Abstract Submitted
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An efficient basis for the modeling of doped and undoped S=1/2 antiferromagnet[1] BAYO LAU, Department of Physics, Columbia University, NY, NY, MONA BERCIU, GEORGE A. SAWATZKY, Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, V6T 1Z1 — We formulate an efficient numerical basis to model both doped and undoped S=$\frac{1}{2}$ Heisenberg antiferromagnet (AFM) with two-dimensional periodic boundary condition (2DPBC). Using a linear combination of Slater determinants with total-spin symmetries, a variational approach is developed to systematically and combinatorially decreases the Hilbert space of the problems, allowing the application of exact diagonalization to record-breaking system sizes. We can now model explicitly the wavefunction of an undoped 64-spin AFM square lattice with 2DPBC. For the doped scenarios, we solve a half-filled lattice with 32 coppers and 64 oxygens with one or two electrons removed. This allows, for the first time, a direct comparison of 32-unit-cell exact diagonalization between multi-band model and the t-J model, quantifying several oxygen-specific properties relevant to the lightly doped cuprate structures.

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