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Spin dynamics algorithms for systems with exchange interactions beyond nearest neighbors[1] XIUPING TAO, D. P. LANDAU, Center for Simulational Physics, University of Georgia, Athens, T. C. SCHULTHESS, Computer Science and Mathematics Division, Oak Ridge National Laboratory, G. M. STOCKS, Metals and Ceramics Division, Oak Ridge National Laboratory — Fast spin dynamics algorithms for classical spin systems with nearest neighbor exchange interactions ($J_1 \neq 0$, and $J_i = 0$ for i^{th} nearest neighbors with $i \geq 2$) were studied extensively years ago[2]. For some realistic magnetic systems, such as Fe, J_i can not be neglected for several shells of neighbors. To study dynamic properties of such systems, fast algorithms are still applicable; however, with n shells of interacting neighbors, a lattice needs to be decomposed into 2^n sublattices and there can be as many as $(5^{2^n} - 3)/2$ factors for the fourth order Suzuki-Trotter decompositions of exponential operators. In comparison, only $2^{n+1} - 1$ factors are needed for second order decompositions. Consequently, only second order decompositions are practical for $n \geq 2$. Examples are given showing the implementation of the algorithms for systems in which as many as four shells of near neighbors play a significant role.

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[2]M. Krech, A. Bunker, and D. P. Landau, Comput. Phys. Commun. **111**, 1 (1998).

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