Introduction to stochastic error correction methods

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Abstract

We propose a method for eliminating the truncation error associated with any subspace diagonalization calculation. The new method, called stochastic error correction, uses Monte Carlo sampling to compute the contribution of the remaining basis vectors not included in the initial diagonalization. The method is part of a new approach to computational quantum physics which combines both diagonalization and Monte Carlo techniques.

1 Introduction

In \cite{1} a new approach was proposed for finding the low-energy eigenstates of very large or infinite-dimensional quantum Hamiltonians. This proposal combines both diagonalization and Monte Carlo methods, each being used to solve a portion of the problem for which the technique is most efficient. The first part of the proposal is to diagonalize the Hamiltonian restricted to a subspace containing the most important basis vectors for each low energy eigenstate. This may be accomplished either through variational techniques or an \textit{ab initio} method such as quasi-sparse eigenvector (QSE) diagonalization. The second step is to include the contribution of the remaining basis vectors by Monte Carlo sampling. The use of diagonalization allows one to consider systems with fermion sign oscillations and extract information about wavefunctions and excited states. The use of Monte Carlo provides tools to handle the exponential increase in the number of basis states for large volume systems.

The first half of this proposal was discussed in \cite{1}. An adaptive diagonalization algorithm known as the quasi-sparse eigenvector method was introduced to find the most important basis vectors for each low energy eigenstate. This technique is especially valuable when little is known about the low energy states. It is also the only method available which can handle non-orthogonal bases, non-Hermitian Hamiltonians, infinite dimensional systems, and which can find several low energy states with like quantum numbers simultaneously. In this paper we discuss the second half of the diagonalization/Monte Carlo scheme. We introduce several new Monte Carlo techniques which we call stochastic error correction (SEC). There are two general varieties of stochastic error correction, methods based on a series expansion and those which are not. The series method starts with an eigenvector of the Hamiltonian restricted to some starting subspace and then includes the contribution of the remaining basis states as terms in an ordered expansion. The idea is to form a perturbative expansion centered around a good non-perturbative starting point.

As an example of a non-series method we discuss a technique called the stochastic Lanczos method. This method again starts with eigenvectors of a Hamiltonian submatrix. Using these as starting vectors, we define Krylov vectors, \(|j\rangle, H |j\rangle, H^2 |j\rangle, \cdots\), similar to standard Lanczos diagonalization. The new ingredient is that matrix elements between Krylov vectors, \(<j' | H^n |j\rangle\), are computed using matrix diffusion Monte Carlo.

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Since the method does not rely on a series expansion, it has the advantage that the starting vectors need not be close to the exact eigenvectors.

One can generate a large class of stochastic error correction methods based on other non-series algorithms, various ways of resumming the series expansion, or combinations of the two techniques. In this introductory paper we concentrate on describing the basic principles and implementation of the series and non-series approaches. We also present three test problems which demonstrate the potential of the new approach for a range of different problems. In the first example we determine the low energy spectrum of $\phi_{2+1}^4$ theory using QSE diagonalization and first order corrections using the series method. In the second example we find the low energy spectrum of compact $U(1)$ in $2+1$ dimensions using the stochastic Lanczos method. In the last example we find the ground state of the $2+1$ dimensional Hubbard model using QSE diagonalization and first order series stochastic error correction. In each case we compare with published results in the literature. We conclude with a summary and some general comments on the new computational scheme.

## 2 Series method

Let $|\phi\rangle$ be the eigenvectors of a Hamiltonian $H$ restricted to some subspace $S$. Let $|A_j\rangle$ be the remaining basis vectors in the full space not contained in $S$. We can represent $H$ as

$$
\begin{pmatrix}
\lambda_1 & 0 & \cdots & \langle 1|H|A_1\rangle & \langle 1|H|A_2\rangle & \cdots \\
0 & \lambda_2 & \cdots & \langle 2|H|A_1\rangle & \langle 2|H|A_2\rangle & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
\langle A_1|H|1\rangle & \langle A_1|H|2\rangle & \cdots & E \cdot \lambda_{A_1} & \langle A_1|H|A_2\rangle & \cdots \\
\langle A_2|H|1\rangle & \langle A_2|H|2\rangle & \cdots & \langle A_2|H|A_1\rangle & E \cdot \lambda_{A_2} & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots 
\end{pmatrix}
$$

(1)

We have used Dirac’s bra-ket notation to represent the terms of the matrix. In cases where the basis is non-orthogonal or the Hamiltonian is non-Hermitian, the precise meaning of terms such as $\langle A_1|H|1\rangle$ is the action of the dual vector to $|A_1\rangle$ upon the vector $H|1\rangle$. We have written the diagonal terms for the basis vectors $|A_j\rangle$ with an explicit factor $E$ for reasons to be explained shortly.

Let us assume that $|\phi\rangle$ is close to some exact eigenvector of $H$ which we denote as $|1_{\text{full}}\rangle$. More concretely we assume that the components of $|1_{\text{full}}\rangle$ outside $S$ are small enough so that we can expand in inverse powers of the introduced parameter $E$. In order to simply the expansion we choose to shift the diagonal entries so that $\lambda_1 = 0$.

The series method of stochastic error correction is based on the $E^{-1}$ expansion,

$$
|1_{\text{full}}\rangle \propto \begin{pmatrix} 1 \\ c'_2 E^{-1} + c''_2 E^{-2} + \cdots \\ \vdots \\ c'_{A_1} E^{-1} + c''_{A_1} E^{-2} + \cdots \\ c'_{A_2} E^{-1} + c''_{A_2} E^{-2} + \cdots \\ \vdots 
\end{pmatrix},
$$

(2)

$$
\lambda_{\text{full}} = \lambda'_1 E^{-1} + \lambda''_1 E^{-2} \cdots.
$$

(3)

It is convenient to choose the normalization of the eigenvector such that the $|1\rangle$ component remains 1. The convergence of the expansion is controlled by the proximity of $|1\rangle$ to $|1_{\text{full}}\rangle$. If $|1\rangle$ is not at all close to $|1_{\text{full}}\rangle$ then it will be necessary to use a non-series method such as the stochastic Lanczos method discussed in the next section.

At first order in $E^{-1}$ we find

$$
c'_{A_j} = -\frac{\langle A_j|H|1\rangle}{\lambda_{A_j}}.
$$

(4)
\[ \lambda_1' = - \sum_j \frac{\langle 1 | H | A_j \rangle \langle A_j | H | 1 \rangle}{\lambda_{A_j}} \]  

(5)

\[ c_j' = \frac{1}{\lambda_j} \sum_k \frac{\langle j | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_k}}. \]  

(6)

At second order the contributions are

\[ c_{A_j}' = \sum_{k \neq j} \frac{\langle A_j | H | A_k \rangle \langle A_k | H | k \rangle}{\lambda_{A_j} \lambda_{A_k}} - \sum_{l \neq 1} \sum_k \frac{\langle A_j | H | l \rangle \langle H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_j} \lambda_{A_l} \lambda_{A_k}} \]  

(7)

\[ \lambda''_1 = \sum_j \sum_{k \neq j} \frac{\langle 1 | H | A_j \rangle \langle A_j | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_j} \lambda_{A_k}} - \sum_j \sum_{l \neq 1} \sum_k \frac{\langle 1 | H | A_j \rangle \langle A_j | H | l \rangle \langle H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_j} \lambda_{A_l} \lambda_{A_k}} \]  

(8)

\[ c_{m}'' = \sum_{j \neq k} \frac{\langle m | H | A_j \rangle \langle A_j | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_m \lambda_{A_j} \lambda_{A_k}} + \sum_{j \neq l \neq 1} \sum_k \frac{\langle m | H | A_j \rangle \langle A_j | H | l \rangle \langle H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_m \lambda_{A_l} \lambda_{A_k}} \]  

(9)

\[ = - \frac{1}{\lambda_m} \left[ \sum_j \frac{\langle 1 | H | A_j \rangle \langle A_j | H | 1 \rangle}{\lambda_{A_j}} \right] - \frac{1}{\lambda_m} \left[ \sum_k \frac{\langle m | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_k}} \right]. \]

These contributions can be calculated by straightforward Monte Carlo sampling. All that is required is an efficient way of generating random basis vectors \(|A_j\rangle\) with known probability rates. Let \( P(A_{\text{trial}}) \) denote the probability of selecting \(|A_{\text{trial}}\rangle\) on a given trial. If for example we are calculating the first order correction to the eigenvalue, then we have

\[ \lambda_1' = - \sum_j \frac{\langle 1 | H | A_j \rangle \langle A_j | H | 1 \rangle}{\lambda_{A_j}} \]  

(10)

\[ = - \lim_{N \to \infty} \frac{1}{N} \sum_{i=1,...,N} \frac{\langle 1 | H | A_{\text{trial}(i)} \rangle \langle A_{\text{trial}(i)} | H | 1 \rangle}{\lambda_{A_{\text{trial}(i)}}} P(A_{\text{trial}(i)}). \]

\[ \text{3 Stochastic Lanczos} \]

We now consider a method called stochastic Lanczos which does not require the starting vectors to be close to exact eigenvectors of \( H \). This is essential if the eigenvectors of \( H \) are not quasi-sparse and require extremely large numbers of basis states to represent accurately.

Let \( V \) be the full Hilbert space for our system. As in the previous section let \( S \) be the subspace over which we have diagonalized \( H \) exactly. Let \( P_S \) be the projection operator for \( S \) and let \( \lambda_j \) and \( |j\rangle \) be the eigenvalues and eigenvectors of \( H \) restricted to \( S \) so that

\[ P_S H P_S |j\rangle = \lambda_j |j\rangle. \]  

(11)

Let \( Z \) be an auxiliary subspace, one which contains \( S \) but excludes very high-energy states. Let \( P_Z \) be the projection operator for \( Z \). We will choose \( Z \) such that \( P_Z H P_Z \) is bounded above. Let \( a \) be a real constant which is greater than the midpoint of the minimum and maximum eigenvalues of \( P_Z H P_Z \). As \( n \to \infty \) the operator \( [P_Z (H - a) P_Z]^n \) maps any given state in \( Z \) to the corresponding lowest-energy eigenvector of \( P_Z H P_Z \) with non-zero overlap.

The stochastic Lanczos method uses the operators \( [P_Z (H - a) P_Z]^n \) to approximate the low-energy eigenvalues and eigenvectors of \( P_Z H P_Z \). The goal is to diagonalize \( H \) in a subspace spanned by vectors

\[ |d, j\rangle = [P_Z (H - a) P_Z]^d |j\rangle, \]  

(12)
for several values of $d$ and $j$. This requires calculating $\langle d', j' | d, j \rangle$ and $\langle d', j' | H | d, j \rangle$. If our Hamiltonian matrix is Hermitian, both of these terms can be written in the general form

$$\langle j' | [P_Z(H - a)P_Z]^n | j \rangle.$$  \hfill (13)

Therefore it suffices to determine the matrix

$$A_n \equiv P_S [P_Z(H - a)P_Z]^n P_S.$$ \hfill (14)

For non-orthogonal bases and non-Hermitian Hamiltonians, the only change is that we use vectors $[P_Z(H - a)P_Z]^d | j \rangle$ \hfill (15)

to generate approximate right eigenvectors of $H$ and vectors in the dual space $\langle j | [P_Z(H - a)P_Z]^d$ to produce approximate left eigenvectors. Adding and subtracting $P_S [P_Z(H - a)P_Z]$, we can rewrite

$$A_n = P_S [P_Z(H - a)P_Z - P_S(H - a)P_S + P_S(H - a)P_S]^n P_S.$$ \hfill (17)

$A_n$ can now be evaluated recursively as

$$A_{n+1} = B_{n+1} + \sum_{m=0, \ldots, n} B_m (H - a) A_{n-m},$$ \hfill (18)

where

$$B_n = P_S [P_Z(H - a)P_Z - P_S(H - a)P_S]^n P_S.$$ \hfill (19)

The components of $B_n$ are computed by matrix diffusion Monte Carlo. One could also directly evaluate the components of $A_n$. However the calculation for $B_n$ eliminates the need to sample the matrix $P_S(H - a)P_S$, which is already known. Any general matrix product $M^{(1)} M^{(2)} \cdots M^{(n)}$ is a sum of degree $n$ monomials,

$$\left[ M^{(1)} M^{(2)} \cdots M^{(n)} \right]_{jk} \equiv \sum_{i_1, \ldots, i_n=1} M^{(1)}_{ji_{i_1}} M^{(2)}_{i_1 i_{i_2}} \cdots M^{(n)}_{i_{n-1} k}.$$ \hfill (20)

We can interpret (20) as a sum over paths through the set of basis vectors of $Z$,

$$|j\rangle \rightarrow |i_1\rangle \rightarrow \cdots \rightarrow |i_{n-1}\rangle \rightarrow |k\rangle,$$ \hfill (21)

with an associated weight $M^{(1)}_{ji_{i_1}} M^{(2)}_{i_1 i_{i_2}} \cdots M^{(n)}_{i_{n-1} k}$. The components of $B_n$ are sampled using ensembles of random walkers. We refer the interested reader to [2] for a review of methods in diffusion Monte Carlo.

We end the section with a discussion of the fermion sign problem. The sign problem is a general issue for any Monte Carlo calculation. For a system with sign oscillations the evaluation of a Euclidean-time Green’s function involves sums

$$\sum_i x_i$$ \hfill (22)

with the property that

$$\frac{\sum_i x_i}{\sum_i |x_i|} \sim \exp(-c \cdot V \cdot T),$$ \hfill (23)

where $V$ is the volume, $T$ is the Euclidean time, and $c$ is a positive constant. We will refer to this term as the cancellation ratio. The exponential dependence on $V$ and $T$ makes computations difficult even for small systems.
The sign problem will affect the calculation of \( B_n \) in the stochastic Lanczos algorithm and terms in the series method discussed in the previous section. The effect however is different from the sign problem in typical Monte Carlo Green’s function calculations. Stochastic error correction is a calculation of eigenvalues and eigenvectors rather than a sampling of the partition function or the time evolution of a given initial state. Therefore the quantity of interest is not \( \exp(-HT) \) but the action of \( H \) or \( H^n \) on approximate eigenvectors of \( H \). Due to homogeneity in \( H \) the explicit volume dependence does not appear in the cancellation ratio. Instead we find

\[
\sum_i \frac{x_i}{|x_i|} \sim \exp(-k \cdot n),
\]

where \( k \) is a positive constant. The sign problem will return if the starting point of the SEC calculation is very poor and it becomes necessary to use \( n \) such that \( k \cdot n \) is large. However in many cases \( k \cdot n \) can be kept small even for large \( n \) since the most important part of the Hamiltonian, \( PSHP_S \), is diagonalized exactly. In short the sign problem is less severe because stochastic error correction uses the result of subspace diagonalization as its starting point.

4 \( \phi^4 \) theory in 2 + 1 dimensions

The first example we consider is \( \phi^4 \) theory in 2 + 1 dimensions near the \( \phi \rightarrow -\phi \) symmetry restoration phase transition. We will use QSE diagonalization and the series version of stochastic error correction to probe the low energy spectrum of the theory on both sides of the phase transition.

In [3] Magruder demonstrated the existence of a phase transition in \( \phi^4_{2+1} \) by extending Chang’s duality argument for \( \phi^4_{1+1} \). The statement of the main result is as follows. Consider the two Lagrange densities

\[
\mathcal{L}_+ = \frac{1}{2} \partial_\nu \phi \partial^\nu \phi - \frac{1}{2} \mu^2 \phi^2 + \frac{3}{4} \phi^4 + \frac{1}{2} \delta^2 \phi^2
\]

\[
\mathcal{L}_- = \frac{1}{2} \partial_\nu \phi \partial^\nu \phi + \frac{1}{2} \mu^2 \phi^2 - \frac{3}{4} \phi^4 + \frac{1}{2} \delta^2 \phi^2.
\]

The counterterm \( \delta^2 \) is defined so that in the \( \mathcal{L}_+ \) system the \( \phi \) self-energy graphs vanish at zero-momentum up to two-loop order. By shifting the field

\[
\phi = \phi' + \sqrt{\frac{3 \mu^2}{g}}
\]

we note that the same counterterm \( \delta^2 \) (same mass dependence but \( \mu_+ \) replaced by \( \mu_- \)) is also sufficient to renormalize \( \mathcal{L}_- \). By equating \( \mathcal{L}_+ \) and \( \mathcal{L}_- \) we obtain a duality constraint between the two theories. One feature of this constraint is that the \( g \rightarrow \infty \) limit of \( \mathcal{L}_- \) is mapped to the \( g \rightarrow 0 \) limit of \( \mathcal{L}_+ \). Therefore \( \mathcal{L}_- \), whose reflection symmetry \( \phi \rightarrow -\phi \) is broken at small \( g \), must eventually reach the symmetric phase for sufficiently large coupling.

The \( \mathcal{L}_- \) phase transition was studied using quasi-sparse eigenvector diagonalization with stochastic error correction. Quantities such as the critical coupling, critical exponents, and the low lying energy spectrum were studied and, where possible, compared with Monte Carlo results. A full discussion methods and results are presented in [3]. We will very briefly summarize some of the results below.

The two spatial dimensions of our system are taken to be a periodic box of size \( 2L \) by \( 2L \). We will use the modal field formalism to describe the Hamiltonian for the theory. In the following we let the vectors \( \vec{n} \) represent ordered integer pairs \((n_x, n_y)\) such that \(|n_x|, |n_y| \leq N_{\text{max}}\). The parameter \( N_{\text{max}} \) corresponds with a momentum cutoff scale of \( \Lambda = N_{\text{max}} \pi / L \). The modal field Hamiltonian has the form\(^1\).

\(^1\)The \( g \rightarrow \infty \) limit of \( \mathcal{L}_+ \) is mapped to the \( g \rightarrow \infty \) limit of \( \mathcal{L}_- \) and so there is no analogous argument for a phase transition in \( \mathcal{L}_+ \). Numerical calculations indicate that there is no phase transition for \( \mathcal{L}_+ \)\(^2\).

\(^2\)We refer the reader to [3] for a short introduction.

\(^3\)Counterterms were calculated using finite volume perturbation theory.
\[ H = \sum _{\vec{n}} \left[ -\frac{1}{2} \partial_{\vec{q}_{\vec{n}}} \partial_{\vec{q}_{\vec{n}}} + \frac{1}{2} \left( \frac{\vec{q}^2}{L^2} - \frac{\mu^2}{2} \right) - \frac{\phi \partial_{\vec{q}}}{(2L)^2} + \frac{48}{(2L)^4} \left( \frac{\vec{q}}{4!} \right)^2 \alpha_{\vec{n}} \right] q_{\vec{n}}^2 \]  \tag{28}

where

\[ b = \sum _{\vec{n}} \frac{1}{2\omega_{\vec{n}}}, \quad \omega_{\vec{n}} = \sqrt{\vec{n}^2 + \mu^2}, \]  \tag{29}

and

\[ \alpha_{\vec{n}} = \sum _{\vec{n}_1, \vec{n}_2} \frac{1}{4\omega_{\vec{n}_1}\omega_{\vec{n}_2}\omega_{\vec{n}_1-\vec{n}_2}(\omega_{\vec{n}_1} + \omega_{\vec{n}_2} + \omega_{\vec{n}_1-\vec{n}_2})}. \]  \tag{30}

In Figure 1 we have plotted the lowest energy eigenstates in the rest frame for \( N_{\text{max}} = 10 \) and \( L = 3\pi \) (in units where \( \mu = 1 \)). This choice of parameters corresponds with 441 different momentum modes and a momentum cutoff scale of \( \Lambda = 3.33\mu \). The states shown in Figure 1 are the three lowest eigenstates in the even and odd \( \phi \rightarrow -\phi \) symmetry sectors, and the energies are measured relative to the ground state energy. In our calculation QSE diagonalization was used keeping 500 Fock states, and the stochastic error correction was computed to first-order using the series method. Error bars shown include statistical error and an estimate of the contribution from higher order corrections. We see clear evidence of a second-order phase transition near \( g = 0.9 \). We have labelled the energies of the states according to their physical interpretation in the symmetric phase. \( E_1 \) is the energy for the one-particle state, \( E_2 (E_3) \) is for the two(three)-particle threshold, and \( E_2' (E_3') \) is for the first state above the two(three)-particle threshold. At finite volume these energies are continuous functions of the coupling \( g \). One feature which was also observed in \( \phi^4_{1+1} \) is the crossing of energy levels due to the double degeneracy of states in the broken symmetry phase. \( E_3 \) is connected to a one-particle state in the broken phase while \( E_2' \) is connected to a two-particle state. The levels \( E_2' \) and \( E_3 \) therefore cross near the critical point.

Another interesting phenomenon is the appearance of a bound state in the broken symmetry phase. In both the odd and even symmetry sectors we can measure the ratio of the two-particle to one-particle energies:

| \( \frac{x}{\pi} \) | \( \frac{E_2'}{E_2} \) | \( \frac{E_3'}{E_3} \) |
|---|---|---|
| 0.2 | 2.01(4) | 1.98(4) |
| 0.3 | 2.01(4) | 2.05(4) |
| 0.4 | 1.95(4) | 1.96(4) |
| 0.5 | 1.87(4) | 1.87(4) |
| 0.6 | 1.86(4) | 1.82(4) |

These results are consistent with the binding energies reported in \( \text{[10]} \) and \( \text{[11]} \), which indicate a ratio of 1.83(3) near the critical point.

5 Compact U(1) in 2+1 dimensions

Compact U(1) lattice gauge theory in 2+1 dimensions is a simple but phenomenologically interesting gauge model. It is asymptotically free and in the usual continuum limit describes massless non-interacting photons. On the other hand if the continuum limit is reached by rescaling the mass gap to remain constant, one instead finds a confining theory of massive bosons \( \text{[13]} \). The Hamiltonian has the form:

\[ H = -\sum _i \frac{\partial^2}{\partial \vec{A}_i^2} - 2x \sum _p \cos \theta _p. \]  \tag{31}

\[ \text{A more complete discussion of the critical coupling as well as critical exponents can be found in \([12]\).} \]
In (31) $A_l$ are link gauge fields, $\theta_P$ is the sum of the links circuiting a plaquette,

$$\theta_P = A_{l_1} + A_{l_2} - A_{l_3} - A_{l_4},$$

and

$$x = e^{-4a^{-2}}$$

is the strong coupling parameter, which tends to infinity as the lattice spacing $a$ goes to 0. We follow the notation of [10] in which an overall constant factor of $\frac{e^2}{2}$ multiplying the right-hand side of (31) is suppressed. The energy levels we measure are therefore in units of $\frac{e^2}{2}$.

The diagonalization of lattice gauge Hamiltonians is constrained by the requirements of gauge invariance. To preserve gauge invariance it is most convenient to use a basis which diagonalizes the electric field part of the Hamiltonian

$$\left[-\sum_l \frac{\partial^2}{\partial A_l^2}\right] \bigotimes_{\nu} |n_{\nu}\rangle \cdots = \left[\sum_l n_l^2\right] \bigotimes_{\nu} |n_{\nu}\rangle.$$  

As our next example of stochastic error correction we will address the $4 \times 4$ lattice system at $x = 1$ using this electric field basis. In [11] it was noted that this poses a challenge to standard diagonalization techniques. Even on the small $4 \times 4$ lattice a surprisingly large number of states, about $10^7 \sim 10^8$, are needed to accurately describe the low energy spectrum at $x = 1$. This problem can be circumvented by modifying the basis states to incorporate more of the physics of the ground state. For example one can introduce a disordered background of magnetic flux as suggested in [14], and that approach is followed in an ongoing project [15]. However we would like to directly address the problem described in [11] and show how the stochastic Lanczos method handles the proliferation of large numbers of basis states in the original electric field basis.

We will choose our starting subspace $S$ to include all basis states

$$\bigotimes_{\nu} |n_{\nu}\rangle$$

which satisfy

$$\sum_l n_l^2 \leq 8,$$

and which can be reached from the strong coupling vacuum by at most two transitions via the plaquette operators $\exp(\pm i\theta_P)$. We take the auxiliary space $Z$ to be the subspace spanned by basis vectors

$$\sum_l n_l^2 \leq L_{\text{max}}^2.$$  

Using matrix diffusion Monte Carlo, we diagonalize the subspace formed by the states

$$|d, j\rangle = [P_Z(H - a)P_Z]^d |j\rangle.$$  

$|j\rangle$ are the eigenvectors of the Hamiltonian restricted to the original subspace $S$. In our calculations we use $a = L_{\text{max}}^2$ and $d = 0, 1, \cdots 12$ for cutoff values,

$$L_{\text{max}}^2 = 24, 28, 32.$$  

In Table 2 we show the results for the ground state energy $E_0$ for the different cutoff values $L_{\text{max}}^2$ and the extrapolated value at $L_{\text{max}}^2 = \infty$. The errors shown are estimated statistical errors. For comparison we show the results of [10] obtained using Green’s function Monte Carlo (GFMC).
Fermion sign problems render Monte Carlo simulations ineffective for the Hubbard model. The difficulties associated with finding the ground state of the model are substantial even for small systems. The summation \( <i,j> \) is over nearest neighbor pairs. \( c_{i\sigma}^\dagger (c_{i\sigma}) \) is the creation (annihilation) operator for a spin \( \sigma \) electron at site \( i \). \( t \) is the hopping parameter, and \( U \) controls the on-site Coulomb repulsion. The model has attracted considerable attention in recent years due to its possible connection to \( d \)-wave pairing and stripe correlations in high-\( T_c \) cuprate superconductors. In spite of its simple form, the computational difficulties associated with finding the ground state of the model are substantial even for small systems. Fermion sign problems render Monte Carlo simulations ineffective for \( U \) positive and away from half-filling, and the collective effect of very large numbers of basis Fock states make most diagonalization approaches very difficult. A brief overview of the history and literature pertaining to numerical aspects of the Hubbard model can be found in [16].

In terms of momentum space variables, the Hubbard Hamiltonian on an \( N \times N \) periodic lattice has the form

\[
H = -t \sum_{<i,j>: \sigma=\uparrow,\downarrow} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}).
\]

The results we find appear in agreement with [10]. Unlike most Monte Carlo algorithms, the SEC method is able to find excited states with the same quantum numbers as lower lying states. This was also evident in the \( \phi_{2+1}^4 \) example where we could track many different states crossing the phase transition. The reason for this advantage goes back to the design of stochastic error correction as a Monte Carlo improvement of a diagonalization scheme. For the \( U(1) \) example one can reliably find the eigenvalues and eigenvectors for the first twenty or so states in the low energy spectrum.

## 6 Hubbard Model

The last example we consider is the two-dimensional Hubbard model defined by the Hamiltonian

\[
H = \sum_{<i,j>,\sigma=\uparrow,\downarrow} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}).
\]

The summation \( <i,j> \) is over nearest neighbor pairs. \( c_{i\sigma}^\dagger (c_{i\sigma}) \) is the creation (annihilation) operator for a spin \( \sigma \) electron at site \( i \). \( t \) is the hopping parameter, and \( U \) controls the on-site Coulomb repulsion. The model has attracted considerable attention in recent years due to its possible connection to \( d \)-wave pairing and stripe correlations in high-\( T_c \) cuprate superconductors. In spite of its simple form, the computational difficulties associated with finding the ground state of the model are substantial even for small systems. Fermion sign problems render Monte Carlo simulations ineffective for \( U \) positive and away from half-filling, and the collective effect of very large numbers of basis Fock states make most diagonalization approaches very difficult. A brief overview of the history and literature pertaining to numerical aspects of the Hubbard model can be found in [16].

In terms of momentum space variables, the Hubbard Hamiltonian on an \( N \times N \) periodic lattice has the form

\[
H = -2t \sum_{p_x,p_y=0,\cdots,N-1} \left( \cos \frac{2\pi p_x}{N} + \cos \frac{2\pi p_y}{N} \right) \left[ c_{p_x,p_y}^\dagger c_{p_x,p_y}^\dagger + c_{p_x,p_y}^\dagger c_{p_x,p_y}^\dagger \right] + \frac{U}{N^2} \sum_{p_x+q_x+r_x+s_x=0 \mod N, \ \ p_y+q_y+r_y+s_y=0 \mod N} \left[ c_{p_x,p_y}^\dagger c_{q_x,q_y}^\dagger c_{r_x,r_y}^\dagger c_{s_x,s_y}^\dagger \right]
\]

As a test of our methods, we use QSE diagonalization with stochastic error correction to find the ground state energy of the \( 4 \times 4 \) Hubbard model with 5 electrons per spin. The corresponding Hilbert space has about \( 2 \cdot 10^7 \) dimensions. For the QSE diagonalization we use momentum Fock states which diagonalize the quadratic part of the Hamiltonian. The Hamiltonian is invariant under the symmetry group generated by

| \( L_s^2 \) | \( L_s^2 = 24 \) | \( L_s^2 = 28 \) | \( L_s^2 = 32 \) | \( L_s^2 = \infty \) | GFMC |
|---|---|---|---|---|
| \( E_0 \) | \(-7.39(3)\) | \(-7.430(3)\) | \(-7.438(3)\) | \(-7.442(4)\) | \(-7.4432(5)\) |

In Table 3 we show the masses for the lightest six particles in the system extrapolated to the limit \( L_s^2 = \infty \). We have labelled the particles according to their spin \( J \) and sign under conjugation \( C : A \rightarrow -A \). We also include results from [10] for the lowest antisymmetric and symmetric glueballs.

| \( J^\pm \) | Mass | GFMC |
|---|---|---|
| \( |0^+\rangle \) | 3.03(2) | 3.01(6) |
| \( |0^+\rangle \) | 4.03(3) | 4.05(8) |
| \( |2^-\rangle \) | 6.8(1) | |
| \( |2^+\rangle \) | 6.8(1) | |
| \( |0^+\rangle \) | 7.0(2) | |
| \( |0^-\rangle \) | 7.1(2) | |
reflections about the $x$ and $y$ axes, interchanges between $x$ and $y$, and interchanges between $\downarrow$ and $\uparrow$. We find it convenient to work with symmetrized Fock states. We will compute stochastic error corrections to first order using the series method.

In Table 4 we present results for the ground state energy. We encountered no trouble with the sign problem, and in fact one can easily see that each term in the first order series expression (7) is negative definite. The energies are measured relative to the energy of the Fermi sea at $U = 0$. The errors reported are statistical errors associated with the first order SEC calculation. Where available, we compare with the results presented in [18], which we label as Exact, Projector Quantum Monte-Carlo (PQMC), and Stochastic Diagonalization (SD). Stochastic diagonalization is a subspace diagonalization technique similar to QSE but one which uses a different method for selecting the subspace and is based on a variational principle [19]. Although the precise number of basis states used in the SD calculations is not listed, we infer from numbers reported for a modified $4 \times 4$ Hubbard system that roughly $10^5$ states were used.

| Coupling | States | QSE   | QSE+SEC | Exact   | SD    | PQMC  |
|----------|--------|-------|---------|---------|-------|-------|
| $U = 2t$ | 100    | -.4797| -.50147(5)| -.50194 | -.5010| -.44(5)|
|          | 500    | -.4945| -.50181(3)|         |       |       |
|          | 1000   | -.5006| -.50198(1)|         |       |       |
|          | 100    | 1.620 | 1.8113(4) |         |       |       |
|          | 500    | 1.748 | 1.8242(3) |         |       |       |
|          | 1000   | 1.800 | 1.8302(1) |         |       |       |
| $U = 4t$ | 500    | 2.558 | 2.7073(4) | -2.7245 | -2.723| -2.9(3)|
|          | 1000   | 2.651 | 2.7208(2) |         |       |       |
|          | 2000   | 2.685 | 2.7231(1) |         |       |       |
| $U = 5t$ | 500    | 2.558 | 2.7073(4) |         |       |       |
|          | 1000   | 2.651 | 2.7208(2) |         |       |       |
|          | 2000   | 2.685 | 2.7231(1) |         |       |       |

Apparently QSE diagonalization with SEC handles the $4 \times 4$ system quite well with relatively few states. Much larger systems are being studied using both higher series corrections and stochastic Lanczos techniques [7].

7 Summary and comments

In this paper we presented two versions of stochastic error correction, the series method and the stochastic Lanczos method. The series method starts with eigenvectors of the Hamiltonian restricted to some optimized subspace and includes the contribution of the remaining basis states as an ordered expansion. The stochastic Lanczos method starts with eigenvectors of a Hamiltonian submatrix and constructs matrix elements of Krylov vectors using matrix diffusion Monte Carlo. This method has the advantage that the starting vectors need not be close to exact eigenvectors.

We presented three different examples which demonstrate the potential of the new approach for strongly coupled scalar, gauge, and fermionic theories. In the first example we calculated the low energy spectrum of $\phi^4_{2+1}$ using the series method, and in the second example we found the spectrum of compact $U(1)$ in $2 + 1$ dimensions using the stochastic Lanczos method. In both examples we found agreement with results from the literature. We also found that unlike typical Monte Carlo results, the SEC method is able to find the eigenvalues and eigenvectors for excited states with the same quantum numbers as lower lying states. This advantage is due to its design as a Monte Carlo improvement of a diagonalization scheme. In the last example we found the ground state of the $2 + 1$ dimensional Hubbard model using QSE diagonalization and first order series stochastic error correction. In this calculation we encountered no fermion sign problem and found that our methods yielded very accurate results with far less effort than existing techniques. We believe that the methods we have presented hold considerable potential for studying a wide range of non-perturbative quantum systems and answering questions difficult to address using other methods.

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5 The discrete symmetries of the system were not utilized in their calculations.
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Figure 1: Energy eigenvalues as functions of $g/4!$ as calculated by QSE diagonalization with first-order error corrections.