Low-rank decomposition for quantum simulations with complex basis functions

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(Dated: 21 September 2021)

Low-rank decompositions to reduce the Coulomb operator to a pairwise form suitable for its quantum simulation are well-known in quantum chemistry, where the underlying basis functions are real-valued. We generalize the result of Ref. [1] to complex basis functions \( \psi_p(r) \in \mathbb{C} \) by means of the Schur decomposition and decomposing matrices into their symmetric and anti-symmetric components. This allows the application of low-rank decomposition strategies to general basis sets.

I. INTRODUCTION

When simulating a second quantized Hamiltonian of a fermionic system with a quantum computer, recent works employed low-rank decomposition strategies known from classical simulation algorithms to express the interaction terms as sums of squares of one-body operators \([1,2,3]\), which allows for a simulation in terms of fermionic Gaussian unitaries and Ising-type interactions\([4,5]\). With the exception of Ref. [6], all such decomposition strategies rely on symmetry properties of the two-body matrix elements in the second-quantized form which result from the the underlying single-particle basis functions being real-valued. This in particular applies to molecular electronic structure type Hamiltonians, which in general do not require complex basis functions\([6]\).

However, other quantum systems exist that are better described by complex basis functions, where the decomposition strategy of Ref. [1] can no longer be applied. One prominent example are Landau-level wave functions\([7]\) used to represent the Hamiltonian describing the fractional quantum Hall effect\([8,9]\). Our work shows how one can employ the low-rank representation of the Hamiltonian terms describing the two-body interaction systems represented by complex-valued single-particle basis functions.

This paper is structured as follows. In Section II we review the low-rank strategy introduced by Motta et al., extend their result to complex-valued basis functions in Section III, and conclude in Section IV.

II. LOW-RANK REPRESENTATION FOR REAL-VALUED BASIS FUNCTIONS

Second quantized time-independent Hamiltonians that describe a non-relativistic system of \( N_f \) interacting fermions are typically of the following form,

\[
\hat{H} = \hat{H}_1 + \hat{H}_2,
\]

where \( \hat{H}_1 (\hat{H}_2) \) contains a linear combination of a quadratic (quartic) polynomial of fermionic annihilation and creation operators, more specifically

\[
\hat{H}_1 = \sum_{p,q=1}^{N_f} f_{p,q} \hat{c}_p \hat{c}_q,
\]

\[
\hat{H}_2 = \frac{1}{2} \sum_{p,q,r,s=1}^{N_f} h_{p,q,r,s} \hat{c}_p \hat{c}_q \hat{c}_r \hat{c}_s,
\]

where \( f \) is a two-dimensional tensor describing the one-body terms such as kinetic energy or local potentials and \( h \) is a four-dimensional tensor describing the physical (e.g. Coulomb-) interaction. Here, \( \hat{c}_p \) and \( \hat{c}_q \) are fermionic creation and annihilation operators acting on the spin-orbitals \( p \) and \( q \), \( f_{p,q} \) and \( h_{p,q,r,s} \) are overlap integrals where the subscript \( p \) corresponds to the \( p \)-th single particle function \( \psi_p(r) \). The factor \( \frac{1}{2} \) corrects for counting the interaction between two indistinguishable fermions twice. The tensors \( f \) and \( h \) carry a structure that depends on the employed basis functions, the quantum system at hand, and naturally reflect the fermionic nature of the problem.

In this section, we will present a condensed version of the method described in Ref. [1], where \( \hat{H} \) (using a real-valued basis set) can be rewritten as the sum-of-squares of one-particle operators, which allows for a relatively simple quantum simulation of its exponential map, e.g. required to simulate its time evolution\([10]\).

For sets of real-valued basis functions \( \psi_p(r) \in \mathbb{R} \), explicit expressions were given for rewriting the Hamiltonian in Eq. (1) as

\[
\hat{H} = \sum_{p,q} f_{p,q} \hat{c}_p \hat{c}_q + \sum_{p,q} S_{p,q} \hat{c}_p \hat{c}_q + \frac{1}{2} \sum_{L=1}^{N_f} \sum_{i,j} \lambda^{(L)}_{i,j} \hat{h}^{(L)}_{i,j} \hat{h}^{(L)}_{i,j}
\]

\[
\equiv \hat{F} + \hat{S} + \sum_{L} \hat{V}^{(L)},
\]

where \( f \) (\( S \)) is a two-dimensional tensor containing all one-body contributions (from the interaction term), \( \hat{h}^{(L)}_{i,j} \) are number operators in a rotated basis, and \( \lambda^{(L)}_{i,j} \) are coefficients. In fact, the coefficients \( \lambda^{(L)}_{i,j} \) are connected to the spectrum of the reshaped tensor \( h \) and can be used to truncate the summation over \( L \), which can lead to a significant reduction in simulation cost at low truncation error\([11]\). Importantly, the creation and annihilation operators in the rotated basis only satisfy the an-
ticommutation relations for a fixed $L$ and not for $L' \neq L$. This implies that $[\hat{U}^{(L)}, \hat{U}^{(L')}] \neq 0$, in general.

As one can see from Eq. (4), the simplicity of its quantum simulation becomes evident when applying the Jordan-Wigner transformation\(^\text{13}\). Then, the fermionic number operators (after applying the single-particle transformation $\hat{U}_L$) is diagonal with no appearance of Pauli-$Z$ strings, allowing for a simple simulation by means of an Ising-type interaction.

The exponential map of the Hamiltonian operator (e.g. for performing a unitary time evolution step) can than be approximated by a Trotter step to first order\(^\text{14}\),

$$e^{i\Delta H} \approx e^{i\Delta (\hat{F} + \hat{S})} \prod_{L=1}^{N^2_f} \left( \hat{U}^{(L)} e^{i\Delta \hat{U}^{(L)}} \left( \hat{U}^{(L)} \right)^\dagger \right),$$

where $\hat{U}^{(L)}$ are basis rotation operations which can be implemented through Givens rotations\(^\text{15}\). As discussed in Ref.\(^\text{1}\), all terms on the right-hand side can be implemented using a low-order polynomial number of Givens rotations and phase gates\(^\text{16}\). The purpose of this work is to give the explicit expressions for the basis rotations for the case that the underlying single-particle basis functions in Eq. (1) are complex-valued.

III. FACTORIZATION OF THE INTERACTION TERM FOR COMPLEX-VALUED BASIS FUNCTIONS

In the following, we will make extensive use of flattening (also known as reshaping) of tensors, which is why we will be rigorous with comma-separated notation in the subscripts, e.g. $h_{p,q,r,s}$ is a $\{N_f \times N_f \times N_f \times N_f\}$-tensor, while $h_{pq,rs}$ denotes the reshaped $\{N_f^2 \times N_f \times N_f\}$-tensor, where the first two dimensions are flattened.

We consider the interaction term

$$\hat{H}_2 = \frac{1}{2} \sum_{p,q,r,s=1}^{N_f} h_{pq,rs} \varepsilon_p^\dagger \varepsilon_q^\dagger \varepsilon_r \varepsilon_s,$$

where the two-body matrix elements are defined as

$$h_{pq,rs} = \frac{1}{4} (v_{p,q,r,s} + v_{q,p,r,s} - v_{p,q,r,s} - v_{p,q,s,r}),$$

$$v_{p,q,r,s} = \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_p^*(\mathbf{r}_1) \psi_q^*(\mathbf{r}_2) \hat{V}(\mathbf{r}_1, \mathbf{r}_2) \times \psi_r(\mathbf{r}_1) \psi_s(\mathbf{r}_2).$$

Here, $\psi_p(\mathbf{r})$ describes the $p$-th basis function for a particle located at position $\mathbf{r}$ and $V(\mathbf{r}_1, \mathbf{r}_2)$ describes the interaction potential between particle 1 and 2, typically given by the Coulomb potential $V(\mathbf{r}_1, \mathbf{r}_2) = 1/|\mathbf{r}_1 - \mathbf{r}_2|$, in appropriate units. We will assume that the resulting tensor elements computed through the two-electron integrals are real-valued, which leads to the property $h_{pq,rs} = (h_{pq,rs})^* = h_{qp,rs}$.

One of the more prominent examples where this holds is for the fractional quantum Hall systems mentioned in the introduction, e.g. Haldane’s spherical model\(^\text{9}\), or the two-dimensional disk geometry\(^\text{10,11}\). Note, that since we have chosen $h_{pq,rs}$ to possess the following symmetries, $h_{pq,rs} = -h_{qp,rs} = -h_{pq,sr} = h_{qp,sr}$, this will also translate to $h_{rs,qp} = -h_{rs,pq}$, resulting in the eight-fold symmetry

$$h_{pq,rs} = -h_{pq,rs} = -h_{pq,sr} = h_{qp,sr} = h_{rs,qp},$$

$$h_{rs,qp} = -h_{rs,pq}.$$  \(\text{(9)}\)

We rewrite Eq. (6) as

$$\hat{H}_2 = \frac{1}{2} \sum_{p,q,r,s=1}^{N_f} h_{pq,rs} \varepsilon_p^\dagger \varepsilon_q^\dagger \varepsilon_r \varepsilon_s + \sum_{p,r=1}^{N_f} h_{pr} \varepsilon_p^\dagger \varepsilon_r,$$

where we defined

$$h_{pr} = -\frac{1}{2} \sum_{q=1}^{N_f} h_{pq,qr}.$$  \(\text{(10)}\)

We begin by transposing the tensor, such that indices belonging to particle 1 (here $p,s$) and particle 2 (here $q,r$) are grouped together. This is followed by flattening the tensor into a $(N_f^2 \times N_f^2)$ matrix, so that $h_{pq,rs} = h_{ps,qr}$. Due to the symmetry properties in Eq. (9), we know that the flattened matrix $h_{ps,qr}$ is real and symmetric, which means that we can diagonalize it by means of a Schur decomposition\(^\text{12}\), which results in

$$h = O^{|h|} \Sigma^{|h|} O^{|h|^T},$$

where $h$ is the flattened tensor with matrix elements $h_{ps,qr}$, $O^{|h|}$ is a $(N_f^2 \times N_f^2)$-real orthogonal matrix, $\Sigma^{|h|}$ is a $(N_f^2 \times N_f^2)$-diagonal matrix with non-negative real-valued entries, and the superscript $|h|$ indicates that $O$ and $\Sigma$ belong here to the decomposition of $h$. With this, we can write the first term on the right-hand side of Eq. (13) as

$$\frac{1}{2} \sum_{p,q,r,s=1}^{N_f^2} h_{ps,qr} \varepsilon_p^\dagger \varepsilon_q^\dagger \varepsilon_s \varepsilon_r = \frac{1}{2} \sum_{p,q,r,s=1}^{N_f^2} \left( O^{|h|} \right)_{ps} \left( \Sigma^{|h|} \right)_{qr} \varepsilon_p^\dagger \varepsilon_q^\dagger \varepsilon_s \varepsilon_r,$$

$$\times \left( O^{|h|} \right)_{ps} \left( \Sigma^{|h|} \right)_{qr} \varepsilon_p^\dagger \varepsilon_q^\dagger \varepsilon_s \varepsilon_r.$$

We now introduce $L$-dependent matrices $O_{L}^{|h|}$ whose matrix elements are given by

$$\left( O_{L}^{|h|} \right)_{ps} = \left( O^{|h|} \right)_{ps,LL}.$$  \(\text{(14)}\)

which can easily be obtained from numpy.\(\text{reshape}()\). We can then write Eq. (13) as

$$\frac{1}{2} \sum_{p,q,r,s=1}^{N_f^2} h_{ps,qr} \varepsilon_p^\dagger \varepsilon_q^\dagger \varepsilon_s \varepsilon_r = \frac{1}{2} \sum_{L=1}^{N_f} \sum_{p,q,r,s} \left( \Sigma^{|h|} \right)_{LL} \left( O_L^{|h|} \right)_{ps} \varepsilon_p^\dagger \varepsilon_s \varepsilon_q \varepsilon_r,$$

and Eq. (12) as

$$h_{ps,qr} = \sum_{L=1}^{N_f^2} \left( O_L^{|h|} \right)_{ps} \left( O_L^{|h|} \right)_{qr}.$$  \(\text{(16)}\)
By introducing the real-valued symmetric and anti-symmetric components of the matrix $O^{[h]}_L$,

$$\mathcal{S}[O_L] = \frac{1}{2} \left( O^{[h]}_L + (O^{[h]}_L)^T \right),$$

$$\mathcal{A}[O_L] = \frac{1}{2} \left( O^{[h]}_L - (O^{[h]}_L)^T \right),$$

we can write Eq. (16) as

$$h_{ps,qr} = \sum_{L=1}^{N_f^2} \sum_{p,s}^{N_f} \sum_{q,r}^{N_f} \left( \mathcal{S}[O_L] \right)_{p,s} \left( \mathcal{S}[O_L] \right)_{q,r} + \sum_{L=1}^{N_f^2} \sum_{ps}^{N_f} \sum_{qr}^{N_f} \left( \mathcal{A}[O_L] \right)_{p,s} \left( \mathcal{A}[O_L] \right)_{q,r},$$

leading to an expression for the interaction term in terms of symmetric and antisymmetric matrices. One might expect two additional terms appearing in Eq. (19), namely the cross terms $\mathcal{S}[O_L] \mathcal{A}[O_L]$ and $\mathcal{A}[O_L] \mathcal{S}[O_L]$, since Eq. (19) is obtained by replacing $O^{[h]}_L$ in Eq. (16) with its symmetric and anti-symmetric components defined in Eqs. (17)-(18). However, the cross terms vanish due to the symmetry constraint $h_{ps,qr} = h_{qp,rs}$, which follows from Eq. (5). If we denote with $L_{\mathcal{S}}$ and $L_{\mathcal{A}}$ the set of indices in $L$ which give a non-zero symmetric matrix $\mathcal{S}[O_L]$ and $\mathcal{A}[O_L]$, respectively, with $L_{\mathcal{S}} \cup L_{\mathcal{A}} = \{1, 2, \ldots, N_f^2\}$ and $L_{\mathcal{S}} \cap L_{\mathcal{A}} = \{\}$, we can write Eq. (19) as

$$h_{ps,qr} = \sum_{L_{\mathcal{S}}}^{N_f^2} \sum_{L_{\mathcal{A}}}^{N_f^2} \sum_{p,s}^{N_f} \sum_{q,r}^{N_f} \left( \mathcal{S}[O_L] \right)_{p,s} \left( \mathcal{S}[O_L] \right)_{q,r} + \sum_{L_{\mathcal{A}}}^{N_f^2} \sum_{L_{\mathcal{S}}}^{N_f^2} \sum_{p,s}^{N_f} \sum_{q,r}^{N_f} \left( \mathcal{A}[O_L] \right)_{p,s} \left( \mathcal{A}[O_L] \right)_{q,r},$$

which leads to

$$\frac{1}{2} \sum_{p,q,r,s=1}^{N_f} h_{ps,qr} \hat{c}_p^\dagger \hat{c}_q \hat{c}_r \hat{c}_s = \frac{1}{2} \sum_{L_{\mathcal{S}}}^{N_f^2} \sum_{L_{\mathcal{A}}}^{N_f^2} \sum_{p,s}^{N_f} \sum_{q,r}^{N_f} \left( \mathcal{S}[O_L] \right)_{p,s} \hat{c}_p^\dagger \hat{c}_q \left( \mathcal{S}[O_L] \right)_{q,r} \hat{c}_r \hat{c}_s + \frac{1}{2} \sum_{L_{\mathcal{A}}}^{N_f^2} \sum_{L_{\mathcal{S}}}^{N_f^2} \sum_{p,s}^{N_f} \sum_{q,r}^{N_f} \left( \mathcal{A}[O_L] \right)_{p,s} \hat{c}_p^\dagger \hat{c}_q \left( \mathcal{A}[O_L] \right)_{q,r} \hat{c}_r \hat{c}_s.$$

We have split the Hamiltonian into the symmetric and anti-symmetric components of the sliced tensor of $O^{[h]}$ that diagonalizes the Coulomb tensor in its flattened form $h_{ps,qr}$. We can now diagonalize the symmetric matrix defined in Eq. (17),

$$\mathcal{S}[O_L] = U^{[\mathcal{S}[O_L]]} \sum_{\mathcal{S}[O_L]}^{[\mathcal{S}[O_L]]} U^{[\mathcal{S}[O_L]]\dagger},$$

where $U^{[\mathcal{S}[O_L]]}$ is a unitary matrix and $\sum_{\mathcal{S}[O_L]}$ a real-valued diagonal matrix. Similarly, one can decompose the antisymmetric matrix defined in Eq. (18) into

$$\mathcal{A}[O_L] = U^{[\mathcal{A}[O_L]]} \sum_{\mathcal{A}[O_L]}^{[\mathcal{A}[O_L]]} U^{[\mathcal{A}[O_L]]\dagger},$$

where $U^{[\mathcal{A}[O_L]]}$ is a unitary matrix and $\sum_{\mathcal{A}[O_L]}$ is a diagonal matrix only possessing purely imaginary entries. Note, that by definition $\mathcal{S}[O_L]^\dagger = \sum_{\mathcal{S}[O_L]}^{[\mathcal{S}[O_L]]} \sum_{\mathcal{A}[O_L]}^{[\mathcal{A}[O_L]]\dagger} \mathcal{A}[O_L]$. By introducing a new set of operators

$$\hat{b}_a^{(L)} = \left\{ \begin{array}{ll} \sum_{p=1}^{N_f} \left( U^{[\mathcal{S}[O_L]]} \right)_{p,a} \hat{c}_p & \text{if } L \in L_{\mathcal{S}}, \\ \sum_{p=1}^{N_f} \left( U^{[\mathcal{A}[O_L]]} \right)_{p,a} \hat{c}_p & \text{if } L \in L_{\mathcal{A}}, \end{array} \right.$$

$$\hat{b}_a^{(L)} = \left\{ \begin{array}{ll} \sum_{p=1}^{N_f} \left( U^{[\mathcal{A}[O_L]]\dagger} \right)_{p,a} \hat{c}_p & \text{if } L \in L_{\mathcal{S}}, \\ \sum_{p=1}^{N_f} \left( U^{[\mathcal{S}[O_L]]\dagger} \right)_{p,a} \hat{c}_p & \text{if } L \in L_{\mathcal{A}}, \end{array} \right.$$
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complex-valued basis functions, one loses a symmetry required to employ the method of Ref. [1], and we showed how this can be overcome by expressing the transformation matrices of the Schur-decomposed reshaped tensor $h$ in terms of its symmetric and antisymmetric components, and using the fermionic nature of the indistinguishable particles to cancel cross terms that mix anti-symmetric and symmetric components. This result allows one to apply low-rank decomposition-based quantum algorithms to general basis sets. Note, that at the time of this writing, a similar result was presented in Ref. [6], which also discusses how to determine a sum-of-squares decomposition of $\hat{H}_2$ by a greedy search algorithm, by means of a low-depth non-orthogonal one-particle bases expansion of $\hat{H}_2$. Since we did not perform numerical experiments and only mentioned truncation strategies to lower the number of elements (by e.g. truncating the sums over the symmetric and anti-symmetric components $L_S$ and $L_A$ by introducing a truncation threshold in the eigenvalues of $\Sigma$ as in Refs. [1] and [6]), future work should focus on explicit error analysis of such strategies to our decomposition.

ACKNOWLEDGMENTS

MPK thanks Simon Balthasar Jäger for discussions. MPK acknowledges funding through S2018-TCS4342 QUITEMAD-CM.

1M. Motta, E. Ye, J. R. McClean, Z. Li, A. J. Minnich, R. Babbush, and G. K. Chan, “Low rank representations for quantum simulation of electronic structure,” arXiv preprint arXiv:1808.02625 (2018).
2J. L. Whitten, “Coulombic potential energy integrals and approximations,” The Journal of Chemical Physics 58, 4496–4501 (1973).
3G. K.-L. Chan, A. Keselman, N. Nakatani, Z. Li, and S. R. White, “Matrix product operators, matrix product states, and ab initio density matrix renormalization group algorithms,” The Journal of chemical physics 145, 041102 (2016).
4B. Peng and K. Kowalski, “Highly efficient and scalable compound decomposition of two-electron integral tensor and its application in coupled cluster calculations,” Journal of chemical theory and computation 13, 4179–4192 (2017).
5Y. Matsuzawa and Y. Kurashige, “Jastrow-type decomposition in quantum chemistry for low-depth quantum circuits,” Journal of Chemical Theory and Computation 16, 944–952 (2020).
6N. C. Rubin, J. Lee, and R. Babbush, “Compressing many-body fermion operators under unitary constraints,” (2021), arXiv:2109.05010 [quant-ph].
7T. Helgaker, P. Jorgensen, and J. Olsen, Molecular electronic-structure theory (John Wiley & Sons, 2014).
8L. Landau, “Diamagnetismus der metalle,” Zeitschrift für Physik 64, 629–637 (1930).
9G. Fano, F. Ortolani, and E. Colombo, “Configuration-interaction calculations on the fractional quantum hall effect,” Physical Review B 34, 2670 (1986).
10E. Tsiper, “Analytic coulomb matrix elements in the lowest landau level in disk geometry,” Journal of Mathematical Physics 43, 1664–1667 (2002).
11M. P. Kaicher, S. B. Jäger, P.-L. Dallaire-Demers, and F. K. Wilhelm, “Roadmap for quantum simulation of the fractional quantum hall effect,” Physical Review A 102, 022607 (2020).
12S. Lloyd, “Universal quantum simulators,” Science 273, 1073–1078 (1996).