

Abstract Submitted
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Variational ground states of 2D antiferromagnets in the valence-bond basis¹ JIE LOU, ANDERS SANDVIK, Boston University — We use a variational method to study two-dimensional $S = \frac{1}{2}$ Heisenberg antiferromagnets in the valence bond basis. The wave function is of the form

$$|\psi\rangle = \prod h(x_{ij}, y_{ij})(i, j),$$

where (i, j) represents a singlet formed by the spins at sites i and j ;

$$(i, j) = \frac{1}{\sqrt{2}}(\uparrow_i \downarrow_j - \downarrow_i \uparrow_j),$$

and $h(x_{ij}, y_{ij})$ is the amplitude corresponding to a bond connecting two spins with separation (x_{ij}, y_{ij}) . The form $h \sim \frac{1}{r^p}$, where r is the distance, was studied previously. The best variational energy was obtained for $p = 4$. Now we optimize all $h(x, y)$ by combining a standard Newton method and a conjugate gradient method. For systems with up to 16×16 spins, the energy of the optimized wave function deviates by less than 0.1% from the exact ground state energy. The spin-spin correlations are also very well reproduced. The exponent $p = 3$ in agreement with recent Monte Carlo simulations. We also investigate this class of wave functions for a quantum-critical bilayer model.

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