Cluster diagonalization in systematically expanded Hilbert spaces: application to models of correlated electrons

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Abstract

A method of cluster diagonalization in a systematically expanded Hilbert space is described. We discuss some applications of this procedure to models of high-$T_c$ superconductors, like the $t - J$ and one and three bands Hubbard models in two dimensions. The results obtained with this method are compared against results obtained with other techniques dealing with truncated
Hilbert spaces. The relation between this method of diagonalization in a reduced Hilbert space, and perturbation theory and variational techniques is also discussed.

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1 Introduction

Since the discovery of high-$T_c$ superconductivity,$^1$ intensive theoretical work has been carried out to understand its properties. Much of this effort was devoted to the analysis of two dimensional electronic models,$^2$ in particular, the Hubbard$^3$ and $t-J$ models.$^4$ In spite of their apparent simplicity, these models are very difficult to study with analytical techniques. Actually, there are no exact solutions of these models except in one dimension (and even in this case, for the $t-J$ model only $J = 0$ and $J = 2t$, i.e. the supersymmetric point, can be solved exactly). In the parameter regime of interest for high-$T_c$ superconductivity, these models can be regarded as strongly correlated electronic systems. It is well known that most analytical methods, like Hartree-Fock$^5$ or RPA approximations, which are reliable for weak coupling systems, have difficulties in dealing with strongly correlated electrons. The same problem arises in approximations like slave boson mean-field techniques.$^6$ In particular, for the $t-J$ model it is not easy to decouple the charge and spin degrees of freedom.

One should also note that in mean field calculations it is necessary to make assumptions about ground state properties. Numerical methods, on the other hand, are not biased by any “a priori” assumptions, and they have provided much of the reliable information available for these models, as well as a useful check of predictions formulated by analytical approximations. Among the most widely used numerical techniques are the Monte Carlo algorithms.$^7$ In particular, the version that uses the Hubbard-Stratonovich transformation has been applied to the Hubbard model$^8$ and
several important results have been obtained. An alternative to Monte Carlo techniques is the Lanczos method \(^9\) which essentially gives the ground state of a given model for a finite lattice. From the ground state, we can compute all static and dynamical properties, and in this sense, we obtain a complete characterization of a model at zero temperature except for finite size effects.\(^{10}\)

This technique has provided important information about models of correlated electrons. For example, let us consider a very recent work\(^{11}\) where the \(t - J\) model at quarter filling has been studied. In this work, strong signals of \(d_{x^2-y^2}\) superconductivity close to the phase separation border were found. These indications come from the study of pairing correlations, Meissner effect and flux quantization in the \(4 \times 4\) lattice. At quarter filling there are an equal number of holes and electrons and we expect that at this point the finite size effects are small. However, if we consider the region physically relevant for high-\(T_c\) superconductivity which is close to half filling (doping fraction \(x \approx 0.10\)), the number of holes is very small (2 for the \(4 \times 4\) lattice) and then we would expect a weak signal for hole superconductivity. Actually, most of the exact diagonalization studies of the \(t - J\) model on this lattice, using realistic couplings, have not found any indications of superconductivity. Then, in order to study the phase diagram of the \(t - J\) model, its properties, and the relation superconductivity-phase separation in the physically relevant region, it appears to be necessary to analyze larger clusters. However, the 32 sites lattice with 4 holes requires the diagonalization of a matrix of \(\sim 2.25 \times 10^{10}\) states, which is unreachable
with present-day computers. Similar Hamiltonian matrix dimensions appear in many other situations.

In this paper we want to stress the need for developing new methods in the context of diagonalization in a reduced basis set in order to answer quantitatively the important questions posed by models of high-$T_c$ superconductivity. There are strong reasons why we should attempt to improve diagonalization schemes, rather than other approaches like Monte Carlo methods. It is well known that Monte Carlo simulations of fermionic models present “the minus sign problem”, which makes very difficult the study of these systems at the physically interesting densities. It is also well known that there are difficulties in the analytical continuation procedure that is necessary to perform in Monte Carlo calculations of dynamical properties, and thus these techniques are not well developed. The diagonalization procedures are free from the minus sign problem, and as we mentioned at the beginning, all quantities static and dynamical, can be computed from the ground state. Thus, it is very important to extend these techniques to large clusters, and the attempt discussed in this paper corresponds to a systematic expansion of the Hilbert space.

2 Systematic expansion of the basis set

As it was described in the Introduction, the sizes of the Hilbert space necessary to study quantitatively problems relevant to high-$T_c$ superconductivity are considerably larger than the dimensions that can be reached with present computers (although
the currently available results for small clusters seem to be qualitatively reliable). In this context, here we want to show that significant results can be obtained by diagonalization of the Hamiltonian in a truncated or reduced Hilbert space.\textsuperscript{13} Some variations of this procedure have been used for many years in other fields such as chemical physics (see, for example, Ref. 14) where similar work has been recently discussed by Wenzel and Wilson.\textsuperscript{15}

The method of diagonalization in a truncated basis is of course justified only if a few coefficients \(x_i\) of the ground state:

\[
\Psi_0 = \sum_i x_i \phi_i, \tag{1}
\]

have significant weight. In some cases, fairly accurate properties of the ground state can be reached even with a small fraction of the total Hilbert space.

There are two questions that must be addressed to implement the proposed technique:

1. It is necessary to choose an appropriate basis \(\{\phi_i\}\) according to the physics of the problem. For example,

   \begin{itemize}
   \item real space \(S^z\) representation for the \(t-J\) model,
   \item momentum space representation for the one-band Hubbard model in weak coupling.
   \end{itemize}
2. The algorithm must be able to find the most significant states that contribute to the ground state wave function.

The outline of the method we have developed and present in this paper, which we call “systematic expansion of the Hilbert space” (SEHS), is the following:

1. start from as few as possible states chosen according to the expected behavior of the system (knowing quantum numbers of the ground state greatly simplifies the work);

2. at each step \( i \) expand the Hilbert space by applying the Hamiltonian, or at least part of it, to the current set of states;

3. diagonalize in the new enlarged Hilbert space using the Lanczos method;

4. retain the states with the largest weight, such that the dimension of the Hilbert space is \( N_i = \lambda N_{i-1} \), \( 1 < \lambda \leq 2 \) (“slow growth” approach);

5. go back to step 2 until convergence in the physical quantities is achieved, or until the largest available dimension in the computer is reached.

In an ideal situation, the states chosen at the starting point should correspond to those that carry most of the weight in the exact ground state. For some sets of parameters (couplings, densities) it is possible to guess these states. However, different sets of parameters may have different behaviors, and usually it is not possible to predict at which point the crossover between them will occur. For example, in the
$t-J$ model, for $J \gg t$ the holes are bound together in pairs, so we can take as starting point states where the holes are in nearest neighbor sites. On the other hand, for $J \ll t$ the holes are not bound and move around independently of each other and then it is not correct to take the same states as before as the initial state for the iterations. In this situation, the “pruning” of the Hilbert space retaining the most weighted states as indicated in point 4 is essential to improve or correct the initial starting set of states. As we discuss below, this procedure effectively works as a systematic method to obtain and improve variational states. Moreover, it allows the dimension of the Hilbert space to grow at a slow rate and the behavior of the energy results smoother than in the case of the straight application of the Hamiltonian. Below we will apply the proposed method to several cases relevant to theories of high-$T_c$ superconductors.

3 Study of the $t-J$ model

Let us apply the SEHS method to the $t-J$ model which is defined by the Hamiltonian:

\[
H = -t \sum_{<ij>,\sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma}) + J \sum_{<ij>} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j),
\]

where the notation is standard. The first term describes the hopping of holes or
kinetic energy, while the second one corresponds to the antiferromagnetic Heisenberg interaction. In this model the size of the Hilbert space grows roughly as $3^{N_s}$, where $N_s$ is the number of sites of the lattice, after taking into account the constraint of no double occupancy. In two dimensions (2D), this model has been studied at all fillings on the $4 \times 4$ cluster.\textsuperscript{10} Up to 2 holes, clusters of up to 26 sites have also been considered.\textsuperscript{16}

First, let us briefly discuss the application of this method to the two dimensional $t-J_z$ model\textsuperscript{17} which is obtained from the $t-J$ model by eliminating the spin exchange term in the Heisenberg interaction. Consider the case of one hole. In the limit of $J_z/t \gg 1$, the ground state of this model consists of a state in which the hole is located at an arbitrary site surrounded by an otherwise perfect Néel state. In this limit the dimension of the Hilbert space needed to get the physics of the problem is just equal to one (plus all states translationally equivalent). Now, as $J_z/t$ is reduced to the most interesting region, i.e. $J_z/t \leq 1$, the hole gains kinetic energy at the expense of magnetic energy and starts to move away from its initial position. As the hole hops, it leaves behind a trail of overturned spins called a “string”.\textsuperscript{18} As $J_z/t$ is lowered, one must take into account longer and longer strings. However the important string excitations are still of finite length, and then in this case it is enough to keep a fraction of the total Hilbert space to describe it. For this model, the application of the Hamiltonian, i.e. the hopping term, to expand the Hilbert space at each step has a direct physical meaning. As we have shown in a previous paper,\textsuperscript{17} it is possible
to converge to the ground state energy with several digits of accuracy by retaining a small fraction of the full Hilbert space. As an example, in Table I, the energy of the system for two holes is shown for a cluster of 50 sites and $J_z/t = 0.3$ as a function of the dimension of the Hilbert space. It is clear that the new technique works very well in this case. For more details see Ref. 17.

Let us now consider the $t - J$ model with the full Heisenberg interaction (Eq. (2)). In this case, even in the absence of holes, the ground state is characterized by the presence of spin wave excitations that reduce the antiferromagnetic order from its Néel (classical) value. Thus, in principle, we not only need to physically describe the modification of the spin background in the vicinity of the holes, but also the spin exchanges that take place at arbitrary distances from the holes which contribute significantly to the spin background. This qualitative difference between the $t - J$ and $t - J_z$ models can be detected by measuring the distribution of weights $S(x)$ defined as the sum of the weights $|x_i|^2$ belonging to the interval $[x, x + \Delta]$. In Fig.1, we show $S(x)$ in the exact ground state of the $4 \times 4$ lattice with two holes at $J_z = 0.6$ and $J = 0.6$ (in general we take $t=1$), for the $t - J_z$ (Fig.1a) and $t - J$ (Fig.1b) models, respectively. It can be seen that in the latter, there is more weight for very small absolute values of the coefficients $x_i$ of the ground state $\Psi_0$ (Eq. (1)).

Let us start the expansion of the Hilbert space from the same sets of states considered for the $t - J_z$ model. At each step, the Hilbert space is expanded by the application of both the hopping term and the spin exchange term of the Heisenberg
interaction. In the language of perturbation theory, this is like a double expansion around the Ising limit \((t - J_z)\) with static holes, namely one or two holes in an otherwise perfect Néel state. The expansion with the spin exchange term of the Heisenberg interaction could be regarded as a perturbation in the spin anisotropic parameter. In Figs. 2-5, we show results for the \(4 \times 4\) lattice. These can be compared with results for the exact ground state which can be easily computed. In Fig. 2, the energy is shown as a function of the dimension of the basis set, for two holes at \(J = 0.2\). The energies obtained with the “truncation” procedure (dot-dashed line) are much better than the energies obtained without it (dashed line) namely diagonalizing at step 3 of the method, but without truncating in step 4. As explained before, this improvement helps in discarding states with very small weight. Finally, both are much better than the energies obtained at each iteration of the conventional Lanczos algorithm (full line). In Fig. 3, the overlap between the variational wave functions in the truncated Hilbert space with the exact ground state are shown for both procedures with (dot-dashed line) and without (dashed line) the elimination of the less weighted states or “truncation”. In Fig. 4, the evolution of the hole-hole correlations at the maximum distance in this lattice is shown as a function of the dimension of the Hilbert space. It can be seen that the convergence with the “truncation” procedure is much faster than without it, even for correlation functions. The notation in these figures is the same as for Fig. 2. A similar behavior was also obtained for the spin-spin correlation at the maximum distance.
Finally, to complete the preliminary study on the $4 \times 4$ lattice, we show in Fig. 5 the energies obtained with the full basis set expansion procedure starting from the Néel state (curve labeled 0); from the Néel state and all the states obtained from it by one spin exchange (curve labeled 1); from the Néel state and all the states obtained from it by two spin exchanges (curve labeled 2); and so on. The energies at the beginning of each set correspond to the variational states discussed in Ref. 20. We see that the energies obtained with the new method starting from the Néel state are considerably better, even for a very small number of iterations, than those corresponding to Dagotto-Schrieffer’s variational states. As a conclusion, even though we cannot reach the ground state as accurately as we did for the $t - J_z$ model, we still can obtain a very good variational state compared with other states discussed in the literature for finite lattices.

Now let us discuss clusters that cannot be studied with the conventional Lanczos approach for lack of enough memory in present-day computers. We will show results obtained for the $t - J$ model on the $6 \times 6$ lattice with two holes, and $J = 0.4$. The dimension of the Hilbert space is, in this case, $2.55 \times 10^9$ states using translational and spin reversal symmetries. In Fig. 6, the energy is plotted as a function of the dimension of the Hilbert space (in a logarithmic scale). With a full line we show the energies obtained at each step of the conventional Lanczos algorithm, while with a dashed line we plot the energies obtained expanding the Hilbert space by applying the Hamiltonian, and at each step diagonalizing in the enlarged space using the Lanczos
method, i.e. steps 2 and 3 of the method described above. Finally, with circles and
diamonds, we show the points obtained by retaining the most weighted states, i.e.
step 4 of our method. The long-dashed line in zig-zag shows the order in which
every point is obtained starting with the circle at the top. It is clear that a better
convergence is achieved with the full procedure of the SEHS method. After reaching
the maximum dimension that can be handled with the available computer, it is also
possible to use an extrapolation procedure to extract results at the dimension of the
total Hilbert space, but we have not attempted such an analysis in the present paper.
(The energy for this particular system has been estimated with a Green’s Function
Monte Carlo technique\textsuperscript{21} to be near $\sim -20.0$.) In principle, one should also compute
other physical quantities of interest at each coupling, and then also extrapolate them
to the full dimension.

Presumably, we can attribute the slow convergence of the ground state energy
with the size of the Hilbert space to the highly nontrivial (and fluctuating) spin-
1/2 background. Then, the convergence is not going to deteriorate if we put more
holes on the lattice. On the other hand, Monte Carlo algorithms typically encounter
increasingly severe problems as the number of holes is increased, at least if one remains
close to half-filling. The number of off-diagonal transitions for both the hopping
(dashed line) and the exchange (full line) parts of the Hamiltonian as a function of
the number of states included in the basis set can be computed at each step. The
result is that successive sets generated during the process of enlargement of the Hilbert
space are increasingly more interacting, i.e. the Hamiltonian matrix becomes more dense (See, for example, Fig. 11 in Ref. 13.)

4 Application to the one-band Hubbard model

The one-band Hubbard model is defined by the Hamiltonian:

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

(3)

where the notation is standard. The size of the Hilbert space grows as $4^{N_s}$, and thus it is even more difficult to study than the $t-J$ model from a numerical point of view. In this case, the largest lattice considered in the literature is the $4 \times 4$ lattice for all dopings.\(^{10,22}\) In momentum space, the Hamiltonian of the Hubbard model takes the form:

$$H = \sum_{k,\sigma} \epsilon(k) c_{k,\sigma}^\dagger c_{k,\sigma} + U \sum_{k_1,k_2,k_3} c_{k_1,\uparrow}^\dagger c_{k_2,\uparrow}^\dagger c_{k_3,\downarrow}^\dagger c_{-k_1-k_2+k_3,\downarrow},$$

(4)

where each $k$ runs over the Brillouin zone. The single particle energies are given by $\epsilon(k) = -2t(\cos(k_x) + \cos(k_y))$. In the absence of Coulomb repulsion, the model reduces to a tight binding model which is easily solved. The total energy is the sum of the single particle energies for all the momentum $k$ up to the Fermi surface. Here,
we have to distinguish between two cases: the closed shell, in which the last shell is completely occupied; and the open shell in which the last shell is partially occupied. In the former case the ground state is not degenerate while in the latter the degeneracy can be very large. In the following, we concentrate on the $6 \times 6$ cluster with 18 ($9^\uparrow$ and $9^\downarrow$) and 26 ($13^\uparrow$ and $13^\downarrow$) electrons which correspond to closed shell situations. The dimensions of the Hilbert space for some closed shell cases in this cluster are: for 10 electrons, $3.95 \times 10^9$; for 18 electrons, $2.46 \times 10^{14}$; and for 26 electrons, $1.48 \times 10^{17}$ well beyond the reach of techniques that fully diagonalize the full Hilbert space of the problem.

For the closed shell situations, our initial Hilbert space consists of only one state, which is the ground state of the $U = 0$ case (remember that we are working in momentum space). The Hilbert space is expanded by applications of the second term of Eq. (4), which contains the off diagonal transitions. These terms create and annihilate pairs of electrons in such a way that the total momentum is conserved. In some other approaches the Hamiltonian is expanded through the creation of single pair electron-hole excitations but then the total momentum is not conserved. In the spirit of the general procedure outlined in Section 2, we expand the Hilbert space by applying the whole second term of Eq. (4). (Another possibility, which we have not yet fully explored, is to expand the Hilbert space by taking only transitions between the shells at both sides of the Fermi level, and then increase successively the number of shells involved.) The expansion of the Hilbert space by application of the
Coulomb term could also be considered as a weak-coupling perturbation expansion in a parameter which is proportional to $U$, but unlike other perturbation schemes, our procedure remains variational in the sense that the energy is always an upper bound to the exact ground state energy.

In Figs. 7 and 8, we show the convergence of the energy as a function of the dimension of the Hilbert space for 18 and 26 electrons respectively, and for several values of $U$. The energies are measured in units of $t$ as usual, and they have been shifted in order to fit them into the same plot and in order to compare their convergence. It can be observed that the convergence is faster the fewer the electrons, and as expected, the convergence is faster for smaller values of $U$. For example, for the case of 26 electrons, for $U = 2$ we obtain a value of -47.907, in good agreement with the Monte Carlo estimate of -47.87 ± 0.05, i.e. the new technique reaches the same accuracy as Monte Carlo methods.

The most important features in these plots are the presence of discontinuities in the derivative of the energy, and a “wrong” concavity of the curves (compared for example with the curvature in Figs. 5 and 6 of the $t - J$ model). We do not have an explanation for this behavior, although perhaps the long-range nature of the Coulomb interaction in momentum space may matter. The wrong curvature of the plots makes it difficult to assess the convergence of the energy and to perform an extrapolation procedure. The points at which there are discontinuities in the derivative are the points obtained by successive application of the Hamiltonian starting from the initial
state. All the other points are obtained by pruning these Hilbert spaces, and by applying the Hamiltonian to the reduced spaces. The somewhat strange behavior of the energy vs. the dimension of the Hilbert space is an artifact of the momentum representation chosen, and perhaps a manifestation of the shell structure of the tight binding limit.

In the interval considered, i.e. $U \leq 4$, we found that the convergence of the energies obtained by working in the momentum representation is much faster than the one obtained by working in real space. Presumably, the opposite is true for larger values of $U$.

Finally, in Table II we provide comparisons of our estimates with the results obtained using Quantum Monte Carlo techniques, as well as the results obtained with a stochastic implementation of the modified Jacobi method also referred to as "stochastic diagonalization" (SD).

To obtain the results quoted in this Table, $N_R \sim 2 \times 10^4$ important states were included in the SD calculation and a CPU time of $\sim 10^4$ seconds (for the $4 \times 4$ lattice) was required. This CPU time is also what is required by our method for $N_h \sim 10^6$. However, as reported in Ref. 28, and as it can be seen in Table II, the energy is not yet converged and presumably $N_R$ has to be increased by a factor of $\sim 10$ in order to obtain the same accuracy as our results. This translates to a factor of $\sim 100$ in the total CPU time, since in the SD algorithm the CPU time grows quadratically with $N_R$. Besides, from the results reported in Ref. 28, it is also evident that for the SD
method the convergence is more difficult for larger values of the Coulomb repulsion.
In summary, it seems that at least in its current implementation, the SD method is
more expensive than the SEHS method reported in this paper for a given accuracy.

5 Application to the three-band Hubbard model

Finally, and for completeness, we briefly consider the three-band Hubbard model
which contains the Coulomb on-site repulsion for both the copper and oxygen sites
($U_d$ and $U_p$ respectively), the energies of each ion ($e_d$ and $e_p$ for copper and oxygen ions), and a Coulomb repulsion between copper and oxygen ions, $V$.$^{29}$ We study the
$\sqrt{8} \times \sqrt{8}$ lattice (24 sites between oxygens and coppers) with two doped holes (10
fermions), and the following set of parameters: $U_d = 7$, $U_p = 0$, $e_p - e_d = 1.5$ and
$V = 3$. As the initial basis set, we took all the states with all the Cu sites having single
occupancy, and the remaining two holes located in O sites (also single occupied). This
is a good starting Hilbert space for the case $V = 0$, but as the algorithm itself has
shown it is not appropriate for all values of the parameters.

In Fig. 9, we show the results obtained using the Hilbert space expansion proce-
dure. The dashed lines show the order in which these points were obtained starting
from the circle at the top right in the same way as was explained in Fig. 6. In Fig.
10, the best points in the set of results shown in Fig. 9 are plotted with circles. In
a second stage, once we have reached $\sim 10^6$ states, we go all the way back (points
indicated with full diamonds), finding that the initial guess was not appropriate (i.e.
the states with the highest weights were not those used in the starting Ansatz), and then we increase the dimension of the basis set again (empty squares). It can be seen that this last set of points behaves very smoothly and the final part of the curve is fairly flat indicating a reasonable convergence. From this set of states, in principle, we could compute all quantities of interest and eventually extrapolate them to the full Hilbert space. However, one should also notice that in this case the largest dimension that we have considered (∼ 2.5 × 10^6) is “only” two orders of magnitude smaller than the dimension of the full Hilbert space, and probably that is the reason for the good convergence of the results.

In Fig. 11 we compare the energies for \( V = 0 \) and \( V = 3 \) as a function of the dimension of the Hilbert space. The energies have been shifted for the sake of comparison. It can be seen that the convergence is better for the \( V = 3 \) case. For \( V = 0 \), following the Zhang-Rice construction, one can map this model to the one-band \( t - J \) model. It is then reasonable to assume that, as in this model, the spin background is responsible for the slow convergence.

The same pattern of convergence was also found for the other set of parameters we have studied: \( U_p = 3, e_p - e_d = 4, \) and \( V = 0, V = 3, \) and the same value of \( U_d = 7. \) In this case, for \( V = 3 \) the convergence is faster than for \( V = 0, \) reflecting the fact that it is easier for the algorithm to find the most relevant states which contain double occupied Cu sites.

Finally, we show in Fig. 12 the spin-spin correlation at the maximum distance on
the lattice, and the density of holes in Cu sites as a function of the dimension of the
Hilbert space for the set of parameters $U_d = 7$, $U_p = 0$, $e_p - e_d = 1.5$ and $V = 3$.
These curves indicate also a reasonable convergence. For this set of parameters we
obtain $n_{Cu} = 0.555$, while for $U_p = 3$, $e_p - e_d = 4$, $n_{Cu} = 1.088$, indicating the
presence of two different regimes for large $V$. This result might be relevant to some
speculation regarding the nature of pairing and phase separation in $Cu-O$ planes.$^{30}$

In any case, it is quite encouraging to observe that the new technique may work
well in the realistic (and complicated) case of the three-band Hubbard model.

6 Discussion and conclusions

The procedure described in this paper can be regarded as a method to generate
and/or improve variational wave functions. In the first place, it should be noted
that since no approximations are done on the Hamiltonian, and since we work in a
reduced Hilbert space, the energies obtained with this procedure are rigorous upper
bounds to the exact ground state energies. The application to the $t-J$ model is one
example in which the initial set of states is “corrected” by this algorithm. In this
case, a direct comparison with a variational state was also given (see also Ref. 19).
Another application in which the elimination at each step of the least weighted states
leads to an improvement or to a correction of the initial guess is the case of the three-
bond Hubbard model. In this case, the initial state depends on the parameters that
determine the \( Cu \) or \( O \) occupancy when the nearest neighbor Coulomb repulsion is large enough. In general, we believe that the technique is promising and may compete against more standard Lanczos and Quantum Monte Carlo methods, at least for some particular Hamiltonians and parameters. A clear example is the \( t - J_z \) model in which the new method has provided the more accurate results reported in the literature thus far\(^{17}\).

For the systems where we cannot arrive at a good approximation for the ground state due to the slow rate of convergence of the results (for example the \( t - J \) model seems to converge only logarithmically), one should resort to some extrapolation procedure to the full Hilbert dimension. In this sense, we are in the same situation as the zero temperature (Green’s function or random walk) Monte Carlo algorithms that cannot reach convergence before the noise becomes very high\(^{21}\).

Besides the possible applications of this reduced Hilbert space approach as indicated above, there are other situations that can also be studied with the SEHS method. One of them is the quarter-filled \( t - J \) model on the 26 sites lattice, which is interesting to study in order to analyze the finite size dependence of the results obtained in Ref. 11 in the context of superconductivity in the \( t - J \) model. The method can also be applied to coupled planes \( t - t_{\perp} - J \) model\(^{31}\). For this system, one could start from the best states of the ground state of each plane separately and then expand the basis set by application of the interplane hopping term of the Hamiltonian. This is equivalent to an expansion around \( t_{\perp}/t = 0 \).
Finally, we want to comment that there are other algorithms that also deal with truncated Hilbert spaces besides the stochastic diagonalization approach and the presently described technique. In an already mentioned paper, the Hubbard model was studied in momentum space with a truncation technique using concepts of renormalization group theory. Another stochastic truncation method has recently been developed for the $Z_2$ gauge model. The computational effort of the SEHS method of systematic expansion of the Hilbert space grows roughly linearly with $N_h$, and currently $N_h \sim 10^6$ for present-day computers. These other methods use a smaller size of the basis set, but the CPU time grows as $N_h^3$ for the methods of references [23] and [32], and quadratically in $N_h$ for the stochastic diagonalization algorithm.

Summarizing, a new algorithm has been discussed that has several of the advantages of the Lanczos approach (specially the possibility of studying dynamical responses), but that can be applied to large clusters. The method works remarkably well in some special cases, while in general it is competitive with other more standard algorithms.

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Table I

| $H_D$ | $E_{2h}$  |
|-------|-----------|
| 234   | -18.707940 |
| 696   | -18.882805 |
| 6204  | -19.026339 |
| 18416 | -19.052528 |
| 52672 | -19.066660 |
| 106435| -19.074957 |
| 212486| -19.079975 |
| 673640| -19.083531 |
| 980681| -19.084816 |
| 1502829| -19.085503 |
| 2249454| -19.085857 |

Table II

| method | 18 electrons | 26 electrons |
|--------|--------------|--------------|
| QMC    | -41.87±0.10  | -41.98±0.15  |
| SEHS   | -41.69       | -41.49       |
| SD     | -41.45       | -40.77       |
TABLE CAPTIONS

Table I

Energy $E_{2h}$ of two holes in the $t-J_z$ model, as a function of the size of the Hilbert space, $H_D$, for a cluster of 50 sites, and coupling $J_z/t = 0.3$.

Table II

Comparison between ground state energies (in units of $t$) obtained with the present method (SEHS), Quantum Monte Carlo (QMC), and Stochastic Diagonalization (SD), for the $6 \times 6$ lattice and $U = 4$. 
FIGURE CAPTIONS

**Figure 1** Distribution of weights $S(x)$ a) for the $t - J_z$ model, b) for the $t - J$ model on the $4 \times 4$ lattice with 2 holes and $J/t = 0.6$.

**Figure 2** Energy vs dimension of the Hilbert space for the $4 \times 4$ lattice with two holes, $J = 0.4$. The full curve corresponds to the energies obtained at each step of the conventional Lanczos iteration. The dot-dashed (dashed) corresponds to the procedure indicated in Sec. 3 with (without) including step 4.

**Figure 3** Overlap between the exact ground state and the states generated during the procedure of expansion of the Hilbert space. The meaning of the curves are as in Fig. 2.

**Figure 4** Hole-hole correlations at the maximum distance on the $4 \times 4$ lattice. The meaning of the curves are the same as for Fig. 2.

**Figure 5** Expansion of the Hilbert space starting from different initial basis sets for the $4 \times 4$ lattice with 2 holes and $J=0.2$. 
Figure 6 Energy vs dimension of the Hilbert space for the $6 \times 6$ lattice, 2 holes, $J=0.4$.

Figure 7 Energy of the Hubbard model on the $6 \times 6$ lattice with 18 electrons vs dimension of the Hilbert space. The asterisk indicate the Monte Carlo estimates.

Figure 8 Energy of the Hubbard model on the $6 \times 6$ lattice with 26 electrons vs dimension of the Hilbert space. The asterisk indicate the Monte Carlo estimates.

Figure 9 Energy of the three-band Hubbard model on the 8 cells square lattice as obtained by application of the SEHS procedure.

Figure 10 Energy of the three-band Hubbard model on the 8 cells square lattice vs the dimension of the Hilbert space. The open circle points correspond to the filled square points of Fig. 12. After reaching $\sim 10^6$ states, we truncate the Hilbert space in successive steps (diamonds), and then we start a new expansion of the basis set (squares).

Figure 11 Energy of the three-band Hubbard model on the 8 cells square lattice vs the dimension of the Hilbert space for different values of the intersite Coulomb repulsion $V$. 

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Figure 12 Spin-spin correlation at the maximum distance and density of holes at Cu sites for the three-band Hubbard model on the 8 cells square lattice vs the dimension of the Hilbert space.