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A dynamical Marshall sign convention KEVIN BEACH, University of Alberta — Monte Carlo sampling of quantum spin models is only practical when it is possible to gauge away simultaneously all negative signs in the coefficients of the ground state wavefunction. The existence of such a transformation is related to the possibility of establishing a bipartite pattern of magnetic order on the lattice and to the choice of a so-called Marshall sign convention. In practice, identifying the correct Marshall sign convention is the responsibility of the QMC practitioner, and the convention itself is generally hard coded. It turns out, however, that a locally optimal sign convention can be determined dynamically within the simulation—meaning that for nonfrustrated systems the simulation quickly establishes a Marshall sign convention that leads to sign-problem-free sampling and that for frustrated systems the Marshall sign convention continually evolves in Monte Carlo time so as to minimize the severity of the sign problem. For concreteness, we focus on a worm algorithm formulated in the basis of singlet product states.

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