and thermodynamic properties of quantum mixed-spin chains of 1/2-1/2-1-1 and 3/2-3/2-1-1 are investigated by a quantum Monte Carlo simulation with the loopcluster algorithm. For 1/2-1/2-1-1 chain, we find it has two phases separated by an energy-gap vanishing point in the ground-state. For 3/2-3/2-1-1 chain, the numerical results show two energy-gap vanishing points isolated by different phases in its ground-state. Our calculations indicate that all these ground state phases can be understood by means of valence-bond-solid picture, and the thermodynamic behavior at finite temperatures is continuous as a function of parameter $\alpha = J_2/J_1$.

PACS: 75.10.Jm, 75.40.Cx, 75.40.Mg Key words: ferrimagnetic, gap, valence-bond-solid (VBS) state

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