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Self-optimized resonating-valence-bond trial wavefunctions[1]
KEVIN BEACH, ANDERS SANDVIK, Boston University — The spin singlet ground state of a quantum antiferromagnet can be expanded in the overcomplete basis of valence bond states. [1] To first approximation, the weight associated with each configuration is factorizable into a product of individual bond amplitudes. For nonfrustrated antiferromagnets with local interactions, mean field calculations indicate that the amplitudes are generically powerlaw in the bond length with exponent d+1, where d is the dimension of the lattice. Such states can be employed as the initial trial state for a valence bond projector calculation of the exact ground state. [2] Moreover, the amplitudes can be determined self- consistently by measuring the statistics of the bonds appear in the projected state and feeding this information back into the trial state. It is also possible to build some of the neglected bond-bond correlations into the trial state itself. The next level of approximation is to factorize the weights in terms of amplitudes that depend on the lengths and orientations of two valence bonds. Again, these amplitudes can be self-optimized in a simulation by matching them to the bond– bond correlations of the projected state.
[1] K. S. D. Beach and A. W. Sandvik, Nucl. Phys. B **750**, 142 (2006).
[2] A. W. Sandvik, Phys. Rev. Lett. **95**, 207203 (2005).

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