THE ROLE OF DIAGNOLIZATION
WITHIN A DIAGNOLIZATION/MONTE CARLO SCHEME

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We discuss a method called quasi-sparse eigenvector diagonalization which finds the most important basis vectors of the low energy eigenstates of a quantum Hamiltonian. It can operate using any basis, either orthogonal or non-orthogonal, and any sparse Hamiltonian, either Hermitian, non-Hermitian, finite-dimensional, or infinite-dimensional. The method is part of a new computational approach which combines both diagonalization and Monte Carlo techniques.

1. Introduction

The methods of Monte Carlo and diagonalization are almost opposite in their strengths and weaknesses. Monte Carlo requires relatively little storage, can be performed using parallel processors, and in some cases the computational effort scales reasonably with system size. But it has great difficulty for systems with sign or phase oscillations and provides only indirect information on wavefunctions and excited states. Diagonalization methods on the other hand do not suffer from fermion sign problems, can handle complex-valued actions, and can extract details of the spectrum and eigenstate wavefunctions. However the required memory and CPU time scales exponentially with the size of the system.

Recently we proposed a new computational approach which takes advantage of the strengths of the two methods in their respective domains. The first half of the approach involves finding and diagonalizing the Hamiltonian restricted to an optimal subspace. This subspace is designed to include the most important basis vectors of the lowest energy eigenstates. Once the most important basis vectors are found and their interactions treated exactly, Monte Carlo is used to sample the contribution of the remaining basis vectors. Much of the sign problem is negated by treating the interactions of the most important basis states exactly, while storage and CPU problems are resolved by stochastically sampling the collective effect of the remaining states.

In our approach diagonalization is used as the starting point of the Monte Carlo calculation. Unfortunately we find that most diagonalization methods are either not sufficiently general, not able to search an infinite or large dimensional Hilbert space, not efficient at finding important basis vectors, or not compatible with the subsequent Monte Carlo part of the calculation. In this brief article we review a new diagonalization method called quasi-sparse eigenvector (QSE) diagonalization. It is a general algorithm which can operate using any basis, either orthogonal or non-orthogonal, and any sparse Hamiltonian, either real, complex, Hermitian, non-Hermitian, finite-dimensional, or infinite-dimensional. It is able to find the most

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important basis states of several low energy eigenvectors simultaneously, including those with identical quantum numbers, from a random start with no prior knowledge about the form of the eigenvectors.

2. **Quasi-sparse eigenvector method**

Let \( |e_i \rangle \) denote a complete set of basis vectors. For a given energy eigenstate

\[ |v \rangle = \sum_i c_i |e_i \rangle , \tag{1} \]

the important basis states of \( |v \rangle \) are defined to be those \( |e_i \rangle \) such that for fixed normalizations of \( |v \rangle \) and the basis states, \(|c_i| \) exceeds a prescribed threshold value. If \( |v \rangle \) can be well-approximated by the contribution from only its important basis states we refer to the eigenvector \( |v \rangle \) as *quasi-sparse* with respect to \( |e_i \rangle \).

Standard sparse matrix algorithms such as the Lanczos or Arnoldi methods allow one to find the extreme eigenvalues and eigenvectors of a sparse matrix efficiently, without having to store or manipulate large non-sparse matrices. However in quantum field theory or many body theory one considers very large or infinite dimensional spaces where even storing the components of a general vector is impossible. For these more difficult problems the strategy is to approximate the low energy eigenvectors of the large space by diagonalizing smaller subspaces. If one has sufficient intuition about the low energy eigenstates it may be possible to find a useful truncation of the full vector space to an appropriate smaller subspace. In most cases, however, not enough is known *a priori* about the low energy eigenvectors. The dilemma is that to find the low energy eigenstates one must truncate the vector space, but in order to truncate the space something must be known about the low energy states.

Our solution to this puzzle is to find the low energy eigenstates and the appropriate subspace truncation at the same time by a recursive process. We call the method quasi-sparse eigenvector (QSE) diagonalization, and we describe the steps of the algorithm as follows. The starting point is any complete basis for which the Hamiltonian matrix \( H_{ij} \) is sparse. The basis vectors may be non-orthogonal and/or the Hamiltonian matrix may be non-Hermitian. The following steps are iterated:

1. Select a subset of basis vectors \( \{e_{i_1}, \ldots, e_{i_n} \} \) and call the corresponding subspace \( S \).
2. Diagonalize \( H \) restricted to \( S \) and find one eigenvector \( v \).
3. Sort the basis components of \( v \) according to their magnitude and remove the least important basis vectors.
4. Replace the discarded basis vectors by new basis vectors. These are selected at random according to some weighting function from a pool of candidate basis vectors.
vectors which are connected to the old basis vectors through non-vanishing matrix elements of $H$.

5. Redefine $S$ as the subspace spanned by the updated set of basis vectors and repeat steps 2 through 5.

If the subset of basis vectors is sufficiently large, then it can be shown that the exact low energy eigenvectors are stable fixed points of the QSE update process. As the name indicates the accuracy of the quasi-sparse eigenvector method depends on the quasi-sparsity of the low energy eigenstates in the chosen basis. If the eigenvectors are quasi-sparse then the QSE method provides an efficient way to find the important basis vectors. In the context of our diagonalization/Monte Carlo approach, this means that diagonalization does most of the work and only a small amount of correction is needed. This correction is found by Monte Carlo sampling the remaining basis vectors, a technique called stochastic error correction. If however the eigenvectors are not quasi-sparse then one must rely more heavily on the Monte Carlo portion of the calculation. The fastest and most reliable way we know to determine whether the low energy eigenstates of a Hamiltonian are quasi-sparse with respect to a chosen basis is to use the QSE algorithm and look at the results of the successive iterations. We generally find that eigenvectors are quasi-sparse with respect to a chosen basis if the spacing between energy levels is not too small compared with the size of the off-diagonal entries of the Hamiltonian matrix.

We regard QSE diagonalization as only a starting point for the Monte Carlo part of the calculation. Once the most important basis vectors are found and their interactions treated exactly, a technique called stochastic error correction is used to sample the contribution of the remaining basis vectors.

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