"Fast Diagonalization of Evolving Matrices: Application to Spin-Fermion Models"

E. F. D'Azevedo*, P. K. Nukala, G. Alvarez
Oak Ridge National Laboratory

Summary

Large scale Monte-Carlo simulation of colossal magnetoresistance effect (CMR) using spin-fermion models is often hampered by the high computational cost associated with computation of all eigenvalues of the Hamiltonian matrix. Consequently, current spin-fermion model simulations contain no more than 6^3 sites in three dimensions. This imposes severe limitations on the kind of physical systems or phenomenon that can be studied. This effort developed an algorithm to directly update the spectrum of successive Hamiltonian matrices based on the spectrum of previous matrices. The updating algorithm significantly reduces the computational cost in re-computing the spectrum of the Hamiltonian matrices each time a local configurational change is accepted. The serial version is an order of magnitude faster than the approaches based on direct diagonalization.

The study of certain manganese oxides exhibiting the "colossal" magnetoresistance effect (CMR) is an important area of research in the theory of strongly correlated electrons. CMR, similar to "gigantic" magnetoresistance (GMR), is a magnetic material property that enables certain materials to be used in data storage applications. For example, GMR technology has been used in hard drives and CMR is two to three orders of magnitude stronger than GMR. Consequently, understanding of CMR has enormous technological implications in terms of developing innovative applications. One of the most commonly used approaches to model CMR manganites is the so-called double-exchange spin-fermion model. The simulation proceeds by visiting each location of the lattice and proposing a local change or event. The probability that the change is accepted is a function of all the eigenvalues of the Hamiltonian. Each time a local change is accepted, the Hamiltonian matrix undergoes a low-rank modification. The simulation proceeds through proposing a new local change, which requires the re-computation of all the eigenvalues of the updated Hamiltonian matrix in the subsequent configuration. This progression of simulation through local changes proceeds for many steps until the observables converge to the desired accuracy of the Monte Carlo procedure. A direct diagonalization method (DDM) that repetitively computes all the eigenvalues of the successive Hamiltonian matrices becomes prohibitively expensive. Consequently, large-scale numerical simulations using this model have often been hampered. In addition, since the frequency that these local events are accepted increases with increasing system sizes, numerical simulation of large systems becomes even more expensive. The computation would scale as $O(N^4)$, where N is the matrix size. Consequently, the largest lattice that can be accessed is limited to at most 6^3 sites in three dimensions or about 14^2 in two dimensions. This imposes limitations on the

*865-576-7925, dazevedoef@ornl.gov

kind of physical systems that can be studied. Furthermore, ensemble averaging of numerical results is necessary to obtain a realistic representation of system response, which further increases the computational cost associated with modeling CMR using Monte Carlo models.

This study presents an algorithm that directly updates the spectrum of a successive Hamiltonian matrix based on the spectrum of previous Hamiltonian matrix. The updating of eigenvalues is similar to a key step in the "divide-and-conqueror" algorithm for computing all eigenvalues of real symmetric matrices. Let $A = Y * D * Y^{'}$ be the eigen-decomposition of matrix *A* and $B = A + \rho zz^{'}$ be the updated matrix under a rank-one modification. Then the new eigenvalues of *B* (γ_j) are obtained as the roots of the secular function $g(\gamma) = 1 + \rho \sum z_i z_i^{'} / (d_i - \gamma)$. An orthogonal matrix of new eigenvectors *U* can be generated from the eigenvalues (γ_j) and vector *z*. The j-th column of matrix *U* is the normalized eigenvector u_j that is parallel to $(D - \gamma_j I)^{-1} z$. The update algorithm proceeds by first computing an initial eigen-decomposition. At each step, low-rank updates are transformed by multiplication of the orthogonal *U* matrices that contain the eigenvectors. The new eigenvalues are computed by finding the roots of the secular function. The low rank updates (*z* vectors) are saved so that the next set of new eigenvectors (matrix *U*) can be reconstructed. A new complete eigen-decomposition is performed occasionally when the cost for saving the updates (*z* vectors) is too high. Figures 1 show the new algorithm is robust and accurate even for large systems. Table 1 shows the new algorithm with incremental update that is an order of magnitude faster than DDM.

Matrix size	Time of update algorithm	Time of LAPACK zheev('N')
288	0.34s	1.6s
800	2.5s	18.5s
1152	9.7s	64s
2048	32s	365s

Table 1: Time for 10 steps of simulation

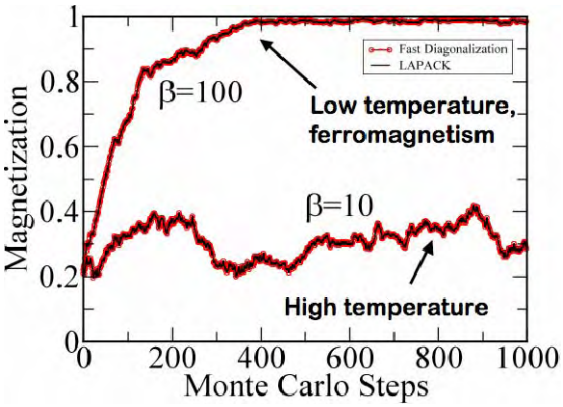

Figure 1: Magnetization in low and high temperature systems

Refereed Journal Publications

1. G. Alvarez, P.K. Nukala, and E. D'Azevedo, *Fast Diagonalization of Evolving Matrices: Application to Spin-Fermion Systems*, Journal of Statistical Mechanics: Theory and Experiment (JSTAT) (2007).

Invited Presentations

2. E. D'Azevedo, P.K. Nukala, and G. Alvarez, *An Eigensolver with Low-rank Updates for Spin-Fermion Models*, Math PI Meeting, Lawrence Livermore National Laboratory, Livermore, May, 2007.
3. P.K. Nukala, E. D'Azevedo, and G. Alvarez, *Low-rank Updates in Statistical Physics Applications*, XXIII StatPhys Conference, Genoa, Italy (2007).

For further information on this subject contact:

Dr. E. F. D'Azevedo
Oak Ridge National Laboratory
dazevedoef@ornl.gov
865-576-7925

Or

Dr. Anil Deane
Applied Mathematics Research Program
Office of Advanced Scientific Computing
Phone: 301-903-1465
deane@ascr.doe.gov