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Quantum Monte Carlo calculations of magnetic couplings in cuprates[1] KATERYNA FOYEVTSOVA, JARON KROGEL, JEONGNIM KIM, FERNANDO REBOREDO, Oak Ridge National Laboratory — Spin excitations are generally believed to play a fundamental role in the mechanism of high temperature superconductivity in cuprates. However, accurate description of the cuprates' magnetic properties and, in particular, calculation of spin exchange couplings have been a long-standing challenge to the electronic structure theory. While the quantum-mechanically more rigorous cluster methods suffer from finite-size effects, the density functional theory approach, on the other hand, is ambiguous due to a rich variety of approximations to the exchange-correlation functional available which often give very different numbers for the spin exchange constants. For example, in some cuprates the theoretically predicted values of the nearest-neighbor superexchange range from 1 eV (local density approximation) to 0.05 eV (periodic unrestricted Hartree Fock) [C. de Graaf *et al*, PRB **63** 014404 (2000)]. We compute spin exchange constants with the fixed-node diffusion Monte Carlo method (FN-DMC). In one-dimensional cuprates, we find that the FN-DMC computed nearest-neighbor spin superexchange is in an excellent agreement with experiment. This both demonstrates that FN-DMC is capable of describing properly the magnetism of strongly correlated oxides as well as positions this technique as the method of choice for theoretical parameterization of spin models.

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