Organization of the Hilbert Space for Exact Diagonalization of Hubbard Model

Medha Sharma and M.A.H. Ahsan

Department of Physics, Jamia Millia Islamia, New Delhi 110025, India

We present an alternative scheme to the widely used method of representing the basis of one-band Hubbard model through the relation $I = I_1 + 2M I_{\uparrow}$ given by H. Q. Lin and J. E. Gubernatis [Comput. Phys. 7, 400 (1993)], where $I_{\uparrow}$, $I_{\downarrow}$ and $I$ are the integer equivalents of binary representations of occupation patterns of spin up electrons, spin down electrons and both spin up and spin down electrons respectively; $M$ being the number of sites. We compute and store only $I_{\uparrow}$ or $I_{\downarrow}$ at a time to generate the Hamiltonian matrix. The non-diagonal part of the Hamiltonian matrix given as $I_{\uparrow} \otimes H_{\uparrow} \oplus I_{\downarrow} \otimes H_{\downarrow}$ is generated using a bottom-up approach by computing the small matrices $H_{\uparrow}$ (spin up hopping Hamiltonian) and $H_{\downarrow}$ (spin down hopping Hamiltonian) and then forming the tensor product with respective identity matrices $I_{\uparrow}$ and $I_{\downarrow}$, thereby saving significant computation time and memory. We find that the total CPU time to generate the non-diagonal part of the Hamiltonian matrix using the new one spin configuration basis scheme is reduced by about an order of magnitude as compared to the two spin configuration basis scheme.

keywords: Hubbard model, Exact diagonalization

I. INTRODUCTION

Hubbard model[1] was introduced as an approximate model for electron-electron interaction in narrow energy band system and serves as the simplest model that captures the essence of strongly-correlated electrons in solids. The one-band Hubbard model is

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

(1)

where $c_{i\sigma}^\dagger$, $c_{i\sigma}$ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ are fermion creation, annihilation and number operators respectively at site $i$ with spin $\sigma(\uparrow \text{ or } \downarrow)$. The angular bracket $\langle i, j \rangle$ denotes the sum over nearest neighbors. The first term of the Hamiltonian describes the kinetic energy of the itinerant electrons and the second term is the on-site Coulomb interaction.

High temperature cuprate superconductors have been described by three-band Hubbard model[2], but it has been argued that the essential physics can be captured by a one-band Hubbard model[3, 4].

An exact solution of Hubbard model in one dimension was given by Lieb and Wu[5] using Bethe Ansatz. The infinite lattice coordination limit introduced by Metzner and Vollhardt[6] forms the basis for the Dynamical Mean Field Theory (DMFT) that maps the Hubbard model onto an Anderson impurity model[7]. Except above two extreme cases, numerical methods are required despite the simplicity of the Hamiltonian and turns out to be quite formidable for any system of interest[8].

Exact Diagonalization (ED)[8][10] is an important technique for studying quantum many-body systems. It provides information about many-body correlations by giving an exact solution of the model albeit on finite lattices. It is a memory expensive technique, apart from being CPU intensive. ED solver is limited to small clusters because of large memory required for an exponentially growing Hilbert space. It also provides flexibility on parameters tuning. When used as an impurity solver in DMFT scheme, ED introduces parameterization of the effective bath which makes it superior to the Quantum Monte Carlo method[11]. Unlike Quantum Monte Carlo simulations at low temperatures, ED suffers no fermionic sign problem. With proper finite size scaling, it helps to gain insight into the many-body system in thermodynamic limit. ED is also advantageous in providing real-frequency information and serves as a check on approximate methods.

The scheme to generate the basis of one-band Hubbard model using both up and down spin was given by H. Q. Lin and J. E. Gubernatis[12] about two decades ago. Since then researchers have been using[13, 14] and recommending[15, 16] the two spin configuration basis, that involves (now) unnecessary computation time and memory requirements. Since in the Hubbard model, up spin and down spin do not mix with each other as no term in the Hamiltonian changes an up spin to a down spin and vice versa, we treat both spin bases in a many-body basis state separately while applying the Hamiltonian to them and present a new scheme that requires only one spin configuration basis at a time to generate the Hamiltonian matrix leading to significant gain in computation time and memory.

The contents of this paper are organised as follows. In section II., we describe the generation of basis states in our scheme. Section III. presents generation of the Hamiltonian matrix. In Section IV., we demonstrate the usefulness of our scheme in diagonalization of the Hamiltonian matrix. In Section V., we present some test runs to compare two-spin and one-spin basis schemes. Finally in section VI., we discuss the advantages of our scheme over the widely used two spin configuration basis scheme.
II. GENERATION OF BASIS STATES

The number operator:

$$N = \sum_i (n_{i\uparrow} + n_{i\downarrow}) = N_\uparrow + N_\downarrow$$  \hfill (2)

and the z-projection of the total spin:

$$S_z = \frac{1}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow}) = \frac{1}{2} (N_\uparrow - N_\downarrow)$$  \hfill (3)

both commute with the Hamiltonian \([11]\). For basis construction we use both these symmetries which is equivalent to conservation of total number of spin up \((N_\uparrow = \frac{1}{2} N + S^z)\) and total number of spin down \((N_\downarrow = \frac{1}{2} N - S^z)\) electrons. We perform diagonalization in a sector \((N_\uparrow, N_\downarrow)\) of total Hilbert space with fixed number of spin up electrons and of spin down electrons. Hilbert space for a sector \((N_\uparrow, N_\downarrow)\) can be constructed by forming the tensor product:

$$|V\rangle = |V^{N_\uparrow}\rangle \otimes |V^{N_\downarrow}\rangle$$  \hfill (4)

The basis states spanning \(|V\rangle\) map uniquely onto an integer \(I\) defined by \([12]\):

$$I = \sum_{i=1}^{M} (n_{i\uparrow} 2^{(i-1)} + n_{i\downarrow} 2^{(M+i-1)})$$  \hfill (5)

where \(n_{i\uparrow}\) and \(n_{i\downarrow}\) are the occupancies of site \(i\) for up spin and down spin respectively; \(M\) being the total number of sites. The basis state of \(|V\rangle\) is written as:

$$|V\rangle = I_\uparrow + 2^M I_\downarrow$$  \hfill (6)

where \(I_\uparrow = \sum_{i=1}^{M} n_{i\uparrow} 2^{(i-1)}\) is the spin up basis state of \(|V^{N_\uparrow}\rangle\) and \(I_\downarrow = \sum_{i=1}^{M} n_{i\downarrow} 2^{(M+i-1)}\) is the spin down basis state of \(|V^{N_\downarrow}\rangle\).

The bits of integer \(I\) represent a specific basis state:

$$|n_{\uparrow}(1), n_{\uparrow}(2), ..., n_{\uparrow}(M), n_{\downarrow}(1), n_{\downarrow}(2), ..., n_{\downarrow}(M)\rangle
= (c_{\uparrow\uparrow}^{1})^{n_{\uparrow}(1)} ... (c_{\uparrow\uparrow}^{M})^{n_{\uparrow}(M)} (c_{\downarrow\downarrow}^{1})^{n_{\downarrow}(1)} ... (c_{\downarrow\downarrow}^{M})^{n_{\downarrow}(M)} |0\rangle$$  \hfill (7)

Like the two-table method of Lin\([18]\), we store \(I_\uparrow\)s and \(I_\downarrow\)s separately. In our scheme, we assign serially ordered indices starting from 1 to spin up basis states spanning \(|V^{N_\uparrow}\rangle\) and to spin down basis states spanning \(|V^{N_\downarrow}\rangle\) and use a relation:

$$\text{Index} = (\text{Index}_\downarrow - 1) \text{count}_\uparrow + \text{Index}_\uparrow,$$  \hfill (8)

where \(\text{Index}\) = index of basis state \((I)\) of \(|V\rangle\), \(\text{Index}_\uparrow\) = index of spin up basis state \((I_\uparrow)\) of \(|V^{N_\uparrow}\rangle\), \(\text{Index}_\downarrow\) = index of spin down basis state \((I_\downarrow)\) of \(|V^{N_\downarrow}\rangle\), \(\text{count}_\uparrow\) = total number of basis states of spin up configuration spanning \(|V^{N_\uparrow}\rangle\). The algebraic relation \([5]\) give the index of \(I\) of \(|V\rangle\) in terms of index of \(I_\uparrow\) of \(|V^{N_\uparrow}\rangle\) and of \(I_\downarrow\) of \(|V^{N_\downarrow}\rangle\) respectively.

| Up | Basis_\uparrow | Index_\uparrow | Down | Basis_\downarrow | Index_\downarrow | Index_\downarrow |
|----|---------------|----------------|------|-----------------|----------------|----------------|
| 011 | 3             | 1              | 001  | 1               | 1              | 1              |
| 101 | 5             | 2              | 001  | 1               | 1              | 2              |
| 110 | 6             | 3              | 001  | 1               | 1              | 3              |
| 011 | 3             | 1              | 010  | 2               | 2              | 4              |
| 101 | 5             | 2              | 010  | 2               | 2              | 5              |
| 110 | 6             | 3              | 010  | 2               | 2              | 6              |
| 011 | 3             | 1              | 100  | 4               | 3              | 7              |
| 101 | 5             | 2              | 100  | 4               | 3              | 8              |
| 110 | 6             | 3              | 100  | 4               | 3              | 9              |

TABLE I. Spin up and down configurations, their bases, their indices and indices of the complete states representing both spin configurations for \(M = 3\) in a sector \((N_\uparrow = 2, N_\downarrow = 1)\).

For example, from table I, the spin up basis state \((|110\rangle\) of \(|V^{N_\uparrow}\rangle\) having \(\text{Index}_\uparrow = 3\) and spin down basis state \((|010\rangle\) of \(|V^{N_\downarrow}\rangle\) having \(\text{Index}_\downarrow = 2\) will result in a basis state \((|110\rangle |010\rangle\) of \(|V\rangle\) with an index=\((2+1)3+3=6\).

All the basis states spanning \(|V^{N_\sigma}\rangle\) where \((\sigma = \uparrow \text{ or } \downarrow)\) and their respective indices are generated using Algorithm I, given in Appendix \([\text{A}]\) which assumes the existence of a bit fiction \(\text{bittest}(i,j)\) that returns true if bit in position \(j\) of \(i\) is 1, else false; \(i\) and \(j\) being integers. Most of high level programming languages such as fortran 90 and C++ have intrinsic functions for bit wise operations on integers. For half filled \((N_\uparrow + N_\downarrow = M)\) sectors, the basis states spanning \(|V^{N_\sigma}\rangle\) can be obtained from the basis states spanning \(|V^{N_\sigma}\rangle\), where if \(\sigma = \uparrow\) \((\downarrow)\) then \(\overline{\sigma} = \downarrow\) \((\uparrow)\) using the following loop:

\[ g = 0 \]

\text{for } i = \text{count}_\sigma : -1 : f \text{ do}
\[ g = g + 1 \]
\[ oo = \text{basis}_\sigma(i) \]
\[ \text{basis}_\sigma(i) = \text{not}(\text{basis}_\sigma(g)) \]
\[ \text{basis}_\sigma(g) = \text{not}(oo) \]
\text{end}

where the function \(\text{not}(k)\) returns the logical compliments of the bits of integer \(k\) and \(f = \text{count}_\sigma + 1\) if \(\text{count}_\sigma\) is even and \(f = \text{count}_\sigma + 1\) if \(\text{count}_\sigma\) is odd.

Total number of basis states spanning \(|V^{N_\sigma}\rangle\) where \((\sigma = \uparrow \text{ or } \downarrow)\) i.e., \(\text{count}_\sigma\) is computed using the number of ways to distribute \(N_\sigma\) electrons among \(M\) sites.

$$\text{count}_\sigma = M C_{N_\sigma} = \frac{M!}{N_\sigma!(M - N_\sigma)!}$$  \hfill (9)

The dimensionality of Hilbert space of a given sector \((N_\uparrow, N_\downarrow)\) is

$$\text{dimension}_V = \text{count}_\uparrow \text{count}_\downarrow$$  \hfill (10)

but we are not required to generate \(I\)'s spanning the full Hilbert space \(|V\rangle\). We work only with \(I_\uparrow\)'s spanning \(|V^{N_\uparrow}\rangle\) or \(I_\downarrow\)'s spanning \(|V^{N_\downarrow}\rangle\) at a time.
III. GENERATION OF THE HAMILTONIAN MATRIX

When the Hamiltonian is applied to each of the basis states, the Hamiltonian matrix is generated.

A. Non-diagonal part of the Hamiltonian matrix

The non-diagonal part of the Hamiltonian matrix is due to the effect of hopping terms \( c_i^\dagger c_j + c_j^\dagger c_i \) that move an electron from site \( i \) to \( j \) or from \( j \) to \( i \).

For generation of the non-diagonal matrix elements the basis states spanning \( \mathcal{V}^N \) are required and only the total number of basis states spanning \( \mathcal{V}^N \sigma \), i.e., \( \text{count}_\sigma \) are required, where if \( \sigma = \uparrow (\downarrow) \) then \( \text{count}_\sigma = \downarrow (\uparrow) \).

1. Spin up hopping

We generate all the spin up basis states spanning \( \mathcal{V}^N \) (using Algorithm I, given in Appendix A) and compute the total number of spin down basis spanning \( \mathcal{V}^N \sigma \), i.e., \( \text{count}_\sigma \) using Eq. [9].

Let the action of \( \uparrow \) spin up hopping term change a state \( \text{basis}_\uparrow(p) \) to \( \text{basis}_\uparrow(l) \),

\[-t(c_i^\dagger c_j + c_j^\dagger c_i)\text{basis}_\uparrow(p) = -t(\text{esign})\text{basis}_\uparrow(l), \tag{11}\]

where \( \text{esign} \) takes care of the sign depending upon the number of occupied sites between the \( i \) and \( j \) sites, i.e., if an electron hops over an even number of electrons, \( \text{esign} = +1 \) and if it hops over an odd number of electrons, \( \text{esign} = -1 \). \( \text{Index}_\uparrow \) \( p \) is known and the \( \text{index}_\uparrow \) \( l \) can be found either by storing the indices of the basis states in a separate array while generating the basis states as in Algorithm I or by using a binary search.

All the elements of the Hamiltonian matrix due to this particular hopping between these two spin up basis states can be computed via a simple loop:

\[
\begin{align*}
\text{for } k = 1 : & \text{count}_\uparrow \\
& r = (k - 1)\text{count}_\uparrow + p \\
& s = (k - 1)\text{count}_\uparrow + l \\
& \text{matrix}(r, s) = -t(\text{esign})
\end{align*}
\]

where \( \text{matrix}(r, s) \) is the \((r,s)\)th element of the Hamiltonian matrix. All the matrix elements generated through this loop are obtained by applying a spin up hopping term to a spin up basis state and enable us to get rid of the repetitive application of the Hamiltonian everytime to get a matrix element.

The above procedure is repeated for each of the spin up hopping terms acting on each of the spin up basis states spanning \( \mathcal{V}^N \) to obtain all the matrix elements due to spin up hopping.

B. Diagonal part of the Hamiltonian matrix

The diagonal part of the Hamiltonian matrix is due to the onsite Coulomb interaction that counts the double occupancy of a site. The onsite interaction term \( U \sum \sigma \sum_i n_{\sigma i} n_{\sigma i} \) acting on a basis state gives the same basis state multiplied by the number of doubly occupied sites times \( U \).

For generation of diagonal matrix elements the basis states of only one configuration (\( \sigma = \uparrow \text{ or } \downarrow \)) spanning \( \mathcal{V}^N \sigma \) are required at a time.

All the diagonal elements of the Hamiltonian matrix can be computed using Algorithm II, given in Appendix B in which \( \text{matrix}(r, r) \) is the \((r,r)\)th element of the Hamiltonian matrix and \( U \) being the onsite interaction. In Algorithm II, if \((N_\uparrow + N_\downarrow) \leq M \) then \( \text{point}_\uparrow = M^{-1}C_{N_\uparrow - 1} \) \( \text{point}_\downarrow = M^{-1}C_{N_\downarrow - 1} \) is the total number of spin up(down) basis states of \( \mathcal{V}^N_\sigma (\mathcal{V}^N_\overline{\sigma}) \) in which any given site is occupied and if \((N_\uparrow + N_\downarrow) > M \) then \( \text{point}_\uparrow = M^{-1}C_{N_\uparrow} \) \( \text{point}_\downarrow = M^{-1}C_{N_\downarrow} \) is the total number of spin up(down) basis states of \( \mathcal{V}^N_\sigma (\mathcal{V}^N_\overline{\sigma}) \) in which any given site is unoccupied. In sectors where either \( N_\uparrow \) or \( N_\downarrow \) is equal to \( M \), all the diagonal elements are equal to \( U \) times \( \text{min}(N_\uparrow, N_\downarrow) \).
Algorithm II is much simplified for the Anderson impurity model \[19\]

\[
H_{\text{Anderson}} = \varepsilon_d \sum_{\sigma} d_\sigma^\dagger d_\sigma + \sum_{i,\sigma} \varepsilon_i a_i^\dagger a_i \sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{i,\sigma} (V_i a_i^\dagger d_\sigma + H.c.), \tag{13}
\]

where the onsite Coulomb interaction is only on one impurity site. DMFT that maps the Hubbard model onto Anderson impurity model uses it efficiently. Even the impurity Green’s function:

\[
G_{\text{imp}}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \langle \langle T_c(\tau)c(0)\rangle \rangle \tag{14}
\]

required for DMFT self consistency loop has been computed by generating the basis states of only one configuration ($\sigma = \uparrow$ or $\downarrow$) spanning $\mathcal{V}^N_{\sigma}$ at a time after solving the impurity model by Exact Diagonalization. The calculation of dynamical properties of a given Hamiltonian using Lanczos method by constructing a full continued fraction \[20\] has also been done by generating the basis states of only one configuration ($\sigma = \uparrow$ or $\downarrow$) spanning $\mathcal{V}^N_{\sigma}$ at a time. A full description of the method along with the analysis of the results will be published elsewhere.

IV. DIAGONALIZATION OF THE HAMILTONIAN MATRIX

After generating the Hamiltonian matrix we diagonalize it to find the eigenvalues and eigenvectors. Owing to the sparseness of the Hamiltonian matrix and the fact that we are interested in the eigenvalues and eigenvectors of the ground state and a few low-lying excited states only, we can use the Lanczos method \[21\] of diagonalizing large, sparse, symmetric matrices. For using the Lanczos algorithm, the matrix does not have to be constructed explicitly, since only its application to a vector is needed to compute the span of the Krylov subspace $K_j(H, q) = q, Hq, ... , H^{j-1}q$. The main computational step in the Lanczos algorithm is the matrix-vector multiplication without having an explicit representation of the matrix. One way is to have some functional representation of the matrix taking its repeating patterns into account so that it can be applied to a vector and the other way is to compute the Hamiltonian matrix every time as and when required. Our scheme will be useful in both the cases.

A. Storage of the nonzero elements of Hamiltonian matrix for matrix-vector multiplication

In each row of the sparse Hamiltonian matrix, there are very few nonzero elements. For the one-band Hubbard model on an one-dimensional ring of $M$ sites, considering only the nearest-neighbours hopping, the Hamiltonian matrix in any given row will have at the most $2M$ nonzero off-diagonal elements; $M$ elements due to the hopping terms of either spin configuration $\sigma(\uparrow$ or $\downarrow$). For an Anderson impurity model on an $M$ site lattice in which the transition is possible between the impurity site and the bath constituted by all other sites, each row of the Hamiltonian matrix will have a maximum of $2M - 2$ nonzero off-diagonal elements; $M - 1$ elements due to the hopping terms of either spin configuration $\sigma(\uparrow$ or $\downarrow$). Let $P$ be the maximum number of finite off-diagonal matrix elements in any given row of the Hamiltonian matrix. For an $R \times R$ matrix, there is an effective $R \times (P + 1)$ matrix, where $R = \text{count}_\uparrow \times \text{count}_\downarrow$

In our scheme both spin up and spin down bases are treated separately.

The diagonal elements of the Hamiltonian matrix corresponding to

\[
H_U = U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{15}
\]

can be generated on-the-fly by storing the integer arrays $\text{index}_U\uparrow$ and $\text{index}_U\downarrow$ of maximum dimension $(M^2/2)$ for even $M$ and $(M, (M-1)^2/2)$ for odd $M$ \cite{Algorithm II, Appendix}\[13\].

By applying the spin up hopping terms to each of the spin up basis states spanning $\mathcal{V}^N\uparrow$, the following Hamiltonian:

\[
H_\uparrow = -t \sum_{<i,j>} (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{j\uparrow} c_{i\uparrow}) \tag{16}
\]

matrix can be generated having effective dimension $\text{count}_\uparrow \times (P/2)$.

Similarly by applying the spin down hopping terms to each of the spin down basis states spanning $\mathcal{V}^N\downarrow$, the following Hamiltonian:

\[
H_\downarrow = -t \sum_{<i,j>} (c^\dagger_{i\downarrow} c_{j\downarrow} + c^\dagger_{j\downarrow} c_{i\downarrow}) \tag{17}
\]

matrix can be generated having effective dimension $\text{count}_\downarrow \times (P/2)$.

The Hubbard Hamiltonian in matrix representation is mathematically given as:

\[
H = \mathcal{I}_\downarrow \otimes H_\uparrow + H_\downarrow \otimes \mathcal{I}_\uparrow + \mathcal{I}_\uparrow \otimes H_U, \tag{18}
\]

where $\mathcal{I}_\uparrow(\mathcal{I}_\downarrow)$ is the identity operator for electrons with spin up(down). Using our scheme we directly obtain the matrices $H_\uparrow$ and $H_\downarrow$ respectively.

Total number of non-zero matrix elements in $H_\uparrow$ where ($\sigma = \uparrow$ or $\downarrow$) is $P \times M^2 - 2C_{N_{\sigma} - 1}$, where $M > 2$ and $0 < N_{\sigma} < M$. Thus number of non-zero matrix elements in $H$ become $P \times M^2 - 2C_{N_{\uparrow} - 1} \times \text{count}_\uparrow + P \times M^2 - 2C_{N_{\downarrow} - 1} \times \text{count}_\downarrow + \text{count}_\uparrow \times \text{count}_\downarrow$, where $M > 2$, $0 < N_{\uparrow} < M$ and $0 < N_{\downarrow} < M$.\[14\]
Since the matrices $H_\uparrow(H_\downarrow)$ are hermitian, we are required to compute and store the symmetric half of their non-zero elements, say the upper triangle or the lower triangle of matrix elements. We store the $esign_\sigma$ (sign of the matrix element depending upon the number of occupied sites between the transition sites as explained earlier) of all the non-zero elements of $H_\sigma$ row-wise in a 1D integer array $nlink_\sigma$ of length $P/2 \times M^2 C_{N_\sigma - 1}$ for $M > 2$ and $0 < N_\sigma < M$ and the column indices of the corresponding matrix elements in another 1D integer array $nlhop_\sigma$ of the same size. We store the number of exact non-zero elements in each row of the matrix in a 1D integer array $\text{count}_\sigma$ of length $N_\uparrow$. We define the matrix elements corresponding to the two values of $esign = 1$ and $esign = -1$ as $ndiag(1) = -t$ and $ndiag(-1) = t$ respectively where $t$ is the hopping amplitude. FIG. 1. shows a matrix stored in this way.

$$H_\sigma = \begin{pmatrix} 0 & -t & t & 0 \\ -t & 0 & 0 & 0 \\ t & 0 & 0 & -t \\ 0 & 0 & -t & 0 \end{pmatrix}$$

$$UpperTriangular H_\sigma = \begin{pmatrix} 0 & -t & t & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -t & 0 \end{pmatrix}$$

$$nsign_\sigma = (1 - 11)$$
$$nlhop_\sigma = (234)$$
$$nhop_\sigma = (2010)$$

FIG. 1. Sparse matrix $H_\sigma$ stored in form of three 1D integer arrays: $nsign_\sigma$, $nlhop_\sigma$ and $nhop_\sigma$ respectively.

We perform the matrix vector multiplication $q_{new} = H_{old} q_{old}$, where $q_{old}$ and $q_{new}$ are the vectors of dimension $\text{count}_\uparrow \text{count}_\downarrow$. The vector product with the non diagonal part of the Hamiltonian matrix due to spin up hopping, i.e. $q_{new} = q_{new} + (I_\downarrow \otimes H_\uparrow H_\downarrow)$ can be computed using the following nested loop:

$$g = 0$$

for $i = 1 : \text{count}_\uparrow$

for $j = 1 : \text{nhop}_\uparrow(i)$

$g = g + 1$

$f = nlink_\downarrow(g)$

$b = nsign_\downarrow(g)$

for $k = 1 : \text{count}_\downarrow$

$r = (k - 1)\text{count}_\uparrow + i$

$s = (k - 1)\text{count}_\uparrow + f$

$q_{new}(r) = q_{new}(r) + ndiag(b)q_{old}(s)$

$q_{new}(s) = q_{new}(s) + ndiag(b)q_{old}(r)$

end

end

end

where $q_{new}$ may be zero or have some initial value at the starting of the loop.

The vector product with the non diagonal part of the Hamiltonian matrix due to spin down hopping, i.e. $q_{new} = q_{new} + (H_\downarrow \otimes I_\uparrow)q_{old}$ can be computed via the following nested loop:

$$g = 0$$

for $i = 1 : \text{count}_\downarrow$

for $j = 1 : \text{nhop}_\downarrow(i)$

$g = g + 1$

$f = nlink_\downarrow(g)$

$b = nsign_\downarrow(g)$

for $k = 1 : \text{count}_\uparrow$

$r = (i - 1)\text{count}_\uparrow + k$

$s = (f - 1)\text{count}_\downarrow + k$

$q_{new}(r) = q_{new}(r) + ndiag(b)q_{old}(s)$

$q_{new}(s) = q_{new}(s) + ndiag(b)q_{old}(r)$

end

end

end

where $q_{new}$ may be zero or have some initial value at the starting of the loop.

The storage requirement of the non-diagonal part of Hamiltonian matrix of effective dimension $(\text{count}_\uparrow \text{count}_\downarrow) \times (P)$ reduces to the storage requirement of two hermitian matrices of effective dimensions $\text{count}_\uparrow \times (P/2)$ and $\text{count}_\downarrow \times (P/2)$ respectively. For the sector $N_\uparrow = N_\downarrow$, i.e. $S^z = 0$, the two hermitian matrices of effective dimensions $\text{count}_\uparrow \times (P/2)$ and $\text{count}_\downarrow \times (P/2)$ are the same, thereby requiring storage only for a hermitian matrix of effective dimension $\text{count}_\uparrow \times (P/2)$. The storage of the Hamiltonian matrix in this form is ideally suited for parallelization. Matrices $H_\uparrow$ and $H_\downarrow$ can be stored on each node using sparse matrix format which in turn lead to significant reduction in inter-node communication on a parallel machine.

B. Computation of non-zero matrix elements for matrix-vector multiplication

In our scheme, to obtain the non-diagonal part of the Hamiltonian matrix we compute only the small matrix $H_\sigma(H_\downarrow)$ and then form the tensor product $I_\downarrow \otimes H_\uparrow(H_\downarrow \otimes I_\uparrow)$ through a nested loop. In other words, for generation of the non-diagonal part of the Hamiltonian matrix due to spin $\sigma$ hopping terms, the operation of $H_\sigma$ acting on each of the $I$'s which is equal to $\text{count}_\uparrow \text{count}_\downarrow$ is split in our scheme into the operation of $H_\sigma$ acting on each of the $I$'s which is equal to $\text{count}_\uparrow$ to generate the matrix $H_\sigma$ and then taking the product of each the non-zero elements of $H_\sigma$ with total non-zero elements of identity matrix $I_\sigma$ which is equal to $\text{count}_\sigma$, where if $\sigma = \uparrow \ (\downarrow)$ then $\sigma = \downarrow \ (\uparrow)$. 
TABLE II. Time taken to generate the non-diagonal part of the 1-D Hubbard model with $U = 4$ and $t = 1$(half-filled, $S^z = 0$) on an intel i7 processor machine by applying the Hamiltonian to the two-spin basis states $I_s$ and one-spin basis states $I_z$ separately.

| $M$ | $N_z$ | $N_s$ | Hilbert Space Dimension | Time Two-spin | Time One-spin |
|-----|-------|-------|-------------------------|---------------|---------------|
| 16  | 8     | 8     | 165 636 900             | 78.66 s       | 8.74 s        |
| 14  | 7     | 7     | 11 778 624              | 5.02 s        | 0.55 s        |

TABLE III. Time taken to generate the non-diagonal part of the $4 \times 4$ square lattice with $U = 4$ and $t = 1$ on an intel i7 processor machine by applying the Hamiltonian to the two-spin basis states $I_s$ and one-spin basis states $I_z$ respectively.

| $M$ | $N_z$ | $N_s$ | Hilbert Space Dimension | Time Two-spin | Time One-spin |
|-----|-------|-------|-------------------------|---------------|---------------|
| 16  | 8     | 8     | 165 636 900             | 186.71 s      | 18.32 s       |
| 14  | 7     | 7     | 130 873 600             | 146.02 s      | 14.24 s       |

The scheme of working with $I_z$ spanning $Y^{N_z}$ or $I_s$ spanning $Y^{N_z}$ at a time to generate the Hamiltonian matrix of one-band Hubbard model that we have presented above has the following advantages as compared to working with $I_s$ spanning the full Hilbert space $Y$:

- Instead of computing and storing $I_s$, we just need to compute and store $I_z$ or $I_s$ at a time, reducing both storage and time requirements. For the specific sector $N_z = N_z$, i.e. $S^z = 0$, the basis states of only one spin configuration $\sigma(\uparrow$ or $\downarrow$) are required to be computed.
- Instead of applying the Hamiltonian to each of the basis states spanning $Y$ which is equal to $\text{count}_\uparrow \times \text{count}_\downarrow$, we just need to apply the Hamiltonian including the hopping terms of only spin up configuration to $\text{count}_\uparrow$ spin up basis states and the Hamiltonian including the hopping terms of only spin down configuration to $\text{count}_\downarrow$ spin down basis states, saving significant computation time. This makes the present algorithm highly parallelizable and can be profitably implemented on a parallel machine.
- The storage requirement of the non-diagonal part of the sparse Hamiltonian matrix of effective dimension $(\text{count}_\uparrow \times \text{count}_\downarrow) \times (P)$ is reduced to the storage requirement of two hermitian matrices of effective dimensions $\text{count}_\uparrow \times (P/2)$ due to spin up hopping and $\text{count}_\downarrow \times (P/2)$ due to spin down hopping respectively, where $P$ is the maximum number of finite off-diagonal elements in any given row of the Hamiltonian matrix. For the $S^z = 0$ sector, the two hermitian matrices of effective dimensions $\text{count}_\uparrow \times (P/2)$ and $\text{count}_\downarrow \times (P/2)$ are the same, thereby requiring storage only for a hermitian matrix of effective dimension $\text{count}_\uparrow \times (P/2)$.
- We just need to store or search the indices of the basis of one spin configuration at a time and not bother about the indices of the basis of the other spin configuration. A binary search would require at the most $O(\log_2(\text{count}_\uparrow))$ or $O(\log_2(\text{count}_\downarrow))$ comparisons to find the index of a given $I_\uparrow$ or $I_\downarrow$ respectively. For $S^z = 0$ or half filled sectors, where $\text{count}_\uparrow = \text{count}_\downarrow$,
the the maximum number of comparisons required in binary search for finding a particular index would be of order half while working with $I_\uparrow$ or $I_\downarrow$ than those with $I$.

- Working with $I$’s and then extracting $I_\uparrow$ and $I_\downarrow$ from $I$ by examining its bits is done away with by working with only $I_\uparrow$ and $I_\downarrow$ at a time.

**ACKNOWLEDGMENTS**

Medha Sharma is thankful to DST for financial assistance in the form of Inspire Fellowship. Medha Sharma also thanks S.R. Hassan and Rajesh Karan for introducing her to the field of DMFT and Centre for Theoretical Physics, Jamia Millia Islamia (New Delhi, India) for providing computational facility.

**Appendix A: Algorithm I**

```plaintext
minrange = 0
maxrange = 0
for i = 1 : Nσ
    minrange = minrange + 2i−1
    maxrange = maxrange + 2M−i
end
countσ = 0
for i = minrange : maxrange
    nbit = 0
    for j = 0 : (M − 1)
        if bittest(i, j)
            nbit = nbit + 1
        end
    end
    if nbit = Nσ
        countσ = countσ + 1
        basisσ(countσ) = i
        indexσ(i) = countσ
    end
end
```

**Appendix B: Algorithm II**

```plaintext
matrix(1 : countσ, 1 : countσ) = 0
{Using Algorithm I compute basisσ(1 : countσ) and store in basisσ(1 : countσ)}
for i = 1 : M
    pointσ = 0
    for j = 1 : countσ
        if Nσ + Nσ ≤ M
            if site i of basisσ(j) is occupied
                pointσ = pointσ + 1
                indexU↑(i, pointσ) = j
            end
            if Nσ = Nσ
                pointσ = pointσ
                indexU↓(i, pointσ) = j
            else
                if site i of basisσ(j) is unoccupied
                    pointσ = pointσ + 1
                    indexU↓(i, pointσ) = j
                end
            end
            if Nσ = Nσ
                g = U(Nσ + Nσ − M)
                for i = 1 : countσ
                    matrix(i, i) = matrix(i, i) + g
                end
            else
                if Nσ + Nσ ≤ M
                    g = UNσ
                else
                    g = U(M − Nσ)
                    for i = 1 : countσ
                        k = (countσ + 1)i − countσ
                        matrix(k, k) = matrix(k, k) + g
                    end
                end
            end
        end
    end
end
for i = 1 : M
    for k = 1 : pointσ
        if l = 1 : pointσ
            if Nσ = Nσ
                if l ≠ k
                    r = (indexU↑(i, l) − 1)countσ + indexU↑(i, k)
                    matrix(r, r) = matrix(r, r) + U
                end
            end
        end
    end
end
```

The code and equations are formatted in a clear, readable manner. The text is divided into sections with appropriate labels for references and acknowledgments. The algorithms are presented with clear, concise instructions, making them easy to understand and implement.
end
else
  $r = (\text{index}_{U}(i, l) - 1)\text{count}_{\uparrow} + \text{index}_{U}(i, k)$
  $\text{matrix}(r, r) = \text{matrix}(r, r) + U$
end

[1] J. Hubbard, Proc. Roy. Soc. London, Ser. A 276, 238 (1963).
[2] V.J. Emery, Phys. Rev. Lett. 58, 2794 (1987).
[3] P. W. Anderson, Science 235, 1196 (1987).
[4] F. C. Zhang and T. M. Rice, Phys. Rev. B 37, 3759 (1988).
[5] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. 20 (1968).
[6] W. Metzner, D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
[7] Antoine Georges, Gabriel Kotliar, Phys. Rev. B 45, 6479 (1992).
[8] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).
[9] D.D. Sarma and S. Ramasesha A. Taraphder, Phys. Rev. B 39, 12286 (1989).
[10] J. Callaway, D.P. Chen, D. G. Kanhere and Qiming Li, Phys. Rev. B 42, 465 (1990).
[11] Michel Caffarel and Werner Krauth, Phys. Rev. Lett. 72, 1545 (1994).
[12] H. Q. Lin and J. E. Gubernatis, Comput. Phys. 7, 400 (1993).
[13] Susumu Yamada, Toshiyuki Imamura, Takuma Kano, Yoji Ohashi, Hideki Matsumoto, and Masahiko Machida, Journal of the Earth Simulator, 7, 23 (2007).
[14] T. Siro, A. Harju, Computer Physics Communications, 183, 1884 (2012).
[15] David Sénéchal, cond-mat/0806.2690v2 (2010).
[16] S. Akbar Safari, cond-mat/0807.4878v1 (2008).
[17] A. Weiße and H. Fehske, in Computational Many-Particle Physics, Lecture Notes in Physics, Vol. 739, edited by H. Fehske, R. Schneider, and A. Weiße (Springer, Heidelberg, 2008), pp. 529-544.
[18] H. Q. Lin, Phys. Rev. B 42, 6561 (1990).
[19] P. W. Anderson, Phys. Rev. 124, 41 (1961).
[20] R Haydock, V Heine and M J Kelly, J. Phys. C: Solid State Phys. 8, 2591 (1975).
[21] C. Lanczos, J. Res. Nat. Bur. Stand. 45, 255 (1950).