Iterative Ground State Approach Algorithm

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The following is the algorithm for performing an iterative diagonalization of fermionic systems. It is mostly similar to DMRG and NRG, and allows obtaining the low-energy spectrum of large many-body Hamiltonians.

I. INTRODUCTION

The broad idea is the following. We have a Hamiltonian describing an interacting set of states (in real or momentum space). We can express the total Hamiltonian in an incremental fashion: $H = \sum_i H_i$, where H_{i+1} involves more number of states than H_i. For example, a tight-binding model can be written in that form, with the definition $H_i = c^\dagger_{i+1} c_i + \text{h.c.}$. The iterative diagonalisation method obtains the low-energy spectrum of this problem in the following manner: We first diagonalise the Hamiltonian H for a smaller value of i, small enough such that this can be done exactly. We then truncate the spectrum to a predefined size, and rotate all existing operators to this truncated basis, including the Hamiltonian H. We then consider the "bonding Hamiltonian" ΔH between the existing sites and the new sites, and rotate the same into the truncated basis. Adding the previous rotated Hamiltonian H and the rotated increment Hamiltonian ΔH gives us a truncated but effective Hamiltonian for the increased number of sites. We again diagonalise this, and again retain only a fixed number of states in the spectrum. We keep repeating this until we reach the required number of sites.

II. STRUCTURE OF HAMILTONIAN AND OPERATORS

A. Jordan-Wigner Matrix Representation of Fermionic Operators

For a single qubit, the creation/annihilation matrices are

$$c = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, c^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \ , \tag{1}$$

given the convention that $|1\rangle = (0 \quad 1)$ is the occupied state. For a many-body system, these must be replaced with field operators that have the canonical fermionic algebra. For a system of N 1-particle levels, this can be accomplished through a *Jordan-Wigner*-like transformation

$$c_j = \left(\otimes_1^j \sigma_z\right) \otimes c \otimes \left(\otimes_1^{N-j} \mathbb{I}\right) \ , j \in [0, N-1] \ , \tag{2}$$

where $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. For example, for spinless electrons on a three-site lattice, we can have three fermionic operators: c_1,c_2, and c_3. Following the above expression, their matrices are

$$c_1 = c \otimes \mathbb{I} \otimes \mathbb{I} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \ ,$$

$$c_2 = \sigma \otimes c \otimes \mathbb{I} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \ ,$$

$$c_3 = \sigma \otimes \sigma \otimes c = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \ ,$$

For later use, we define the *antisymmetriser matrix* $S(j)$ and identity matrix $\mathbb{I}(j)$,

$$\begin{aligned} S(j) &= \otimes_1^j \sigma_z = \sigma_z \otimes \ldots j \text{ times } \ldots \otimes \sigma_z, \\ \mathbb{I}(j) &= \otimes_1^{N-j} \mathbb{I} = \mathbb{I} \otimes \ldots j \text{ times } \ldots \otimes \mathbb{I} \ , \end{aligned} \tag{3}$$

to express the fermionic representation compactly:

$$c_j = S(j) \otimes c \otimes \mathbb{I}(N-j) \ . \tag{4}$$

B. Structure of Hamiltonian

We consider a general impurity model, of L number of sites (excluding the impurity site):

$$H_{\text{sys}}(L) = H_{\text{imp}} + H_{\text{imp-bath}} + -t \sum_{\sigma,j=1}^{L-1} \left(c^\dagger_{j,\sigma} c_{j+1,\sigma} + \text{h.c.} \right) \ , \tag{5}$$

where H_{imp} is the Hamiltonian for the decoupled impurity site and $H_{\text{imp-bath}}$ is the impurity-bath coupling. Such a system has $2L+2$ single-particle levels in the full system (2 spin levels for each of the $L+1$ sites).

Iteration scheme (the initial number of states is L_0):

$$\begin{aligned} H_0(L_0) &= H_{\rm sys}(L_0)\ , \\ H_{r+1}(L_0) &= H_r(L_0) + \Delta H_r(L_0),\ r \geq 0\ , \\ \Delta H_r(L_0) &= -t \sum_\sigma \left(c^\dagger_{L_0+r,\sigma} c_{L_0+r+1,\sigma} + \text{h.c.} \right). \end{aligned} \tag{6}$$

H_0 is the initial Hamiltonian, consisting of L_0 lattice sites in the bath, $H_{r+1}(L_0)$ is the Hamiltonian after $r+1$ iterations having started with L_0 sites, and $\Delta H_r(L_0)$ is the increment term that gets added to $H_r(L_0)$ during the $(r+1)^{\rm th}$ iteration to give rise to $H_{r+1}(L_0)$.

III. THE ALGORITHM

A. Iterative Diagonalization

Let the starting Hamiltonian be $H_0(L_0)$, consisting of L_0 single-particle levels (hence a Hilbert space dimension of 2^{L_0}). We start with a single-particle computational basis and construct the L_0 fermionic operators $c_1, c_2, \ldots, c_{L_0}$ in this basis, using eq. 4. We also keep track of a large antisymmetriser matrix $S(L_0)$ that will be used to attach new sites when we expand the system. Let M_s be the maximum number of eigenstates we retain in the spectrum at any given step. The value of M_s should be chosen so that a $M_s \times M_s$ matrix can be diagonalised in reasonable time.

S1. Construct the complete Hamiltonian matrix H_0 in our present basis using the field operators $\{c_j\}$. Diagonalise the Hamiltonian (of size $D_0 \times D_0$) and obtain the eigenvalues E_n and eigenstates X_n. Each X_n is a column vector of size D_0.

S2. Retain at most M_s number of eigenstates, preferring the ones with lower energy. The reduced basis for this rotated truncated subspace is constructed by stacking the column vectors X_n horizontally:

$$R = [X_1 X_2 \ldots X_{M_s}]_{D_0 \times M_s}\ . \tag{7}$$

This matrix also acts as the transformation to rotates and truncate all operators from the old basis into the new one.

S3. We rotate our Hamiltonian H_0, our fermionic operators $\{c_j\}$ and the large antisymmetrizer matrix $S(L_0)$ into the new reduced basis, using the transformation $\mathcal{O} \to R^\dagger \mathcal{O} R$.

S4. We now need to expand our system by adding the increment Hamiltonian ΔH_0. Let the number of *new* 1-particle levels in ΔH_0 be L_Δ. These new levels will be indexed as $L_0+1, \ldots, L_0+L_\Delta$. We need to define antisymmetrized fermionic operators for the new sites:

$$\begin{aligned} c_{L_0+1} &= c \otimes \mathbb{I}(2^{L_\Delta - 1}), \\ c_{L_0+2} &= \sigma_z \otimes c \otimes \mathbb{I}(2^{L_\Delta - 2}), \\ &\cdots \\ c_{L_0+L_\Delta} &= (\otimes_1^{L_\Delta - 1} \sigma) \otimes c\ . \end{aligned} \tag{8}$$

These have to be calculated in the local computational basis (of size 2^{L_Δ}) of the new levels.

S5. Combining the new sites with the old sites leads to a combined Hilbert space dimension of $(M_s + 2^{L_\Delta}) \times (M_s + 2^{L_\Delta})$. To allow all operators to act on the enlarged Hilbert space, we expand both sets of operators:

$$\begin{aligned} c_j &= S(L_0) \otimes c_j;\quad j = L_0+1, \ldots, L_\Delta\ , \\ c_j &= c_j \otimes \mathbb{I}(2^{L_\Delta});\quad j = 1, 2, \ldots, L_0\ , \\ H_0 &\to H_0 \otimes \mathbb{I}(2^{L_\Delta}), \\ S(L_1) &= S(L_0) \otimes \mathbb{I}(2^{L_\Delta})\ . \end{aligned} \tag{9}$$

where $\mathbb{I}(2^{L_\Delta})$ is an identity matrix of dimension $2^{L_\Delta} \times 2^{L_\Delta}$. Note that the operators in the last three equations are the rotated ones (following Step 3).

S6. Using the transformed operators $c_{L_0+1}, \ldots, c_{L_0+L_\Delta}$ for the new sites, construct the difference Hamiltonian matrix ΔH_0 and hence the updated Hamiltonian $H_1 = H_0 + \Delta H_0$ for the next step. Repeat the process starting from step 2 with the new Hamiltonian H_1, the new operators c_j and the new matrix $S(L_1)$ replacing the old counterparts.

B. Static Correlations

We are in general interested in $n-$point correlations of the form $\langle \mathcal{O}_1 \mathcal{O}_2 \ldots \mathcal{O}_n \rangle$, where $\mathcal{O}_i$ are operators that act on 1-particle Hilbert spaces. Let the earliest step of the iterative diagonalisation procedure at which all these operators have entered the system be r. At this step r, construct the correlation operator $\mathcal{O}_1 \mathcal{O}_2 \ldots \mathcal{O}_n$ using the fermionic matrices c_j at that step (recall that these matrices will be highly rotated versions of the matrices we started with). Having constructed the operator O, we expand and rotate it after the completion of every future step: $O_{n+1} = (R_n^\dagger O_n R_n) \otimes \mathbb{I}(2^{L_\Delta})$, where R_n is the rotation matrix for the $n^{\rm th}$ step. The last step n^* of the iterative diagonalisation consists of only a diagonalisation and no expansion, resulting in a final set of eigenstates $\{X_i\}$. The form of the correlation operator in this basis is $O_{n^*} = R_{n^*-1}^\dagger O_{n^*-1} R_{n^*}$. The expectation value can now be calculated using the matrix O_{n^*} and the ground state of $\{X_i\}$.

IV. EXAMPLES AND BENCHMARKS

A. Single-Impurity Anderson Model

The single-impurity Anderson model at half-filling is obtained by setting $H_{\text{imp}} = -\frac{U}{2}\left(n_{d\uparrow} - n_{d\downarrow}\right)^2$ and $H_{\text{imp-bath}} = -V\sum_\sigma \left(c^\dagger_{d\sigma} c_{0\sigma} + \text{h.c.}\right)$ in eq. 5. We studied this model using the above approach to benchmark the ground state energy and spin-flip correlation $\left\langle \frac{1}{2} S^+_d S^-_0 + \text{h.c.} \right\rangle$ against exact diagonalization (ED). In order to extend the ED to a larger number of sites, we restricted ourselves to just the $N = 2$ sector, N being the total occupancy. We find very good agreement for $M_s \sim 1000$ and above. These results are shown in Fig. IV A.