Compression algorithm for multi-determinant wave functions

Gihan L. Weerasinghe, Pablo López Ríos, and Richard J. Needs
Theory of Condensed Matter Group, Cavendish Laboratory,
J J Thomson Avenue, Cambridge CB3 0HE, United Kingdom
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A compression algorithm is introduced for multi-determinant wave functions which can greatly reduce the number of determinants that need to be evaluated in quantum Monte Carlo calculations. We have devised an algorithm with three levels of compression, the least costly of which yields excellent results in polynomial time. We demonstrate the usefulness of the compression algorithm for evaluating multi-determinant wave functions in quantum Monte Carlo calculations, whose computational cost is reduced by factors of between 1.885(3) and 25.23(4) for the examples studied. We have found evidence of sub-linear scaling of quantum Monte Carlo calculations with the number of determinants when the compression algorithm is used.

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I. INTRODUCTION

The variational and diffusion [1, 2] quantum Monte Carlo (VMC and DMC) methods are the most accurate known for computing the energies of large numbers of interacting quantum particles. The crucial ingredient is an approximate trial wave function which should be easy to evaluate, while giving a good approximation to the true many-body wave function. A standard approach is to use a Slater-Jastrow trial wave function which consists of the product of determinants for the up and down-spin electrons, multiplied by a Jastrow factor that describes dynamical correlation [3, 4]. We omit the Jastrow factor in the rest of this paper for conciseness. Static correlation can be included by replacing the determinant product by a multi-determinant expansion,

$$\Psi_{MD}(\mathbf{R}) = \sum_{k=1}^{N_s} c_k \Phi^\uparrow_k(\mathbf{R}_\uparrow)\Phi^\downarrow_k(\mathbf{R}_\downarrow),$$

(1)

where $\Phi^\sigma_k(\mathbf{R}) = \det \left( \phi_{a^\sigma_{i,k}}(\mathbf{r}_j^\sigma) \right)$ and $\Phi_k^\sigma(\mathbf{R}) = \det \left[ \phi_{a^\sigma_{i,k}}(\mathbf{r}_j^\sigma) \right]$ are determinants of up- and down-spin single-particle orbitals, $a^\sigma_{i,k}$ is an index that selects the orbital which occurs in the $i$th row of the $\sigma$-spin determinant in the $k$th term of the expansion, $\mathbf{R}_\sigma$ denotes the set of $\sigma$-spin electron coordinates, $\mathbf{R} = \{ \mathbf{R}_\uparrow, \mathbf{R}_\downarrow \}$, and $c_k$ is the coefficient of the $k$th term in the expansion. The accuracy of $\Psi$ can be further improved by, for example, increasing the number of terms in the expansion, $N_s$, or by introducing a backflow transformation [5, 6].

VMC and DMC calculations are normally performed by displacing electrons one at a time, because this has been shown to be the most efficient way to decorrelate consecutive electronic configurations [6, 7]. The displacement of a single electron requires the calculation of the ratio of the wave functions at the new and old coordinates, $\Psi(\mathbf{R}')/\Psi(\mathbf{R})$. In a standard single-determinant calculation this requires the replacement of a single row of the Slater matrix by the vector of the orbitals at the new position $\mathbf{R}'$, and the required calculation is performed using the Sherman-Morrison formula [2]. In a multi-determinant calculation $N_s$ such calculations must be performed. In a backflow calculation each electronic coordinate in the Slater part of the wave function is replaced by a “quasiparticle coordinate”, which depends on all of the electronic coordinates, so that each entry within each Slater matrix must be recalculated when an electron is displaced, and its determinant must be reevaluated, which is achieved using standard LU decomposition. In a multi-determinant backflow calculation, $N_s$ Slater determinants for each spin must be constructed and evaluated.

The repeated evaluation of the trial wave function and its first two derivatives for different electronic coordinates $\mathbf{R}$ is the main contribution to the computational cost of a QMC calculation, which is, as discussed above, approximately proportional to $N_s$. Methods to reduce the cost of evaluating multi-determinant wave functions during QMC calculations have been developed in previous studies [8, 9]. In this paper we introduce a determinant compression algorithm which can significantly reduce the cost of evaluating a multi-determinant trial wave function by reducing the number of determinants in the expansion, by as much as a factor of 26.57 in the examples presented here. We have used the CASINO code [10] for the QMC calculations reported here.

II. METHODOLOGY

Quantum chemistry methods are often used to provide appropriate multi-determinant wave functions for electronic systems. In practice, the determinants contain $M_\ell$ distinct orbitals, and different determinants often differ by only a single orbital. Moreover, quantum chemistry methods group determinants into configuration state functions (CSFs), and different CSFs may contain the same determinant product $\Phi^\uparrow_k \Phi^\downarrow_k$. The compression method we present here exploits these two facts.
A. Basic determinant operations

1. Identical determinants

To achieve greater efficiency we combine repeated determinant products so that each of them need only be evaluated once at each \( \mathbf{R} \), which is equivalent to simply adding together the terms from identical determinant products, i.e.,

\[
c_1 \Phi^\dagger \Phi^\dagger + c_2 \Phi^\dagger \Phi^\dagger = (c_1 + c_2) \Phi^\dagger \Phi^\dagger = c'_1 \Phi^\dagger \Phi^\dagger,
\]

where \( c' \) is the coefficient of the term arising from the combination of two repeated determinant products.

We refer to this procedure as “de-duplication”, which is the first operation in our compression algorithm, and its computational cost scales as \( O(N_s^2) \), since all pairs of determinants need to be compared to determine if they are equal. The number of determinants in the resulting expansion is \( N_d \leq N_d \), while the number of distinct orbitals \( M_d \) is equal to \( M_a \). Later stages of the compression algorithm can be simplified based on the assumption that the expansion has been de-duplicated.

2. Determinants differing by a single orbital

It is convenient to express each Slater determinant in Eq. (1) using a compact vector notation consisting of the list of orbitals that the determinant contains,

\[
[\phi_{a_1}, \phi_{a_2}, \ldots, \phi_{a_n}] = \begin{bmatrix}
\phi_{a_1}(r_1) & \phi_{a_2}(r_1) & \cdots & \phi_{a_n}(r_1) \\
\phi_{a_1}(r_2) & \phi_{a_2}(r_2) & \cdots & \phi_{a_n}(r_2) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_{a_1}(r_n) & \phi_{a_2}(r_n) & \cdots & \phi_{a_n}(r_n)
\end{bmatrix}.
\]

(3)

Central to the algorithm is an elementary identity from linear algebra which allows two determinants to be combined if they differ by a single row or column. This is applicable to a multi-determinant expansion for terms where the determinants of one spin type are equal and can be factored out, and the determinants of the other spin type differ by a single column, e.g.,

\[
c'_1[\phi_{a_1}, \phi_{a_3}, \ldots, \phi_{a_4}]\Phi^\dagger + c'_2[\phi_{a_2}, \phi_{a_3}, \ldots, \phi_{a_4}]\Phi^\dagger = [c'_1 \phi_{a_1} + c'_2 \phi_{a_2}, \phi_{a_3}, \ldots, \phi_{a_4}]\Phi^\dagger
\]

\[
= \tilde{c}_1[\tilde{\phi}_{a_1}, \phi_{a_3}, \ldots, \phi_{a_4}]\Phi^\dagger,
\]

(4)

where \( \tilde{\phi}_{a_1} \) is a new orbital resulting from the linear combination of two of the original orbitals and \( \tilde{c}_1 \) is a new coefficient, satisfying

\[
\tilde{c}_1 \tilde{\phi}_{a_1} = c'_1 \phi_{a_1} + c'_2 \phi_{a_2}.
\]

(5)

This operation can be applied to sets of more than two determinant products, provided they all differ in the same column of the same-spin determinant.

The compression algorithm we have developed applies this basic operation repeatedly to all possible sets of determinants. However, there may be multiple mutually-exclusive ways of combining the determinants, and the size of the resulting expansion depends on the choice of operations. We discuss this in Sec. II C.

B. Representation of compressed expansions

A compressed multi-determinant expansion is of the form

\[
\Psi_{MD}(\mathbf{R}) = \sum_{k=1}^{N_c} \tilde{c}_k \det [\tilde{\phi}_{a_{ik}}(r^j)] \det [\tilde{\phi}_{a_{jk}}(r^l)],
\]

(6)

where \( N_c \) is the number of terms in the compressed expansion, \( \tilde{c} \) are the compressed expansion coefficients, \( \tilde{\phi} \) are the compressed orbitals, and \( \tilde{\phi}_{a_{ik}}(r^j) \) is an index that selects which compressed orbital occurs in the \( j \)th row of the \( \sigma \)-spin determinant in the \( k \)th term of the compressed expansion. The expansion coefficients are

\[
\tilde{c}_k = \pm c_{\nu_1} \prod_{p=2}^{P} \frac{c'_{\delta_{kp}}}{c'_{\delta_{kp}}},
\]

(7)

and the compressed orbitals are

\[
\tilde{\phi}_{a}(r) = \sum_{x=1}^{X_a} \sum_{q=1}^{Q_{ax}} c'_{axq} \phi_{\mu_{ax}}(r),
\]

(8)

where \( P, X, \) and \( Q \) are sum and product lengths, and \( \nu, \delta, n, d, \) and \( \mu \) are indices, all of which arise from the application of the compression operations described above. The \( \pm \) signs account for any required row exchanges in the determinants. In this notation, the compression operation exemplified in Eq. (1) is such that

\[
\tilde{c}_1 = +c'_1,
\]

(9)

and

\[
\tilde{\phi}_{a_{1}}(r) = +\phi_{a_{1}}(r) + \frac{c'_1}{c'_2} \phi_{a_{2}}(r),
\]

(10)

which satisfies Eq. (5), as required. Therefore in this case \( P_1 = 1, \nu_{1,1} = 1, X_{a_1} = 2, Q_{a_1,1} = 0, \mu_{a_1,1} = a_1, Q_{a_1,2} = 1, n_{a_1,2,1} = 2, d_{a_1,2,1} = 1, \) and \( \mu_{a_1,2} = a_2 \).

A compressed expansion is fully determined by specifying \( a, P, X, Q, \nu, \delta, n, d, \mu, \) and the signs in Eqs. (7) and (8). Expressing the compressed expansion in this manner is useful because the orbitals and coefficients can be quickly reconstructed using Eqs. (7) and (8) when the original expansion coefficients, the \( \{c_k\} \) of Eq. (1), change, as is the case during wave function optimization within QMC.
C. Choosing the optimal set of operations

It is convenient to express the principles of the compression algorithm using set theory notation. Let $P$ be a set whose elements are the terms in the de-duplicated multi-determinant expansion, $P = \{p_k \equiv c_k^j \Phi_k^j \Phi_k^j\}$, of size $|P| = N_d$. Let $u_i$ be a subset of $P$ such that its elements can be combined via the compression operation of Sec. II.A.2 and $U$ the set of all possible such sets, $U = \{u_i\}$. Note that $u_i$ is allowed to contain only one term, and that any two elements $u_i$ and $u_j$ may contain the same term $p_k$.

A valid compressed expansion can be obtained by finding a subset $V = \{v_i\}$ of $U$ that satisfies the conditions that (a) $V$ contains all terms in $P$, $\bigcup_i v_i = P$, and (b) each term in $P$ is contained in only one element of $V$, $v_i \cap v_j = \emptyset \forall i \neq j$. The resulting compressed expansion will contain one term for each element of $V$, and therefore the optimal compression is that for which $V$ has the fewest elements.

Finding the minimal set of sets $V$ that covers a set $P$ is otherwise known as the set-covering problem. This can be expressed as a binary linear program \[11\], that is, an optimization problem where a linear objective function $f$ of the binary unknowns $\{x_i\}$ is to be optimized subject to a set of linear equalities and/or inequalities involving the unknowns. In the binary linear program associated with a set-covering problem there are $|U|$ unknowns $\{x_i\}$ that determine whether a subset $u_i$ is present in $V$ ($x_i = 1$) or not ($x_i = 0$). The objective function that must be minimized is the number of subsets in $V$,

$$f(\{x_i\}) = \sum_{i=1}^{|U|} x_i , \quad (11)$$

constrained so that each element in $P$ appears exactly once in $V$,

$$\sum_{j=1}^{|U|} a_{ij} x_j = 1 , \quad (12)$$

where the binary element $a_{ij}$ of the constraint matrix indicates whether the term $p_i$ is contained within subset $u_j$.

The size of the enumeration set $U$ can become very large if large sets of combinable determinants are present in the original expansion, since all possible combinations of those determinants are required to be individual elements of $U$. In practice we construct a set $W$ which only contains the sets in $U$ that are either of size one or not wholly contained in another set. The maximum size of $W$ is linear with the original expansion size. The process of constructing $V$ from $W$ differs slightly from that described earlier, in that when an element $w_i$ is added to $V$ we now require that the terms contained in $w_i$ be removed from all other $\{w_j\}_{j \neq i}$. Note that by construction the order in which elements of $W$ are added to $V$

$$g(\{y_i\}) = \sum_{i=1}^{|W|} y_i , \quad (13)$$

and the constraints which guarantee that $V$ covers $P$ are

$$\sum_{j=1}^{|W|} b_{ij} y_j \geq 1 , \quad (14)$$

where the binary element $b_{ij}$ of the constraint matrix indicates whether the term $p_i$ is contained within subset $w_j$.

We further reduce the size of the linear program by partitioning $W$ into subsets such that each term $p_i$ appears in only one of the subsets. Solving the linear programs for each of the partitions independently is equivalent to solving the linear program for $W$.

There exist efficient methods to solve binary linear programs, such as the iterative simplex method implemented in the LPsolve library \[12\]. However, solving a binary linear program, or otherwise solving the set-covering problem, is in general NP-hard \[13\], and therefore a good determinant compression algorithm should implement an approximate fall-back method for cases where it is infeasible to obtain the exact solution in a reasonable amount of time. A good approximate solution to the set-covering problem can be found in polynomial time using a “greedy” algorithm \[14\], in which $V$ is constructed by adding to it the largest element of $W$, removing all the terms contained in this element from the other elements of $W$, and repeating this process until no non-empty elements remain in $W$. In the examples we have studied in the present work we have not found any cases where we had to resort to the greedy algorithm.

D. Multiple Iterations

In some cases it is possible for a set of compressed determinants to be combined in order to yield an even shorter expansion. For example the sum

$$[\phi_{a_1}, \phi_{a_3}] + [\phi_{a_2}, \phi_{a_3}] + [\phi_{a_1}, \phi_{a_4}] + [\phi_{a_2}, \phi_{a_4}] , \quad (15)$$

can be compressed into

$$[\phi_{a_1} + \phi_{a_2}, \phi_{a_3}] + [\phi_{a_1} + \phi_{a_2}, \phi_{a_4}] , \quad (16)$$

which can be further compressed into

$$[\phi_{a_1} + \phi_{a_2}, \phi_{a_3} + \phi_{a_4}] . \quad (17)$$
The presence of multiply compressible sets of terms is a property of the original expansion. Note that the result of applying a compression operation to already-compressed determinants continues to be of the form given by Eqs. \((6), (7), \) and \((8).\)

The most straightforward method of dealing with multiply compressible terms is to apply the procedure described in the previous section iteratively until no further decrease in the length of the expansion occurs, which we refer to as the “simple iterative method”. By construction this method will operate on a different row of the determinants at each iteration, and therefore the maximum number of iterations is the number of electrons in the system.

However, the simple iterative method is not guaranteed to give the optimal solution for two reasons. Firstly, the choice of which terms are grouped in earlier iterations affects the size of the final expansion, in such a way that making sub-optimal choices at individual iterations (e.g., using the greedy algorithm) may yield a better overall compression than solving the set-covering problem exactly at all iterations. And secondly, terms in the original expansion should be allowed to contribute to more than one term of the compressed expansion. For example, consider the following compression of a six term expansion into two terms,

\[
\begin{align*}
[\phi_{a_1}, \phi_{a_2}] & \pm 2[\phi_{a_1}, \phi_{a_3}] + \phi_{a_4} \\
[\phi_{a_1}, \phi_{a_2}] & \pm 2[\phi_{a_2}, \phi_{a_4}] + \phi_{a_3} \\
[\phi_{a_1}, \phi_{a_2}] & + [\phi_{a_1} + \phi_{a_2}, \phi_{a_3}] \\
[\phi_{a_1} + \phi_{a_2}, \phi_{a_4}] & + [\phi_{a_2} + \phi_{a_1}, \phi_{a_4}] \\
[\phi_{a_1} - \phi_{a_3}, \phi_{a_2} + \phi_{a_3}] & + [\phi_{a_1} + \phi_{a_2}, \phi_{a_3} + \phi_{a_4}] \\
\end{align*}
\]

This compression operation is possible only if the second and fifth terms of the original expansion are used twice; otherwise the result would be a three-term compressed expansion at best. Note that, in the absence of multiply compressible terms, the resulting compressed expansion will contain the same number of terms regardless of whether a term can be used more than once or not.

We have developed a multiple iteration algorithm that solves the first of these issues, although not the second which would require an entirely different methodology, and in our opinion the resulting method would not give significantly better compression ratios. This method, which we refer to as the “unified iteration method”, is similar to that outlined in Sec. III\(\text{C}\). First the enumeration set \(U\), which we refer to as \(U^{(0)}\) in this context, is constructed. We define \(u_i^{(1)}\) as a subset of \(U^{(0)}\) such that its elements can be combined, and \(U^{(1)}\) is the set of all possible such sets, \(U^{(1)} = \{u_i^{(1)}\}\). A similar set can be defined for each recursion level \(n > 1\), so that \(U^{(n)}\) is formed by all possible sets of elements of \(U^{(n-1)}\) that can be combined together. Recursion stops at \(n = n_{\text{max}}\) if \(U^{(n_{\text{max}})}\) does not contain any terms that can be combined together.

The unknowns of the linear program for the unified iteration method are \(x_i^{(n)}\), where \(x_i^{(n)}\) indicates whether set \(u_i^{(n)}\) is in \(V\) or not. The objective function that is minimized is the number of sets in \(V\),

\[
f(\{x_i^{(n)}\}) = \sum_{i=0}^{n_{\text{max}}} \sum_{i=1}^{U^{(n)}} x_i^{(n)},
\]

constrained by

\[
\sum_{i=0}^{n_{\text{max}}} \sum_{i=1}^{U^{(n)}} a_{ij}^{(n)} x_j^{(n)} = 1,
\]

where the binary element \(a_{ij}^{(n)}\) of the constraint matrix indicates whether or not the term \(p_i\) is present in \(u_i^{(n)}\).

As in the case of the simple iterative method, it is possible to avoid constructing the enumeration set \(U^{(0)}\) and instead construct a set \(W^{(0)}\) that contains all elements of \(U^{(0)}\) that are not contained in other elements. However this simplification cannot be applied to higher recursion levels, and one must construct \(U^{(n)}\) explicitly for \(n > 0\). The reason for this is that eliminating a single term \(p_i\) from all \(w_j^{(n)}\) during the construction of \(V\) may cause the compression operation represented by \(w_j^{(n)}\) to become invalid in the absence of \(p_i\), an event which is not taken into account by the linear program. Therefore the simplified linear program has the unknowns \(\{y_i\}\) and \(\{x_i^{(n)}\}_{n=1}^{n_{\text{max}}}\), and the objective function

\[
f(\{y_i\}, \{x_i^{(n)}\}) = \sum_{i=1}^{W^{(0)}} y_i + \sum_{n=1}^{n_{\text{max}}} \sum_{i=1}^{U^{(n)}} x_i^{(n)},
\]

constrained so that each term of the original expansion appears at least once in the selected operations,

\[
\sum_{j=1}^{W^{(0)}} b_{ij} y_j + \sum_{n=1}^{n_{\text{max}}} \sum_{j=1}^{U^{(n)}} a_{ij}^{(n)} x_j^{(n)} \geq 1,
\]

and each term of the original expansion appears at most once in operations of recursion level \(n > 0\),

\[
\sum_{n=1}^{n_{\text{max}}} \sum_{j=1}^{U^{(n)}} a_{ij}^{(n)} x_j^{(n)} \leq 1.
\]

Operations of recursion level \(n > 0\) must be added to \(V\) before those with order \(n = 0\) to prevent the application of the latter from invalidating the former, as mentioned earlier.

Partitioning can be also applied at recursion level \(n = 0\) to reduce the potential cost of solving the linear program.

III. IMPLEMENTATION

We have implemented the multi-determinant expansion compressor as a stand-alone utility \([13]\) which can be
used with any suitably modified quantum Monte Carlo code, and we have modified the CASINO code [10] to be able to use compressed multi-determinant expansions produced by the utility.

The compression utility uses the LPSOLVE library [12] to solve the linear programs described in Secs. III.C and III.D. This utility implements four operational levels: (a) “de-duplicate”, which performs the de-duplication stage of the compression only (polynomial time); (b) “quick”, which performs de-duplication and uses the greedy algorithm to find an approximate solution to the set-covering problems posed by the simple iterative method (polynomial time); (c) “good”, which performs de-duplication and solves the set-covering problems posed by the simple iterative method exactly using a linear program (potentially NP-hard), and (d) “best”, which performs de-duplication and solves the set-covering problem posed by the unified iteration method exactly using a linear program (potentially NP-hard).

The “best” operational level should be used whenever feasible. The “good” mode is provided for cases where the construction of the enumeration sets $U^{(n)}$ makes the “best” mode too expensive, and the “quick” mode is useful for expansions which make the “good” algorithm exhibit its potential NP-hardness. The utility specifies the compressed expansion in terms of the variables introduced in Eqs. (6), (7), and (8).

We have modified the CASINO code to enable it to compute the compressed orbitals as appropriate linear combinations of the original orbitals, as per Eq. (8). During optimization, the original expansion coefficients are exposed to the optimizer, and the linear coefficients of the compressed determinants and orbitals are re-evaluated when the parameters change.

### IV. RESULTS

We have tested our compression algorithm on multi-determinant expansions for the N, O, Li, B, Be, Ne, and F atoms generated using the ATSP2K multi-configurational Hartree-Fock (MCHF) package [16], and with a multi-determinant expansion for the Be$_2$ molecule generated using the GAMESS code [17]. The test cases are intended to represent realistic calculations, such as the multi-determinant calculations of Seth et al. [18].

The wave functions produced by ATSP2K are arranged in CSFs, each of which comprises a set of determinants with a certain symmetry. Since the same determinant product may be contained in different CSFs, the atomic wave functions in our tests benefit from de-duplication. In contrast, the GAMESS code performs de-duplication internally, and as a result the de-duplication stage of our compression utility does not yield any gains for the Be$_2$ wave function.

The results for the compression algorithm are presented in Table IV, which gives the number of determinants and distinct orbitals for the original and compressed expansions at the different operational levels of the compression utility. Also given is the CPU time taken by the compression utility, averaged over 20 trials, on a modest CPU. (The compression tests were performed on a single core of a 2007 Intel Core 2 Quad CPU.)

De-duplication results in significant reductions in the size of the multi-determinant expansions for the atoms, with $N_d/N_b$ ranging between 1.0 and 3.3. The compression stage provides an even greater reduction, with values of $N_d/N_b$ ranging between 2.1 and 10.8. In total, the compression utility yields compression factors of up to $N_d/N_b = 26.57$.

The different compression levels “quick”, “good”, and “best” yield very similar compression sizes, with “good” giving a small improvement over “quick” of up to $N_d/N_g = 1.024$, and “best” yielding a smaller change over “good” of $N_d/N_b = 1.005$ at most. The CPU times required by the three compression levels are also very similar, which indicates that the linear programs do not exhibit their potential NP-hardness in any of the cases studied here.

The number of distinct orbitals in the compressed expansions appears to be roughly of the order of the number of terms in the compressed expansion, $M \sim N$. For

| $N_{CSF}$ | $N_d$ | $M_d$ | $N_g$ | $M_g$ | $N_b$ | $M_b$ |
|-----------|-------|-------|-------|-------|-------|-------|
| Be$_2$    | 61    | 200   | 12    | 200   | 60    | 0.001(1) |
| N         | 50    | 1271  | 51    | 764   | 51    | 0.012(1) |
| O         | 100   | 3386  | 53    | 1271  | 53    | 0.058(1) |
| Li        | 500   | 8140  | 105   | 5824  | 105   | 0.332(6) |
| B         | 500   | 14057 | 105   | 5703  | 105   | 0.79(1) |
| Be        | 500   | 14212 | 105   | 10600 | 105   | 1.18(1) |
| Ne        | 400   | 22827 | 105   | 1271  | 51    | 0.012(1) |
| F         | 600   | 57456 | 105   | 17174 | 105   | 11.43(1) |

TABLE IV: Number of terms $N$, number of orbitals $M$, and CPU times $t$ taken by the compression algorithm on a modest CPU.
TABLE II: Speed-up provided by the “best” compression algorithm over the uncompressed \((T_s/T_b)\) and de-duplicated \((T_d/T_b)\) expansions for a fixed number of moves in a multi-determinant VMC calculation. The relative expansion sizes \(N_s/N_b\) and \(N_d/N_b\) are also shown for comparison.

| \(N_s/N_b\) | \(T_s/T_b\) | \(N_d/N_b\) | \(T_d/T_b\) |
|-------------|-------------|-------------|-------------|
| Be\(_2\)   | 2.06        | 1.88(5)(3)  | 2.06        | 1.905(6)  |
| N          | 3.92        | 3.718(9)    | 2.36        | 2.276(8)  |
| O          | 6.34        | 6.09(1)     | 2.38        | 2.309(5)  |
| Li         | 6.73        | 6.50(2)     | 4.81        | 4.64(1)   |
| B          | 26.57       | 25.23(4)    | 10.78       | 10.05(2)  |
| Be         | 6.57        | 6.48(1)     | 4.90        | 4.83(2)   |
| Ne         | 12.65       | 13.17(2)    | 9.01        | 9.34(1)   |
| F          | 20.92       | 21.77(5)    | 6.25        | 6.48(1)   |

The data for the other systems show that the value of \(T_s/T_b\) is between 91% and 99% that of \(N_s/N_b\), implying that handling the determinants in the expansion is by far the leading contribution to the CPU time of the QMC calculation, and that reducing \(N\) produces an almost equal reduction in \(T\). The additional CPU time required to compute the orbitals for the compressed expansion as linear combinations of the original orbitals has an insignificant impact on the benefits of using the compression scheme for the examples in Table II.

We have also run VMC and DMC calculations using Jastrow factors and backflow transformations with identical conclusions, but we have omitted the results from Table II for the sake of conciseness.

We have applied our “best” compression algorithm to expansions of different sizes to investigate how \(N_b\) varies with \(N_s\). Results for the Be, B, and F atoms with up to 600 CSFs are plotted in Fig. 1 where we also show fits to \(N_b = a N_s^\alpha\). The active space used in the generation of the MCHF wave function included up to double excitations (D) and up to triple excitations (DT). The results, ignoring the plateau in the case of B, were fitted to \(N_b = a N_s^\alpha\).
have repeated the scaling tests for B with an active space that includes up to triple excitations, as shown in Fig. [2]. As we expected, the plateau disappears when the larger active space is used.

We conclude that the use of the compression algorithm can make multi-determinant QMC calculations scale as $N_s^\alpha$, with $1/2 \leq \alpha < 1$.

V. CONCLUSION

In this paper we have presented a compression algorithm for multi-determinant expansions based on a simple identity for combining determinants, which can provide computational cost savings in QMC calculations of about the compression factor $N_s/N_b$, which in our tests ranges between 2.06 and 26.57.

In addition to the full compression algorithm we have implemented a polynomial-scaling fallback algorithm which has been shown to yield nearly the same compression ratios as the full method. This algorithm avoids the NP-hardness associated with solving the set-covering problem, but in none of our tests did the full algorithm incur costs excessive enough to require the use of the fallback algorithm.

We find that the compression algorithm makes QMC calculations scale sub-linearly with the number of determinants in the expansion. The cost savings provided by using compressed determinant expansions are expected to permit QMC calculations using much larger multi-determinant expansions than would otherwise be possible. Our compression algorithm can be used in combination with methods for the optimized evaluation of multi-determinant wave functions [8, 9] for additional efficiency.

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