Approximate diagonalization method for many-fermion Hamiltonians

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The limits of direct unitary transformation of many-fermion Hamiltonians are explored. Practical application of such transformations requires that effective many-body interactions be discarded over the course of a calculation. The truncation of the Hamiltonian leads to finite errors and in some cases divergences. A new formalism is proposed to manage errors and avoid divergences. Removing all interactions from a many-fermion Hamiltonian reduces it to fermion number operators allowing for direct calculation of eigenvalues. If the same transformations are applied to the bare fermions, eigenfermions are produced whose Slater determinants form eigenstates. This enables a hierarchy of diagonalization methods of increasing accuracy as fewer interactions are discarded from the Hamiltonian.

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I. INTRODUCTION

Simulation of interacting fermions is difficult. The root of the difficulty is the large size of the fermion configuration space, which is exponential in the number of fermion degrees of freedom. Brute force calculations on the large space are only tractable for small model systems and small molecules. Approximations are necessary, but there is no consensus on an approximate method that is sufficiently accurate and efficient for systems of interest. Development is split mainly between a few popular approaches based on well-established ideas: many-body perturbation theory with a variety of resummations and empirical parameterization, quantum Monte Carlo to statistically sample large configuration spaces, and methods based on renormalization group (RG) principles. The two most popular RG methods are based on the extreme limits of one and infinite spatial dimensions.

Another, less popular RG approach exists that is based on preserving the form of a many-fermion Hamiltonian under unitary transformations. With no reference to spatial dimension or scale, it is less fundamentally restricted than other RG approaches. Its primary use to date has been in decoupling weakly correlated fermions from a system to produce a smaller strongly correlated subsystem to be solved using other methods. Attempts to decouple all fermions with this method have resulted in slow convergence and the appearance of numerical divergences. What remains unclear are the source of these problems, and whether they present a fundamental barrier to improvement or merely a technical barrier.

The work presented in this paper addresses the technical problems of previous many-fermion transformation methods. The fundamental source of error in these methods is the truncation of the Hamiltonian after each transformation, to remove terms outside a prescribed Hamiltonian form. Divergences resulting from truncation can be eliminated by conserving a set of quantities that are naturally conserved by exact unitary transformation. The restrictions placed on operator truncation specify a unique form. In a flow equation framework, the continuous transformation of the Hamiltonian results in continuous growth of truncation errors. All previous errors get locked into the solution. To minimize the total truncation error, the continuous transformation is grouped into discrete fragments, each of which is carefully optimized based on an error minimization criteria. Some finite amount of truncation error inevitably remains and can only be reduced further by truncating fewer terms from the transformed Hamiltonian.

Completely decoupling all fermions in a many-fermion Hamiltonian reduces it to a diagonal form containing only fermion number operators. The transformation that diagonalizes a many-fermion Hamiltonian can be applied either directly to the Hamiltonian or the elementary fermion operators. The transformed fermions are called eigenfermions. Eigenstates are Slater determinants of eigenfermions. Whereas the eigenvalue decomposition of a matrix produces a list of all eigenvalues, the eigenfermion decomposition of a many-fermion Hamiltonian produces a function of eigenfermion number operators. Eigenvalues are evaluated by replacing number operators with occupation numbers. The complete set of eigenstates is parameterized by a configuration space of eigenfermion occupation numbers much like the states of a classical system lie in a configuration space of classical variables. Based on this analogy, the diagonalization of a many-fermion Hamiltonian can be interpreted as a quantum-to-classical mapping.

The paper proceeds as follows. Section II defines and discusses the concept of an eigenfermion. Section III constructs a general mathematical theory of truncated unitary transformations and truncated eigenvalue decomposition. Section IV applies the general theory to the many-fermion case. Section V discusses what can be computed as a result of a truncated eigenfermion decomposition and the associated computational costs.
II. THE EIGENFERMION CONCEPT

The many-fermion Hamiltonians that describe physical systems typically contain only 1&2-fermion interactions. The structure of these Hamiltonians is compactly encoded in the standard language of second quantization,

\[ \hat{H} = \sum_{i,j} h_{ij} \hat{c}^\dagger_i \hat{c}_j + \sum_{i,j,k,l} V_{ijkl} \hat{c}^\dagger_i \hat{c}^\dagger_j \hat{c}_k \hat{c}_l. \]  

(1)

If \( \hat{H} \) is diagonalized in the basis of Slater determinants by a unitary transformation \( \hat{U} \), then the transformed Hamiltonian contains only fermion number operators, \( \hat{n}_i = \hat{c}^\dagger_i \hat{c}_i \),

\[ \hat{U}^\dagger \hat{H} \hat{U} = E_0 + \sum_i E_i \hat{n}_i + \sum_{i,j} E_{ij} \hat{n}_i \hat{n}_j + \cdots. \]  

(2)

All possible products of \( \hat{n}_i \) operators can appear in this expression. The 1&2-fermion form of \( \hat{H} \) in Eq. (1) cannot generally be preserved by the diagonalization procedure. The eigenvalues and eigenstates of \( \hat{H} \) are parameterized by an occupation vector \( \mathbf{f} \) with entries \( f_i \in \{0,1\} \),

\[ E(\mathbf{f}) = E_0 + \sum_i E_i f_i + \sum_{i,j} E_{ij} f_i f_j + \cdots \]  

(3a)

\[ |\Psi(\mathbf{f})\rangle = \hat{U} |\mathbf{f}\rangle = \hat{U} \prod_i [(1 - f_i) + f_i \hat{c}^\dagger_i] |0\rangle. \]  

(3b)

Each \( |\mathbf{f}\rangle \) is a Slater determinant and \( |0\rangle \) is the zero-fermion vacuum state.

Occupation vectors are convenient mathematical labels for eigenstates in Eq. (3), but to have physical significance they must describe the occupations of a physical object. This object is a fermion and because of its special relationship to eigenstates, it is named an eigenfermion. The \( \hat{U} \) that diagonalizes \( \hat{H} \) can be used to define eigenfermion operators from the bare fermions of the system,

\[ \hat{\hat{q}}_i = \hat{c}^\dagger_i \hat{U}^\dagger \]  

and \( \hat{n}_i = \hat{\hat{q}}_i \hat{\hat{q}}_i^\dagger \). \hspace{1cm} (4)

The anti-commutation relations of \( \hat{\hat{c}}_i \) are inherited by \( \hat{\hat{q}}_i \). By rearranging Eq. (2), the original Hamiltonian can be written solely in terms of eigenfermion number operators,

\[ \hat{\hat{H}} = E_0 + \sum_i E_i \hat{n}_i + \sum_{i,j} E_{ij} \hat{n}_i \hat{n}_j + \cdots. \]  

(5)

The eigenstates can be written as a Slater determinant of eigenfermions acting on a new vacuum, \( |0\rangle = \hat{U} |0\rangle \),

\[ |\Psi(\mathbf{f})\rangle = \prod_i [(1 - f_i) + f_i \hat{\hat{q}}^\dagger_i] |0\rangle. \]  

(6)

If \( \hat{U} \) preserves total fermion number, then \( |\mathbf{f}\rangle = |0\rangle \). It is clear from Eqs. (5) and (6) that occupation vectors labelling the eigenstates specify eigenfermion occupation numbers.

The only properties that eigenfermions are guaranteed to share with the bare fermions of a system are those preserved by symmetry. Such symmetries must be explicitly preserved by \( \hat{U} \) in Eq. (4). If total fermion number is conserved, then the number of eigenfermions in a state corresponds to the number of fermions. If total fermion spin is conserved, then eigenfermions will have the same well-defined spin as the bare fermions. If translational invariance is conserved, then eigenfermions will have a well defined crystal momentum. Unless completely constrained by symmetry, the eigenfermions that diagonalize a Hamiltonian are non-unique. However, it is possible to define a unique set of eigenfermions that are in some sense most similar to the bare fermions.

Practical calculations of Eq. (2) will require approximations. The generic form of an approximately diagonalized Hamiltonian is

\[ \hat{U}^\dagger \hat{H} \hat{U} = \hat{D} + \hat{R}, \]  

(7)

where \( \hat{D} \) contains only fermion number operators and \( \hat{R} \) is a residual interaction. The physical effect of \( \hat{R} \) is to scatter eigenfermions, reducing \( |\Psi(\mathbf{f})\rangle \) from an eigenstate to a finite-lifetime nearly-stationary state. This situation resembles a theory of fermion quasiparticles that are adiabatically connected to the bare fermions. Such a quasiparticle theory can be cast in the form of Eq. (7) with a 1-fermion diagonal term, \( \hat{D} = \sum_i \epsilon_i \hat{n}_i \), and \( \hat{R} \) that weakly scatters between a ground state \( |\Psi(\mathbf{f}_{GS})\rangle \) and certain few-quasiparticle excited states \( |\Psi(\mathbf{f}_X)\rangle, \langle \mathbf{f}_X | \hat{D} | \mathbf{f}_{GS} \rangle \approx 0 \). Eigenfermions generalize these fermion quasiparticles to allow for strong non-scattering interactions in \( \hat{D} \) while requiring a weak residual interaction between all states, \( \hat{R} \approx 0 \). If \( \hat{R} \) is sufficiently small, then \( \hat{U} \) exactly diagonalizes a perturbed Hamiltonian,

\[ \hat{U}^\dagger (\hat{H} + \Delta \hat{H}) \hat{U} = \hat{D} \]  

with \( \Delta \hat{H} = -\hat{U} \hat{R} \hat{U}^\dagger \). \hspace{1cm} (8)

Constructing the exact solution to a system slightly different from what was intended is similar to experimenting on impure samples.

There are many distinct approaches in the literature\textsuperscript{6–8,10–12} for approximating \( \hat{U}^\dagger \hat{H} \hat{U} \) for a general 1&2-fermion Hamiltonian and a wide class of transformations. Unfortunately, none of these methods have claimed to generally and reliably solve Eq. (7) with a small residual error \( \hat{R} \). The deficiency is often attributed to nearly degenerate states or strong fermion correlations. Inadequate closure of equations can result in uncontrolled growth of \( \hat{R} \) and numerical divergences\textsuperscript{7}. No analysis has yet isolated the fundamental source of divergences. No \textit{a priori} criteria has yet to guarantee the existence of solutions. Recent progress has focused on unitary transformations that only partially diagonalize a Hamiltonian, leaving the rest of the problem to other many-fermion methods. A lack of progress in full diagonalization might be blamed on the complexity of many-fermion algebra. It proves productive to step back from the many-fermion case and construct a general
theory of operator diagonalization in the presence of non-negligible truncation errors.

III. TRUNCATED EIGENVALUE DECOMPOSITION THEORY

The goal of this section is to develop a basic theory for the effect of truncation errors on continuous unitary transformations. A continuous unitary transformation of an operator $\hat{X}$ is defined by a differential equation of a real variable $\lambda$,

$$\frac{d}{d\lambda} \hat{X}(\lambda) = [\hat{A}(\lambda), \hat{X}(\lambda)], \quad (9)$$

specified by an anti-Hermitian generator function $\hat{A}(\lambda)$ and starting from $\hat{X}(0) = \hat{X}$. Operator truncation will modify this equation. Diagonalization of a Hermitian operator $\hat{H}$ is possible if the modified form of Eq. (9) can be evolved to a diagonalized form, $\hat{H}(\infty) = \hat{D}$. A theory should provide a priori conditions that guarantee the success of the diagonalization process. Specifically, the evolution of $\hat{H}(\lambda)$ should contain no divergences and no stable, non-diagonal fixed points.

The form of truncation assumed by the theory is that $\hat{X}(\lambda)$ is restricted to a given model subspace of the full operator space. There is a corresponding restriction of $\hat{A}(\lambda)$ to a given generator subspace. If the elements of the model and generator subspaces form a Lie algebra, then no truncations are necessary and an established diagonalization method exists. Otherwise, Eq. (9) cannot be calculated exactly and a truncation procedure must be defined to close the equation. For the application to many-fermion systems, a wide variety of physically motivated truncation procedures have been proposed. What is more suitable for a general theory is a truncation that preserves $\text{Tr}[\hat{X}^\dagger(\lambda)\hat{X}(\lambda)]$ as a conserved quantity over $\lambda$. This criteria prevents divergences during the truncated transformation process and heavily constrains the form of truncation.

The constraint on truncation is clarified by elevating the space of operators to a Hilbert space, which requires the definition of an operator inner product,

$$\langle \hat{X}, \hat{Y} \rangle = \text{Tr}[\hat{X}^\dagger \hat{Y}]. \quad (10)$$

An operator inner product naturally defines an operator outer product $\hat{X} \otimes \hat{Y}$,

$$\langle \hat{X} \otimes \hat{Y} \rangle \hat{Z} = \hat{X} \langle \hat{Y}, \hat{Z} \rangle, \quad (11)$$

which can be used to construct linear maps between operators, commonly referred to as superoperators. Without constraint, the most general possible form for truncation of Eq. (9) is

$$\frac{d}{d\lambda} \hat{X}_M(\lambda) = \hat{T}(\lambda)[\hat{A}(\lambda), \hat{X}_M(\lambda)], \quad (12)$$

where $\hat{T}(\lambda)$ is a truncation superoperator acting on the result of the commutator. $\hat{X}_M(\lambda)$ is an approximation of $\hat{X}(\lambda)$ restricted to the model subspace, initialized to $\hat{X}_M(0) = \hat{T}(0)\hat{X}$. The range of $\hat{T}(\lambda)$ must be the model operator subspace to close the equation.

The target conserved quantity is now the natural norm of the operator Hilbert space,

$$\|\hat{X}\| = \sqrt{\langle \hat{X}, \hat{X} \rangle} = \sqrt{\text{Tr}(\hat{X}^\dagger \hat{X})}. \quad (13)$$

If Eq. (12) is suggestively rewritten as

$$\frac{d}{d\lambda} \hat{X}_M(\lambda) = \hat{A}(\lambda)\hat{X}_M(\lambda), \quad (14)$$

then $\hat{A}(\lambda)$ must be anti-Hermitian to conserve $\|\hat{X}_M(\lambda)\|$

$$\frac{d}{d\lambda} \|\hat{X}_M(\lambda)\|^2 = \langle \hat{X}_M(\lambda), [\hat{A}(\lambda) + \hat{T}(\lambda)]\hat{X}_M(\lambda) \rangle. \quad (15)$$

Since $\hat{T}(\lambda)$ restricts the range of $\hat{A}(\lambda)$, anti-Hermiticity correspondingly restricts the domain.

Specifying the constrained forms of $\hat{A}(\lambda)$ and $\hat{T}(\lambda)$ requires the definition of a few more pieces of notation. First, the commutator can be written as a superoperator, which is anti-Hermitian for an anti-Hermitian argument,

$$\hat{C}[\hat{X}]\hat{Y} = [\hat{X}, \hat{Y}]. \quad (16)$$

Second, a Hermitian projection superoperator is defined for the model subspace,

$$\hat{P}_M = \sum_i M_i \otimes \hat{M}_i, \quad (17)$$

where $\{\hat{M}_i\}$ is an orthonormal basis of the model subspace. In terms of these new superoperators, the most general truncation that conserves $\|\hat{X}_M(\lambda)\|$ is

$$\hat{T}(\lambda) = k\hat{P}_M + \hat{P}_M\hat{C}[\hat{A}(\lambda)]\hat{K}(\lambda), \quad (18a)$$

$$\hat{A}(\lambda) = \hat{T}(\lambda)\hat{C}[\hat{A}(\lambda)]\hat{P}_M, \quad (18b)$$

where $k$ is real and $\hat{K}(\lambda)$ is anti-Hermitian.

Simple error minimization arguments complete the specification of $\hat{T}(\lambda)$. The residual error of the truncated transformation is

$$\frac{d}{d\lambda} \hat{X}_R(\lambda) = [\hat{Z} - \hat{T}(\lambda)][\hat{A}(\lambda), \hat{X}_M(\lambda)] + [\hat{A}(\lambda), \hat{X}_R(\lambda)], \quad (19)$$

with the identity superoperator $\hat{I}$ and initial condition $\hat{X}_R(0) = \hat{X} - \hat{X}_M(0)$. The second term just rotates the residual and is cancelled by considered a prerotated form, $\hat{X}_{R2}(\lambda) = \hat{U}(\lambda)\hat{X}_R(\lambda)\hat{U}^\dagger(\lambda)$, defined by

$$\frac{d}{d\lambda} \hat{U}(\lambda) = -\hat{U}(\lambda)\hat{A}(\lambda) \quad \text{and} \quad \hat{U}(0) = \hat{I}. \quad (20)$$
Assuming the details of \( \hat{X}_R(\lambda) \) are unknown, the best strategy for minimizing \( \| \hat{X}_R(\lambda) \| \) is to minimize

\[
\|d\hat{X}_R(\lambda)/d\lambda\|^2 = \| (\hat{L} - \hat{P}_M) [\hat{A}(\lambda), \hat{X}_M(\lambda)] \|^2 
+ \| [\hat{P}_M - \hat{T}(\lambda)] [\hat{A}(\lambda), \hat{X}_M(\lambda)] \|^2 .
\] (21)

The growth of error is minimized by a unique choice of truncation, \( \hat{T}(\lambda) = \hat{P}_M \) \((k = 1 \text{ and } \hat{K}(\lambda) = 0)\), which cancels the second term. Operator truncation is now determined solely by the choice of model subspace.

By combining Eqs. (12), (19), and (20), the exact transformation of \( \hat{X} \) can be separated into

\[
\hat{U}^\dagger(\lambda) \hat{X} \hat{U}(\lambda) = \hat{X}_M(\lambda) + \hat{X}_R(\lambda) .
\] (22)

To conform to the notation in Eq. (7), the truncated eigenvalue decomposition of a Hermitian operator \( \hat{H} \) is defined as

\[
\hat{U}^\dagger(\infty) \hat{H} \hat{U}(\infty) = \hat{D} + \hat{R} ,
\] (23)

for a diagonal operator \( \hat{D} = \hat{H}_M(\infty) \) and a residual error \( \hat{R} = \hat{H}_R(\infty) \). The rest of the section is devoted to the theoretical issues of existence and uniqueness of solutions and the technical issues of efficient computability and error minimization.

The diagonalization of a Hermitian operator places special emphasis on Hermitian and diagonal operators. Truncation should preserve both of these properties. This can be enforced with restrictions on the model subspace. If \( \hat{X} \) is in the subspace, then \( \hat{X}^\dagger \) must also be in the subspace. The model subspace must also be completely separable into a purely diagonal and purely off-diagonal subspace. Projection superoperators can separate diagonal from off-diagonal ("coupling") operators,

\[
\hat{P}^D = \sum_i \langle i | \langle i | \otimes \langle i | \langle i | 
\] (24a)

\[
\hat{P}^C = \sum_{i \neq j} \langle i | \langle j | \otimes \langle i | \langle j | ,
\] (24b)

where \( \{ | i \rangle \} \) is an orthonormal basis of states that defines diagonality. The model projector can be separated into \( \hat{P}_M = \hat{P}_M^D + \hat{P}_M^C \), where \( \hat{P}_M^D = \hat{P}_M \hat{P}_M^D \) and \( \hat{P}_M^C = \hat{P}_M \hat{P}_M^C \). Model operators can similarly be split into \( \hat{X}_M^D(\lambda) = \hat{P}^D \hat{X}_M(\lambda) \) and \( \hat{X}_M^C(\lambda) = \hat{P}^C \hat{X}_M(\lambda) \).

### A. Existence and computability

The most straightforward way to prove the existence of a solution to Eq. (23) is to construct one. This simultaneously demonstrates that solutions are computable and lays the groundwork for a solution method. Construction of a solution is guided by a convergence metric,

\[
\Omega(\lambda) = \frac{1}{2} \| \hat{H}_M^C(\lambda) \|^2 ,
\] (25)

which approaches zero as Eq. (23) is satisfied. A solution exists if it is possible to choose \( \hat{A}(\lambda) \) to monotonically reduce \( \Omega(\lambda) \) to zero. This places important constraints on the generator subspace that contains \( \hat{A}(\lambda) \).

It is almost always possible to reduce \( \Omega(\lambda) \) by enforcing \( d\Omega(\lambda)/d\lambda < 0 \). The first derivative of \( \Omega(\lambda) \) is

\[
\frac{d}{d\lambda} \Omega(\lambda) = - \langle [\hat{H}_M^D(\lambda), \hat{H}_M^C(\lambda)], \hat{A}(\lambda) \rangle .
\] (26)

To maximize the rate of decrease of \( \Omega(\lambda) \), the two operators in the inner product should be made as close to parallel as possible. This criterion is limited by the restriction of \( \hat{A}(\lambda) \) to the generator subspace, which is enforced with a projection superoperator defined by an orthonormal basis \( \{ \hat{G}_i \} \) of the generator subspace,

\[
\hat{P}_G = \sum_i \hat{G}_i \otimes \hat{G}_i ,
\] (27)

The most parallel \( \hat{A}(\lambda) \) is

\[
\hat{A}(\lambda) = \hat{P}_G [\hat{H}_M^D(\lambda), \hat{H}_M^C(\lambda)] .
\] (28)

Without truncation, this procedure produces anti-Hermitian, off-diagonal operators. These properties are preserved by truncation if the generator subspace is similarly restricted to contain only anti-Hermitian, off-diagonal operators.

In some cases, diagonalization can get stuck at a non-diagonal fixed point with \( d\Omega(\lambda)/d\lambda = 0 \) and \( \Omega(\lambda) \neq 0 \). This occurs when \( \hat{A}(\lambda) = 0 \) and \( \hat{H}_M^C(\lambda) \neq 0 \) in Eq. (28) and signifies that \( \hat{H}_M^C(\lambda) \) is contained in the right null space of \( \hat{P}_G \hat{C} \hat{H}_M^D(\lambda) \hat{P}_M^C \). To further reduce \( \Omega(\lambda) \), the second derivative must be considered,

\[
\frac{d^2}{d\lambda^2} \Omega(\lambda) = - \left\langle [\hat{H}_M^D(\lambda), \hat{H}_M^C(\lambda)], \frac{d}{d\lambda} \hat{A}(\lambda) \right\rangle 
+ \langle \hat{P}_M [\hat{H}_M^D(\lambda), \hat{A}(\lambda)], \hat{H}_M^C(\lambda), \hat{A}(\lambda) \rangle 
+ \| \hat{P}_M [\hat{H}_M^D(\lambda), \hat{A}(\lambda)] \|^2 
- \| [\hat{H}_M^D(\lambda), \hat{A}(\lambda)] \|^2 .
\] (29)

Monotonicity requires \( d^2\Omega(\lambda)/d\lambda^2 \leq 0 \), but further reduction of \( \Omega(\lambda) \) requires either \( d^2\Omega(\lambda)/d\lambda^2 < 0 \) or the consideration of even higher derivatives of \( \Omega(\lambda) \).

To guarantee that \( \Omega(\lambda) \) can be reduced to zero, the effects of the null space of \( \hat{P}_G \hat{C} \hat{H}_M^D(\lambda) \hat{P}_M^C \) have to be addressed. If this superoperator’s domain is restricted to the Hermitian off-diagonal model subspace and the range to the generator subspace, then constraining the dimensions of the subspaces to be equal is a necessary condition for the absence of a null space. If a null space remains, then the right null space has a corresponding left null space. When \( d\Omega(\lambda)/d\lambda = 0 \), the second derivative of \( \Omega(\lambda) \) can be made non-positive by restricting \( \hat{A}(\lambda) \) to the left null space,

\[
\frac{d^2}{d\lambda^2} \Omega(\lambda) = - \langle [\hat{H}_M^D(\lambda), \hat{A}(\lambda)], \hat{A}(\lambda) \rangle .
\] (30)
The \( d\Omega(\lambda)/d\lambda = 0 \) fixed point is unstable if the second derivative can be made negative and nonzero. A sufficient existence criteria is that for any \( \tilde{H}_M^D(\lambda) \) in the right null space of \( \tilde{P}_M \tilde{C}[\tilde{H}_M^D(\lambda)] \tilde{P}_M^C \), there must exist an \( \hat{A}(\lambda) \) in the left null space such that Eq. \( (30) \) is nonzero. To demonstrate that the existence criteria is necessary, the untruncated case is considered. Without truncation, there is analytic eigenvalue decomposition of \( \tilde{C}[\tilde{H}_M^D(\lambda)] \),

\[
\tilde{C}[\tilde{H}_M^D(\lambda)]|j\rangle = \left( \langle i|\tilde{H}_M^D(\lambda)|i\rangle - \langle j|\tilde{H}_M^D(\lambda)|j\rangle \right) |i\rangle |j\rangle.
\]

(31)
The off-diagonal eigenoperators naturally come in pairs with eigenvalues of opposite sign, \( \{ |i\rangle |j\rangle, |j\rangle |i\rangle \} \). When

\[
\langle i|\tilde{H}_M^D(\lambda)|i\rangle = \langle j|\tilde{H}_M^D(\lambda)|j\rangle,
\]

the eigenoperator pairs are degenerate and in the null space of \( \tilde{C}[\tilde{H}_M^D(\lambda)] \). This signifies a case where \( d\Omega(\lambda)/d\lambda = 0 \) and \( \Omega(\lambda) \neq 0 \) if \( \tilde{H}_M^D(\lambda) \propto |i\rangle |j\rangle + |j\rangle |i\rangle \). To satisfy the existence criteria for this case, the choice \( \hat{A}(\lambda) \propto |i\rangle \langle j| - |j\rangle \langle i| \) makes Eq. \( (30) \) nonzero.

A unique solution is defined by Eq. \( (28) \) if the derivative of \( \Omega(\lambda) \) remains nonzero until the problem is solved. Uniqueness is lost when \( d\Omega(\lambda)/d\lambda = 0 \) because any \( \hat{A}(\lambda) \) that satisfies the existence criteria is an arbitrary sign. Each choice of sign leads to a different solution. This almost always unique solution minimizes \( R \) in Eq. \( (23) \) in a weak and indirect way. The growth of truncation errors in Eq. \( (21) \) is proportional to \( \|\hat{A}(\lambda)\| \), and a smaller total error results from less transformation. Orthogonal components could be added to Eq. \( (28) \) to produce different solutions, but this increases \( \|\hat{A}(\lambda)\| \) and thus truncation errors without affecting convergence to a solution as measured by \( d\Omega(\lambda)/d\lambda \). While a more sophisticated technique may be possible, this simple choice of solution establishes both uniqueness and error minimization for solutions to Eq. \( (23) \) in a weak but practical form.

**B. Efficient solution method**

The continuous minimization of \( \Omega(\lambda) \) can be used to construct solutions to Eq. \( (23) \), but it is not the most efficient method. Numerical evolution of a differential equation is required to calculate \( \tilde{H}_M(\lambda) \). \( \hat{A}(\lambda) \) has to be stored at many \( \lambda \) values to transform operators after \( \tilde{H} \) has been diagonalized. These problems are avoided if \( \hat{A}(\lambda) \) is restricted to a piecewise constant function defined by a finite set of generators \( \{ \hat{A}_i \} \). The continuous transformation in Eq. \( (12) \) can be analytically integrated over each constant generator to produce a sequence of unitary superoperator exponentials,

\[
\hat{X}_{M,i} = \exp(\hat{A}_i)\hat{X}_{M,i-1},
\]

(32)

with \( \hat{X}_{M,0} = \tilde{P}_M \hat{X} \) and \( \hat{A}_i = \tilde{P}_M \tilde{C}[\hat{A}_i] \tilde{P}_M \). Some many-fermion methods \textsuperscript{5,10,14} use a single exponential for transformations, but section III A cannot guarantee solutions in this case. Efficiency is improved by reducing the cost of calculating each \( \hat{A}_i \) and minimizing the number required to diagonalize \( \hat{H} \).

Eq. \( (32) \) can be efficiently evaluated as a Taylor series cast in a recursive form,

\[
\begin{align*}
\hat{Z}_j &= \frac{1}{j} \tilde{P}_M[\hat{A}_i, \hat{Z}_{j-1}] \\
\sum_{j=0}^{\infty} \hat{Z}_j &= \exp(\hat{A}_i)\hat{X}_{M,i-1},
\end{align*}
\]

(33a)

(33b)

with \( \hat{Z}_0 = \hat{X}_{M,i-1} \). If \( \hat{X}_{M,i-1} \) is overwritten with the sum over \( \hat{Z}_j \), then the total memory requirement of this process is the storage of \( \hat{X}_{M,i-1}, \hat{A}_i, \hat{Z}_j, \) and \( \hat{Z}_{j-1} \). The calculation is terminated with a desired accuracy is reached, as estimated by \textit{a posteriori} and \textit{a priori} error bounds,

\[
\left\| \sum_{j=d+1}^{\infty} \hat{Z}_j \right\| \leq d! \max_{|x| \leq \|\hat{A}_i\|} |\exp(ix) - \sum_{j=0}^{d} (ix)^j/j!|.
\]

(34a)

(34b)

\textit{a}_d(x) \text{ bounds the error of a finite Taylor series approximation of the imaginary exponential,}

\[
\text{a}_d(x) = \left| \exp(ix) - \sum_{j=0}^{d} (ix)^j/j! \right|.
\]

(35)

Eq. \( (34) \) is derived using the superoperator spectral norm and a superoperator function inequality,

\[
\|f(\hat{A}_i)\hat{X}\| \leq \|\hat{X}\| \max_{\|\hat{A}_i\| \leq \|\hat{Y}\|} |f(\hat{Y})|.
\]

(36a)

(36b)

\( \|\hat{A}_i\| \) can be efficiently calculated by restricting \( \hat{Y} \) to the model subspace and using the Lanczos method\textsuperscript{15}.

To guarantee the existence of solutions as in section III A, a method must calculate the \( \hat{A}_i \) sequentially by reducing a discrete analogue of \( \Omega(\lambda) \),

\[
\Omega_i[\hat{A}_i] = \frac{1}{2} \|\tilde{P}_C \exp(\hat{A}_i) \tilde{H}_{M,i-1} \|^2.
\]

(37)

Direct minimization of \( \Omega_i[\hat{A}_i] \) requires the calculation of an accurate gradient, which is prohibitively expensive for large \( \|\hat{A}_i\| \). The gradient of \( \Omega_i[\hat{A}_i] \) can be avoided by constructing a cheaper bounding functional, \( \Omega_i[\hat{A}_i] \leq \Lambda_i[\hat{A}_i] \). Minimization of \( \Lambda_i[\hat{A}_i] \) approximately minimizes \( \Omega_i[\hat{A}_i] \). With this strategy, the exponential of \( \hat{A}_i \) only needs to be accurately evaluated once per \( i \) to calculate \( \tilde{H}_{M,i} \). The tightness of the \( \Lambda_i[\hat{A}_i] \) bound will determine the number of generators required to solve Eq. \( (23) \). Specifically, if \( \Lambda_i[\hat{A}_i] - \Omega_i[\hat{A}_i] \propto \|\hat{A}_i\|d \) for small \( \|\hat{A}_i\| \), then the asymptotic convergence will be \( \Omega_i[\hat{A}_i] \propto \Omega_{i-1}[\hat{A}_{i-1}]^d \). The only
limitation on the choice of \( \Lambda_i[\hat{A}_i] \) is that it must match \( \Omega_i[\hat{A}_i] \) up to second order in \( \hat{A}_i \) to correctly treat the cases in section III A where \( d^2\Omega(\lambda)/d\lambda^2 \) is required to calculate \( \tilde{\Lambda}(\lambda) \).

Ultimately, the choice of \( \Lambda_i[\hat{A}_i] \) must be guided by the specific details of a particular application and computing environment. Some examples of bounds on \( \Omega_i[\hat{A}_i] \) are

\[
\sqrt{2\Omega_i[\hat{A}_i]} \leq \left| \mathcal{P}_C \sum_{j=0}^{d} \frac{\hat{A}_i^j}{j!} \hat{H}_{M,i,j-1} \right| + a_d([\hat{A}_i])\|\hat{H}_{M,i,j-1}\|, \tag{38}
\]

derived by splitting the exponential Taylor series with the triangle inequality and applying Eq. (36a). If one of these bounds is minimized, \( a_d([\hat{A}_i]) \) effectively acts as a Lagrange multiplier to constrain the size of \( [\hat{A}_i] \) and thus reduce unnecessary transformations and their associated truncation errors. Whatever the choice of \( \Lambda_i[\hat{A}_i] \), standard methods can be used for functional minimization. Convergence of the minimization procedure will depend on the condition number of the Hessian matrix and the ability to effectively precondition the gradient.

### IV. APPLICATION TO FERMIONS

Several ingredients are required to apply the theory developed in section III to many-fermion systems. First, new notation is introduced to simplify many-fermion operator algebra. Second, model and generator subspaces are chosen to satisfy the existence criteria in section III A. Third, a bounding functional \( \Lambda_i[\hat{A}_i] \) and its gradient preconditioner are specified to satisfy the requirements in section III B.

A few basic but non-standard occupation vector operations are used throughout this section. Vector-valued operations are modular addition and three set-theoretic operations, defined by their components as

\[
\begin{align*}
[f \oplus g]_i &= (f_i + g_i) \mod 2 \tag{39a} \\
[f \cap g]_i &= f_i g_i \tag{39b} \\
[f \cup g]_i &= f_i + g_i \tag{39c} \\
[f \setminus g]_i &= f_i - g_i \tag{39d}
\end{align*}
\]

An occupation vector norm is defined as \( \|x\| = \sum_i |x_i| \). Also useful is a fermion sign function,

\[
s(f, g) = (-1)^{\sum_i (f_i \Sigma_{j<i} g_j)}, \tag{40}
\]

which obeys several useful identities,

\[
\begin{align*}
&s(f, g)s(h, g) = s(f \oplus h, g) \tag{41a} \\
&s(f, g)s(f, h) = s(f, g \oplus h) \tag{41b} \\
&s(f, f) = (-1)^{\|f\|/2} \tag{41c} \\
&s(f, g)s(g, f) = (-1)^\|f\|\|g\| - f^g, \tag{41d}
\end{align*}
\]

and accounts for all sign changes resulting from fermion anti-commutations.

Operator algebra is simplified by indexing operator basis elements with pairs of occupation vectors. A simple example of such an operator is an outer product of Slater determinants, \( |f\rangle |g\rangle \). However, physical many-fermion operators such as in Eq. (1) are compactly represented with products of elementary fermion operators and not Slater determinant outer products. Two types of operator basis elements of this form are considered,

\[
\begin{align*}
\hat{B}(f, g) &= i\|f \oplus g\|/2 \mod 2 \\
&\times \prod_j [1 - f_j(1 - g_j) + (1 - 2\tilde{n}_j)f_jg_j + (\tilde{c}_j^\dagger + \tilde{c}_j)f_j(1 - g_j) + i(\tilde{c}_j^\dagger - \tilde{c}_j)(1 - f_j)g_j], \tag{42a} \\
\hat{C}(f, g) &= \prod_j [1 - f_j(1 - g_j) + (1 - 2\tilde{n}_j)f_jg_j + \tilde{c}_j^\dagger f_j(1 - g_j) + \tilde{c}_j(1 - f_j)g_j], \tag{42b}
\end{align*}
\]

each with distinct advantages and disadvantages.

\( \hat{B}(f, g) \) and \( \hat{C}(f, g) \) share several basic properties. They are both off-diagonal for \( f \neq g \) and diagonal for \( f = g \). Also, \( \hat{B}(f, f) = \hat{C}(f, f) \). Each set of elements is trace-orthogonal and both have simple normalizations,

\[
\|\hat{B}(f, g)\|^2 = 2^n \quad \text{and} \quad \|\hat{C}(f, g)\|^2 = 2^{n-\|F \oplus G\|}, \tag{43}
\]

where \( n \) is the total number of fermion degrees of freedom. Operators can be decomposed in either basis,

\[
\begin{align*}
\hat{X} &= 2^{-n} \sum_{f, g} \text{Tr}[\hat{B}(f, g)\hat{X}]\hat{B}(f, g) \tag{44a} \\
\hat{X} &= 2^{-n} \sum_{f, g} 2^{\|F \oplus G\|} \text{Tr}[\hat{C}(f, g)\hat{X}]\hat{C}(f, g). \tag{44b}
\end{align*}
\]

Basis transformations can be calculated by representing the elements of one basis in another basis,

\[
\begin{align*}
\hat{C}(f, g) &= i^{-\|F \oplus G\|/2} \mod 2 + |g\rangle |f\rangle \mod 2 - |F \oplus G\| \\
&\times \sum_{h, \{f, g\}=0} \hat{B}(f \oplus h, g \oplus h) \tag{45a} \\
\hat{B}(f, g) &= i^{-\|F \oplus G\|/2} \mod 2 - |g\rangle |f\rangle \\
&\times \sum_{h, \{f, g\}=0} (-1)^{\Sigma_h} \hat{C}(f \oplus h, g \oplus h). \tag{45b}
\end{align*}
\]

Further properties of the operators deviate.

The \( \hat{B}(f, g) \) operators are Hermitian and unitary and have simple algebraic properties. The action of \( \hat{B}(f, g) \) on a Slater determinant produces another Slater determinant with an \( i^n \) phase factor,

\[
\begin{align*}
\hat{B}(f, g)|h\rangle &= \theta(f, g, h)|f \oplus g \oplus h\rangle \tag{46a} \\
\theta(f, g, h) &= (-1)^{\Sigma_h} s(f \oplus g, h) \\
&\times i^{-\|F \oplus G\|/2} \mod 2 + |g\rangle |f\rangle. \tag{46b}
\end{align*}
\]
The product of two $\hat{B}(f, g)$ basis operators is a single other basis operator with another $i^m$ phase factor,

$$\hat{B}(f, g) \hat{B}(h, k) = \phi(f, g, h, k) \hat{B}(f \oplus h, g \oplus k)$$  \hspace{1cm} (47a)

$$\phi(f, g, h, k) = s(f \oplus h, g \oplus k)(-1)^{\|f\oplus h\|\cdot\|g\oplus k\|}$$

$$\times \left( -1 \right)^{(f \cap g) \cdot (k \cap h) + (f \cap g) \cdot (h \cap k)}$$

$$\times j\left((f \cap g) \cdot (h \cap k) - \|f \oplus g\| \|h \oplus k\| \right) \text{ mod 2}$$

$$\times j\left((f \cap h) \cdot (g \cap k) \right) \text{ mod 2}. \hspace{1cm} (47b)$$

The commutator formula is equally simple,

$$[\hat{B}(f, g), \hat{B}(h, k)] = 2i \text{Im} \phi(f, g, h, k) \hat{B}(f \oplus h, g \oplus k). \hspace{1cm} (48)$$

The algebra of the $\hat{B}(f, g)$ operators bears similarities to the Pauli matrices and they might be considered as a many-fermion analogue.

The important advantage of $\hat{C}(f, g)$ over $\hat{B}(f, g)$ is its ability to exploit 1-fermion symmetries. These symmetries arise from 1-fermion invariant operators that commute with a Hamiltonian, $[\hat{S}, \hat{H}] = 0$. Without loss of generality, $\hat{S}$ is Hermitian. The vanishing commutator allows $\hat{S}$ and $\hat{H}$ to be simultaneously diagonalized. The fermion operators can be chosen to diagonalize $\hat{S}$, resulting in the simple commutation relations

$$[\hat{S}, \hat{c}_i] = s_i \hat{c}_i. \hspace{1cm} (49)$$

Examples of common 1-fermion invariant operators are total fermion number, total fermion spin, lattice vector translations, and point group operations. The $\hat{C}(f, g)$ operators retain the simple commutation relations,

$$[\hat{S}, \hat{C}(f, g)] = \hat{C}(f, g) \sum_i s_i (g_i - f_i). \hspace{1cm} (50)$$

Only $\hat{C}(f, g)$ operators that commute with $\hat{S}$ are required to represent $\hat{H}$ and the symmetry-preserving generators $\hat{A}$ that diagonalize it.

The disadvantage of the $\hat{C}(f, g)$ operators is their more complicated operator algebra. They are not Hermitian and are related to their Hermitian conjugates by

$$\hat{C}^\dagger(f, g) = (-1)^{\|f \oplus g\|/2} \hat{C}(g, f). \hspace{1cm} (51)$$

The action of $\hat{C}(f, g)$ on Fock states can now produce zero,

$$\hat{C}(f, g)|\mathbf{h}\rangle = \mathbf{v}(h - g + f)(-1)^{(f \cap g) \cdot h}$$

$$\times s(f \oplus g, h)|f \oplus g \oplus h\rangle, \hspace{1cm} (52)$$

encoded in an occupation vector validity function,

$$\nu(x) = \begin{cases} 1, & x \in \{0, 1\}^n \\ 0, & \text{otherwise} \end{cases} \hspace{1cm} (53)$$

The product of two basis operators is no longer always a single basis operator,

$$\hat{C}(f, g) \hat{C}(h, k) = \mathbf{v}(f - g + h - k)s(f \oplus g, h \oplus k)(-1)^{(f \cap h) \cdot (g \cap h) \cdot 2 - (f \cap g) \cdot (h \cap k)}$$

$$\times \sum_{\mathbf{z} \setminus \{f \cap g\} \setminus \{h \cap k\} = \emptyset} (-1)^{\|\mathbf{z}\| \cdot (g \cap h)} \hat{C}(x \oplus \mathbf{z}, y \oplus \mathbf{z}) \hspace{1cm} (54)$$

In this arrangement, $\hat{C}(x, y)$ is the contribution with the smallest value of $\|\{x \oplus \mathbf{z}\} \cup \{y \oplus \mathbf{z}\}\|$. The commutator formula is just two applications of the product formula and does not further simplify except to cancel some terms in the sum over $\mathbf{z}$ and vanish when

$$(f \oplus g) \cdot (h \oplus k) = 0 \hspace{1cm} \text{and} \hspace{1cm} (f \cap k) \cdot (g \cap h) + (g \oplus h) \cdot (f \cap k)$$

$$+ \|f \oplus g\| \|h \oplus k\| \text{ mod } 2 = 0. \hspace{1cm} (55)$$

### A. Model and generator subspaces

The model subspace of a many-fermion system should contain all operators necessary for an accurate physical description of the Hamiltonian as it is transformed to a diagonal form. It is generally observed that basis operators containing fewer elementary fermion operators have more physical importance. In systems where the physics is geometrically local, geometric constraints may also determine the importance of basis operators. Careful study might reveal further crucial system-specific sets of basis operators, distinct from either general criterion. To allow for all these possibilities, the model subspace is defined
by an allowed set of occupation vectors $V$ as
\begin{equation}
\{ \hat{B}(f, g) : f \cup g \in V \}, \; f \in V \implies f \setminus x \in V.
\end{equation}
\(\hat{B}(f, g)\) and \(\hat{C}(f, g)\) are interchangeable in this definition.

The constraints on $V$ are minimal and it is straightforward to expand any set to satisfy them. Operators in the span of this basis are defined to be $V$-sparse.

The generator subspace is chosen to contain all off-diagonal and anti-Hermitian operators in the model subspace. In terms of $\hat{B}(f, g)$, this means basis elements of the form $i\hat{B}(f, g)$, $f \neq g$. In terms of $\hat{C}(f, g)$, this means basis elements of the form $\hat{C}(f, g) - \hat{C}^\dagger(f, g)$ for a real operator space. For a complex operator space, the subspace must also include $i(\hat{C}(f, g) + \hat{C}^\dagger(f, g))$, $f \neq g$. This choice minimizes the truncation errors in a weak, "greedy" way. For a given $f$ in $V$, if a Hamiltonian contains only terms of the form $\hat{B}(g, h)$ with $(g \cup h) \setminus f = 0$, then diagonalization can be performed exactly.

The use of $\hat{B}(f, g)$ or $\hat{C}(f, g)$ as both an operator basis and subspace basis simplifies operator truncation. Since the basis elements are trace-orthogonal, projections using $\mathcal{P}_M$ or $\mathcal{P}_G$ just discard elements not in the subspace. This can be physically interpreted as a form of normal ordering based truncation. The standard normal ordering rules for a reference Slater determinant $|z\rangle$ arrange all number operators into the form $n_m - z_m$ as in $\hat{C}^\dagger(f, g)$ defined below in Eq. (65). If the reference is an ensemble of Slater determinants with statistically uncorrelated occupations, $z_m \in [0, 1]$, the standard normal ordering rules still apply. The $\hat{C}(f, g)$ operators and truncation derived in section III correspond to the infinite temperature thermal ensemble, $z_m = 1/2$, that equally weights all fermion configurations. This prevents the physics from being biased by a choice of reference state. For a truncation process meant to approximate the entire spectrum of a many-fermion system, it is unreasonable to expect any one reference state to be suitable for the description of all eigenstates.

The suggested choice of model and generator subspace defined by $V$-sparsity satisfies all the criteria established in section IIIA to guarantee Hamiltonian diagonalization. The only criterion that requires discussion is the existence of non-zero values for Eq. (38). The analysis is simplest in the $\hat{C}(f, g)$ basis because the truncated diagonal commutator $\hat{P}_G \hat{C}^\dagger \hat{M}^D \hat{P}_M^C$ preserves the vector $f - g$. This property can be exploited by writing the Hamiltonian in the form
\begin{equation}
\hat{H}_M = \hat{H}_M^D + \sum_{f \neq g} \hat{C}(f, g) \hat{D}(f, g),
\end{equation}
where $\hat{D}(f, g)$ are non-zero diagonal Hermitian operators that commute with $\hat{C}(f, g)$. If $\hat{H}_M$ is in the right null space of $\mathcal{P}_G \hat{C}^\dagger \hat{M}^D \mathcal{P}_M^C$, then each non-zero term of the form $\hat{C}(f, g) \hat{D}(f, g)$ is also in the null space. The generator $\hat{A}$ can be chosen as any anti-Hermitian combination of these null operators. If the generator is chosen to be $[\hat{C}(f, g) - \hat{C}^\dagger(f, g)] \hat{D}(f, g)$ then the existence condition reduces to
\begin{equation}
\|\hat{P}_M \hat{D}^2(f, g)[\hat{C}(f, g), \hat{C}(f, g)]\| \neq 0.
\end{equation}
The left hand side of Eq. (58) can be bounded from below by replacing $\hat{D}^2(f, g)$ by its trace. For $\hat{D}(f, g) \neq 0$, the trace of $\hat{D}^2(f, g)$ is non-zero and can be ignored. The remaining commutator is unaffected by the truncation and can be explicitly calculated as
\begin{equation}
\|\hat{C}(f, g)\| \leq 2\|f \otimes g\| \sqrt{2^n + b(\|f \oplus g\|)}
\end{equation}
\begin{equation}
b(i) = \sum_{j=0}^{[(i-1)/2]} \frac{i!}{(i-2j-1)!(2j+1)!}.
\end{equation}
The commutator always has a non-zero norm, which establishes that Eq. (58) is satisfied.

\section{B. Bounding functional and preconditioner}

The bounding functional is chosen to match the form of Eq. (38) for $d = 2$, which is the simplest allowed functional of that form. With this choice, the asymptotic convergence is $\|\hat{H}_{M,i}^C\| \propto \|\hat{H}_{M,i-1}^C\|^3$. The functional can be written suggestively as
\begin{align}
\Lambda_i[\hat{A}_i] &= \frac{1}{2}\|\hat{H}_{M,i-1}^C + \hat{P}_G \hat{C} \hat{M}^D \hat{P}_M^C[\hat{A}_i, \hat{H}_{M,i-1}^C]\| \\
&+ a_2(\|\hat{A}_i\|)\|\hat{H}_{M,i-1}^C\|^2 \tag{60a}
\end{align}
\begin{align}
\hat{H}_{M,i-1}^C &= \hat{H}_{M,i-1}^C + \frac{1}{2} \hat{P}_M[\hat{A}_i, \hat{H}_{M,i-1}^C] \tag{60b}
\end{align}
\begin{align}
\alpha &= \|\hat{A}_i\|/\|\hat{A}_i\| \tag{60c}
\end{align}
This form enables the calculation of $\|\hat{A}_i\|$ to be weakly coupled to the minimization of $\Lambda_i[\hat{A}_i]$ if $\alpha$ has a weak dependence on $\hat{A}_i$.

A preconditioner is constructed by approximating the inverse Hessian of $\Lambda_i[\hat{A}_i]$. This is straightforward in the untruncated case. When diagonalization is converged, the Hessian reduces to $\hat{C} \hat{D}^2$. A preconditioner that is exact in this limit is
\begin{align}
\hat{F} &= \sum_{f \neq g} \frac{\langle f | g \rangle \otimes \langle f | g \rangle}{\Delta(f, g)}, \tag{61a}
\end{align}
\begin{align}
\Delta(f, g) &= (\langle f | \hat{H}_{M,i-1}^C | f \rangle - \langle g | \hat{H}_{M,i-1}^C | g \rangle)^2 \\
&+ 4 \|\langle f | \hat{H}_{M,i-1}^C | g \rangle\|^2 + \beta. \tag{61b}
\end{align}
This form includes approximate off-diagonal corrections using the quadratic formula and an extra uniform shift $\beta$. The shift acts as either a tuning parameter to adjust the size of the preconditioned gradient or to approximate the effects of $a_2(\|\hat{A}_i\|)$ on the Hessian when $\|\hat{A}_i\|$ gets large. (WIP)
There is no natural extension of Eq. (61a) to the truncated case using the $\hat{B}(f, g)$ or $\hat{C}(f, g)$ basis elements. However, this preconditioner can be approximated by defining a basis $\hat{E}_V^z(f, g)$ of the $V$-sparse subspace that mimics the Slater determinant outer products,

$$\langle f \oplus z | \hat{E}_V^z(h, k) | g \oplus z \rangle = \delta(\|h\| \delta(\|g - k\|)) \quad (62)$$

for $f \cup g \in V$ and $h \cup k \in V$. $\delta(\cdot)$ is the Kronecker delta function ($\delta(0) = 1, \delta(i \neq 0) = 0$). These operators are defined with respect to a reference Slater determinant $|z\rangle$. A $V$-sparse operator $\hat{X}_V$ can be decomposed in this basis using its matrix elements,

$$\hat{X}_V = \sum_{f \cup g \in V} \langle f \oplus z | \hat{X}_V | g \oplus z \rangle \hat{E}_V^z(f, g). \quad (63)$$

The analogue of Eq. (61a) using $\hat{E}_V^z(f, g)$ is

$$\hat{F} = \sum_{f \cup g \in V} \frac{\hat{E}_V^z(f, g) \otimes (f \oplus z) | g \oplus z \rangle}{\Delta(f \oplus z, g \oplus z)} \quad (64)$$

The choice of $z$ is arbitrary, but it should not have a strong effect on the quality of the preconditioner.

An efficient explicit construction of $\hat{E}_V^z(f, g)$ requires the definition of an intermediate operator basis,

$$\hat{C}(f, g) = s(f \oplus g, g \oplus z)$$

$$\times \prod_{i} \{ (1 - f_i)(1 - g_i) \} + \hat{n}_i f_i g_i + (1 - 2\hat{n}_i) z_i f_i g_i + \hat{c}_i^{}[f_i(1 - g_i) + z_i(g_i - f_i)] + \hat{c}_i^{}[(1 - f_i)g_i + z_i(f_i - g_i)] \quad (65)$$

This is a variant of $\hat{C}(f, g)$ that is normal ordered with respect to $|z\rangle$. $\hat{E}_V^z(f, g)$ can be constructed by writing $|f \oplus z \rangle |g \oplus z \rangle$ in terms of $\hat{C}^z(f, g)$ and projecting into the $V$-sparse subspace,

$$\hat{E}_V^z(f, g) = \sum_{\substack{f \cup g \in V \\{f, g\} \otimes h \in V \\{f, g\} \otimes h = 0}} \{ (1 - f_i)(1 - g_i) \} \hat{C}^z(f \oplus h, g \oplus h) \quad (66a)$$

$$\hat{C}^z(f, g) = \sum_{\substack{f \cup g \in V \\{f, g\} \otimes h \in V \\{f, g\} \otimes h = 0}} s(f \oplus g, h) \hat{E}_V^z(f \oplus h, g \oplus h). \quad (66b)$$

The inverse transformation is calculated using Eq. (63). The transformations between $\hat{E}_V^z(f, g)$ and $\hat{C}^z(f, g)$ are independent of $z$.

A few remaining formulas are required to transform between the $\hat{B}(f, g)$ basis and $\hat{E}_V^z(f, g)$ basis. The missing intermediate steps are the transformations between $\hat{C}(f, g)$ and $\hat{C}^z(f, g)$,

$$\hat{C}(f, g) = (1 - f \cup g) s(f \oplus g, g \oplus z) \quad (67a)$$

$$\times \sum_{h \{f \cup g\} = 0} (-2) \|h\| s(f \oplus g, h) \times \hat{C}^z(f \oplus h, g \oplus h)$$

$$\hat{C}^z(f, g) = 2^{-f \cdot g} s(f \oplus g, g \oplus z) \quad (67b)$$

$$\times \sum_{h \{f \cup g\} = 0} (-1) \|h\| \|z\| \hat{C}(f \oplus h, g \oplus h),$$

with $f' = (f \setminus z) \oplus (g \cap z) \oplus (f \cap g)$ and $g' = (g \setminus z) \oplus (f \cap z) \oplus (f \cap g)$. (67c)

The complete transformation is performed as a sequence of three intermediate steps: $B \leftrightarrow C$ using Eq. (45), $C \leftrightarrow C^z$ using Eq. (67), and $C^z \leftrightarrow \hat{E}_V^z$ using Eq. (66).

### V. TRUNCATED EIGENFERMION DECOMPOSITION

Many-fermion methods, especially those in quantum chemistry, are often arranged as a systematic hierarchy of increasing cost and accuracy. While it is possible to construct a TED for a flexible choice of operator basis limited only by Eq. (56), this section considers only a specific hierarchy of methods. The methods are referred to as TEDr for an integer $r$ and defined by the model operator subspace

$$\{ \hat{C}(f, g) : \|f \cup g\| \leq r \}. \quad (68)$$

TEDr is exact for $r = n$ and accuracy should systematically improve with increasing $r$. Computational scaling of the methods depend on $r$ and the total number of fermion degrees of freedom $n$. The memory required to store each operator scales as $O(n^r)$. Commutation of operators is the most computationally expensive step of the TED and scales as $O(n^{1.5r})$ operations. $O(n^r)$ memory and $O(n^{1.5r})$ operations are taken to be the computational budget of TEDr for calculating physical properties following the diagonalization of a Hamiltonian.

A Hamiltonian diagonalized by TEDr as in Eq. (7) has the form

$$\hat{D} = \sum_{\|f\| \leq r} d(f) \hat{C}(f, f). \quad (69)$$

An eigenvalue $E(z)$ can be calculated with this formula by replacing $\hat{n}_i$ with $z_i$. This calculation scales as $O(n^r)$ operations. Only $O(n^{1.5r}/r)$ eigenvalues can be calculated this way before the computational budget is exhausted. A specialized alternative is to transform $\hat{D}$ into the $\hat{E}_V^z(f, f)$ operator basis,

$$\hat{D} = \sum_{\|f\| \leq r} E(f \oplus z) \hat{E}_V^z(f, f). \quad (70)$$
This simultaneously calculates $O(n^r)$ eigenvalues corresponding to few-fermion excitations from a reference eigenstate $|\Psi(z)\rangle$. Each of these transformations costs $O(n^r)$ operations, which increases the total number of computable eigenvalues to $O(n^{1.5r})$.

It is in the study of energetics that the TED can be considered a quantum-to-classical mapping. All energies come from $E(f)$ in Eq. (3a), which for TED$_r$ has a form that resembles the total energy cluster expansions used in the study of alloys. The complexity of finding the ground state is dramatically reduced from the initial Hamiltonian,

$$ \langle \Psi | H | \Psi \rangle $$

from $\min \langle \Psi | H | \Psi \rangle / f$ to $\min E(f)$. \hspace{1cm} (71)

A minimization over $2^n$ complex numbers is reduced to $n$ binary choices. Complexity theory still classifies both problems as hard, QMA-complete for the quantum problem and NP-complete for the classically-mapped problem. Practically, many physical systems of interest are unfrustrated and will result in easy instances of minimization over $E(f)$. Even in hard cases, simple heuristics can give good results. Eq. (70) can be calculated for random sets of $z$ and energy-lowering few-fermion excitations can be successively applied. In an easy problem, most or all initial configurations will relax to the ground state. A hard “glassy” problem will have many distinct local minima in configuration space. In “exotic” systems where the low-energy excitations are not few-fermion excitations, this procedure might help to map out the energy landscape.

To calculate eigenstate matrix elements of an operator $X$, a truncated unitary transformation is performed. This exactly calculates $U^\dagger X^r U$ for a perturbed operator $X^r = X - U X_0 U^\dagger$ as in Eq. (22). The transformation costs $O(n^{1.5r})$ operations, which exceeds the computational budget if more than $O(1)$ operators are calculated in this manner. Calculations of this nature are able to produce a large amount of spectral information for a small number of operators. This might be useful for categorizing eigenstates and transitions based on a small number of important observables. By rewriting the transformed operator in the $E^r(f, g)$ operator basis,

$$ \hat{U}^\dagger X^r \hat{U} = \sum_{\|f-g\| \leq r} \langle \Psi(f+z) | X^r | \Psi(g+z) \rangle E^r(f, g), \hspace{1cm} (72) $$

a set of approximate matrix elements close to a reference eigenstate $|\Psi(z)\rangle$ can be efficiently computed.

The calculation of reduced density matrices is an established application of truncated unitary transformations. They can be calculated as a subset of $\langle \Psi(z)|C(f, g)|\Psi(z)\rangle$ for a chosen eigenstate and all elements of the model subspace. To close this calculation, the infinitesimal transformation of a matrix element must be related back to the untransformed matrix elements. The key step is performing the transformation backwards by defining a new unitary operator $\hat{V}(\lambda)$ that evolves as

$$ \frac{d}{d\lambda} \hat{V}(\lambda) = -\hat{A}(\lambda_F - \lambda) \hat{V}(\lambda), \hspace{1cm} (73) $$

with initial condition $\hat{V}(0) = \hat{I}$. The entire transformation that defines $\hat{U}$ must occur in the interval $[0, \lambda_F]$, resulting in $\hat{V}(\lambda_F) = \hat{U}$. Using the same truncation as in the transformation of operators, the truncated transformation of matrix elements is defined as

$$ \frac{d}{d\lambda} \langle \hat{C}(f, g) \rangle / \lambda = \langle \hat{F}_M [\hat{A}(\lambda_F - \lambda), \hat{C}(f, g)] \rangle / \lambda, \hspace{1cm} (74) $$

with $\langle \hat{C}(f, g) \rangle / \lambda \approx \langle z | \hat{V}^\dagger (\lambda) \hat{C}(f, g) \hat{V}(\lambda) | z \rangle$. For a piecewise constant generator, the transformation can be evaluated as a sequence of superoperator exponentials,

$$ \langle \hat{C}(f, g) \rangle_i = \langle \exp(\hat{A}_{m-i+1}) \hat{C}(f, g) \rangle_{i-1}, \hspace{1cm} (75) $$

where $m$ is the number of generator segments. As with operator transformations, the cost of this calculation scales as $O(n^{1.5r})$ operations.

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1. J. Olsen, P. Jørgensen, and J. Simons, Chem. Phys. Lett. 169, 463 (1990).
2. G. Oinada, L. Reining, and A. Rubio, Rev. Mod. Phys. 74, 601 (2002).
3. W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal, Rev. Mod. Phys. 73, 33 (2001).
4. U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005).
5. A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
6. F. Wegner, J. Phys. A 39, 8221 (2006).
7. S. R. White, J. Chem. Phys. 117, 7472 (2002).
8. T. Yanai and G. K.-L. Chan, J. Chem. Phys. 127, 104107 (2007).
9. F. Wegner, Ann. Physik 3, 77 (1994).
10. A. G. Taube and R. J. Bartlett, Int. J. Quantum Chem.
106, 3393 (2006).

11 A. Hübsch, S. Sykora, and K. W. Becker arXiv:0809.3360.

12 D. A. Mazziotti, Phys. Rev. Lett. 97, 143002 (2006).

13 N. J. Wildberger, P. Am. Math. Soc. 119, 649 (1993).

14 R. J. Bartlett and M. Musial, Rev. Mod. Phys. 79, 291 (2007).

15 B. N. Parlett, H. Simon, and L. M. Stringer, Math. Comput. 38, 153 (1982).

16 J. M. Sanchez, F. Ducastelle, and D. Gratias, Physica A 128, 334 (1984).

17 J. Kempe, A. Kitaev, and O. Regev, SIAM J. Comput. 35, 1070 (2006).

18 F. Barahona, J. Phys. A 15, 3241 (1982).