Variational Ansätze for frustrated quantum magnetism: reconstructing correlations, entanglement and the sign structure

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Exotic quantum spin states stabilised by magnetic Hamiltonians are fundamentally characterised by their correlation/fluctuations properties, and by their entanglement pattern - namely by the properties which are completely missed at the mean-field level. The sign problem in quantum Monte Carlo generally leaves us without unbiased numerically approaches to reconstruct the above properties of models of quantum frustrated magnetism for large ($N \gg 10$) systems. A general strategy to circumvent this fundamental difficulty is offered by the variational approach, which is at the core of the most successful algorithms to study frustrated quantum magnetism; namely, the density-matrix renormalisation group approach — which variationally optimises matrix-product states — and its generalisations, which optimise so-called tensor-network states. Such states, while very powerful, are fundamentally limited in their entanglement content by the number of variational parameters (the so-called bond dimension), and their optimisation becomes very complex in dimension d=2 and higher (implying the contraction of a d-dimensional tensor network). Here we propose an alternative strategy to the variational study of frustrated quantum magnetism, based on a class of wavefunctions called entangled-plaquette states [1] or correlator-product states [2]. Such states have a very transparent structure in terms of correlations, which can be made to be scale invariant and therefore reproduce faithfully the structure at quantum critical points; they can be efficiently optimised using Monte Carlo techniques; and they can accommodate for an arbitrary amount of entanglement with a polynomial number of variational parameters. Most importantly, our recent progress shows us that, by complexifying the wavefunction coefficients, we can variationally reconstruct their correct sign structure, biased uniquely by the form of the Ansatz - something which is generally considered to be hard in frustrated magnetism [Becca, Sorella in [3]]. We demonstrate the power of our variational Ansatz in the paradigmatic case of the J1-J2 Heisenberg chain, whose quantum phase transition is correctly reproduced, as well as its intricate sign structure induced by the appearance of incommensurate spin correlations.

[1] F. Mezzacapo et al, New Journal of Physics, 11, 083026 (2009)

[2] H. Changlani et al., Phys. Rev. B 80, 245116 (2009)

[3] J.Chalker, Introduction to frustrated magnetism (Springer, 2011)