Efficient $6j$ symbol evaluations for atomic calculations

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We have developed an efficient tabulation scheme to evaluate $6j$ symbols for atomic calculations. The scheme is appropriate for coupled-cluster based calculations. In particular, for perturbed coupled-clusters calculations, which has another perturbation in addition to the residual Coulomb interaction. The scheme relies on the symmetry of the $6j$ symbol and the triangular conditions.

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I. INTRODUCTION

The use of angular momentum algebra is inevitable in many body calculations of atoms and nuclei. It is essential to couple the single particle states to form many particle states or to evaluate matrix elements of tensor operators. To couple two angular momentum states, Clebsch-Gordan coefficients are the weight factors in the linear combinations of the direct product states. It reflects the geometric aspect of the coupled many particle state. Then, for three angular momenta, it is the Wigner $6j$ symbols $\{\}$ which are closely related to the Racah recoupling coefficients $\{\}$. Higher $3nj$ symbols are required to couple larger number of angular momentum states $\{\}$. As mentioned earlier, these coefficients also occur while evaluating the matrix elements of tensor operators in the angular momentum basis. In atomic many body theory, $6j$ symbols occur frequently while evaluating the matrix elements of the two-electron Coulomb interaction $\{\}$. The number of times $6j$s symbols are calculated increases substantially in structure or properties calculations, where the the Coulomb interaction is treated perturbatively to high orders or non-perturbatively to all orders.

In this paper, we address the $6j$ symbol evaluation requirements of coupled-cluster calculations, a non-perturbative many body theory $\{\}$, of heavy atoms. The theory is applicable to both, atomic structure and properties calculations. In these calculations, depending on the number of orbitals in the basis set chosen, the number of $6j$ symbol evaluations could be as large as $10^9$. It is found that, the $6j$ symbol evaluations of this magnitude take a large fraction, in many instances about 30–40 %, of the total computational time. This has severe implications in coupled-cluster calculations, where the working equations are a set of non linear algebraic equations. The number of $6j$ symbol evaluations increases manifold in perturbed coupled-cluster theory, where the perturbation is an operator of rank one or higher in the electron space. The theory is appropriate to calculate the effects of discrete symmetry violations in atoms $\{\}$ and transition properties. The large number of $6j$ symbol in the perturbed cluster equations, set of linear algebraic equations, is a serious issue for calculating the properties of heavy atoms. Further, the evaluations are repetitive as iterative schemes suitable method to solve the equations.

One solution to avoid the repeated evaluations of the $6j$ symbols and reduce the time of calculation is, evaluate all the needed $6j$ symbols and tabulate it. However, this is easier said than done. The possible number of $6j$ symbols up to a maximum value of angular momentum $j_{\text{max}}$ grows rapidly as $j_{\text{max}}$ is increased. Then the tabulation require large arrays, which is an undesirable feature in large scale computations. Employing the symmetry properties, it is possible to reduce the number significantly. But the disadvantage of incorporating the symmetries is, large number of binary operations are essential to retrieve the tabulated values. An optimal scheme is to tabulate with selected symmetry properties. The other approach is to improve efficiency of the $6j$ symbol calculations is to employ a fast evaluation scheme $\{\}$. This scheme would be faster than the calculations with factorials. But it involves several binary operations as it has a summation, so the tabulation is a better choice.

The paper is organized as follows in Section$\{\}$ the expression and properties of $6j$ symbols are described in brief. Then in Section$\{\}$ the reason for larger number of $6j$ symbols in perturbed coupled-cluster calculations is discussed with an example. We have chosen an example from electric dipole moment calculations. Then the method of tabulation and retrieval we have developed are given in Section$\{\}$ This is followed by results and discussions, and conclusions.

II. $6J$ SYMBOLS

A. Symmetry and representation

Consider a many particle system consisting of three particles, each having individual angular momenta $j_1$, $j_2$ and $j_3$. Then the total angular momentum $J$ of the system is the vector sum of $j_1$, $j_2$ and $j_3$.

In general, there are three distinct ways of coupling the three angular momenta. These are $|J_{12}, j_3, JM\rangle$, $|J_{13}, j_2, JM\rangle$ and $|j_1, J_{23}, JM\rangle$, where $J_{ij}$ represents coupling of $j_i$ and $j_j$, and $JM$ is the total angular momentum. Among these possibilities, states of two different coupling schemes are related through a unitary transfor-
The elements of the transformation are the recoupling coefficients \( \langle \cdots | \cdots \rangle \). The symmetric representation of these coefficients is

\[
\langle J_{12}, J_3, J M | j_1, J_{23}, J M \rangle = (-1)^{j_1+j_2+j_3+J} [J_{12}, J_{23}] \times \\
\left\{ \begin{array}{c}
 j_1 \ J_{12} \ j_2 \\
 j_3 \ J_{23} \ J
\end{array} \right\},
\]

where \( \{ \cdots \} \) is the 6j symbol. It is invariant with respect to any column permutation and rows interchange for a pair of columns, which explains why it is the symmetric representation of recoupling coefficients. Counting the number of invariant transformations, column permutations and row interchange, one 6j symbol has 24 equivalent representations. Then, the angular momenta in a 6j symbol satisfy the triangular conditions

\[
\begin{align*}
|j_1 - j_2| & \leq J_{12} \leq j_1 + j_2, \\
|j_2 - j_3| & \leq J_{23} \leq j_2 + j_3, \\
|J - j_3| & \leq J_{12} \leq J + j_3, \\
|J - j_1| & \leq J_{12} \leq J + j_1.
\end{align*}
\]

The 6j symbols are products of four Clebsch-Gordan coefficients or equivalently four 3j symbols, the symmetric representation of Clebsch-Gordan coefficients. Besides coupling of angular momenta, the 6j symbols are part of the angular factors in the matrix elements of coupled tensor operators.

![Diagrammatic representation of 6j symbol](image)

**FIG. 1:** Diagrammatical representation of 6j symbol.

Atomic structure and properties calculations involve calculations of matrix elements of a tensor operator in the single particle basis, which comprises of the radial and angular parts. The evaluation of the angular part involves the expansion of the matrix elements using the Wigner-Eckart theorem and rearranging the angular momenta couplings and tensor coupling of the operators. It then simplifies to product of 3j and 6j symbols, phase factors and constant factors. This procedure is sometimes tedious especially when the matrix element has several angular momenta and operators. A simpler way is to use angular momentum diagrams. In atomic many-body theory, these are the Goldstone diagrams where operator and angular momenta representations replace the interaction and orbital lines respectively [4]. The diagrams are then simplified and evaluated based on rules which separate close or open parts to diagrammatic representation of angular momenta coupling identities. In this scheme, the diagrammatic representation of 6j symbols is shown in Fig. [4] The diagram has a high degree of symmetry, which are equivalent to the symmetry of the algebraic representation. It is non-zero only if the angular momenta meeting at each vertex satisfy the triangular conditions listed in the earlier section.

**B. 6j symbol calculation and unique representation**

The 6j symbols are normally calculated using the Racah formula

\[
\left\{ \begin{array}{c}
 j_1 \ j_2 \ j_3 \\
 l_1 \ l_2 \ l_3
\end{array} \right\} = \sqrt{\Delta(j_1 j_2 j_3) \Delta(l_1 l_2 l_3) \Delta(l_1 j_2 j_3)} \times \\
\sqrt{\Delta(l_1 l_2 l_3)} \sum_{\ell} (-1)^{\ell}(t + 1)!,
\]

where \( \Delta(abc) \) is a triangle coefficient

\[
\Delta(a, b, c) = \frac{(a + b - c)!(a - b + c)!(a + b + c)}{(a + b + c + 1)!}
\]

and

\[
f(t) = (t - j_1 - j_2 - j_3)!(t - j_1 - l_2 - l_3)!
\times (t - l_1 - j_2 - l_3)!(t - l_1 - l_2 - j_3)!
\times (j_1 + j_2 + l_1 + l_2 - t)!(j_2 + j_3 + l_2 + l_3 - t)!
\times (j_3 + j_1 + l_3 + l_1 - t)!. 
\]

The summation is over all integer values of \( t \) for which \( f(t) \) is defined. In other words, values of \( t \) which make the arguments of factorials in \( f(t) \) non negative. Often, theoretical atomic and nuclear physics calculations require several values of 6j symbols, for which one can refer to one of the several published tabulations. Usually, in these tables, as mentioned earlier each 6j symbol has twenty four equivalent representations, only one of the representations is listed.

\[
\left\{ \begin{array}{c}
 j_1 \rightarrow j_2 \rightarrow j_3 \\
 l_1 \ l_2 \ l_3
\end{array} \right\}
\]

A unique choice of selecting the one representation is to impose the inequalities \( j_1 \geq j_2, j_2 \geq j_3, j_1 \geq l_1, j_2 \geq l_2 \) and \( j_2 \geq l_3 \). The relations are symbolically represented in Eq. (7), where \( \cdots \rightarrow \cdots \) denotes \( \cdots \geq \cdots \).

**III. 6j SYMBOLS IN COUPLED-CLUSTER CALCULATIONS**

Coupled-cluster theory [3] is considered to be one of the most accurate many-body theory. This is evident
from the fact that it is an all order theory and proved through extensive calculations in atom, molecules and nuclei. Recently, we have developed a coupled-cluster based method to calculate electric dipole moments of closed-shell atoms [3]. The theory has cluster amplitudes arising from two interaction Hamiltonians. First, the residual Coulomb interaction $V_{es}$ and second, the discrete symmetry violating interaction $H_{PTV}$. As a result, the angular parts of the cluster equations have large number of $6j$ symbols. To demonstrate, consider the single excitation diagram with $V_{es}$ as interaction shown in Fig.2. The equivalent algebraic expression is

$$ \langle bp | \frac{1}{\gamma_{12}} | aq \rangle \times \langle q | O_1^{(1)} | b \rangle $$

where $O_1^{(1)}$ is a rank zero and one cluster operators for $V_{es}$ and $H_{PTV}$ respectively, $a$ and $b$ are the occupied orbitals, and $p$ and $q$, are the virtual orbitals. The angular factor of the diagram (a) in the the figure is

$$ (-1)^{j_b - j_a + k} \sqrt{2j_b + 1} \delta(j_a, j_q) \delta(j_b, j_p), $$

where $k$ are the allowed multipoles of the $V_{es}$ interaction and $j_b$ are the angular momenta of the orbitals. This angular factor, consisting of phase factor, a constant and Kronecker delta is computationally not demanding. However, for the diagram (b), where the cluster operator is rank one, the angular factor is

$$ (-1)^{j_a + j_b + 1} \left\{ \begin{array}{ccc} j_b & j_q & 1 \\ j_p & j_a & k \end{array} \right\}. $$

From the expression of $6j$ symbol, given in Eq.4, it’s evaluation has far larger number of arithmetic operations than calculation of Eq.8. The present comparison is for one of the simpler diagrams. The occurrence of $6j$ symbol is larger in diagrams of doubles and more complicated. Calculating a larger number of $6j$ symbols to solve the perturbed cluster amplitude equations is a serious performance issue. It is particularly severe for properties calculations of heavy atoms, the number of cluster amplitudes is in millions. Another factor adding to the inefficiency is the repeated occurrence of the same $6j$ symbol in several diagrams, the multiple evaluations is expensive. A trivial solution is tabulating the $6j$ symbols, however this is not simple to implement.

**IV. STORAGE AND RETRIEVAL**

**A. Symmetry considerations**

The optimal basis sets chosen for accurate structure and properties calculations of heavy atoms have single particle wave functions of high angular momenta. For example, for structure and properties calculations of atomic ytterbium, in $jj$ coupled scheme. The optimal basis set consist of orbitals upto $h$ symmetry, which has angular momenta $9/2$ and $11/2$. This is an important consideration to describe the electron-electron correlation energies accurately. An immediate outcome is the large values of the angular momenta in the angular part of the matrix elements. Then, the number of possible $6j$ symbols which can occur is extremely large. For a basis set consisting of orbitals upto $h$ symmetry, the maximum angular momenta which can occur in $6j$ is 11. That is the maximum rank of the operator which satisfies triangular condition for matrix elements between two $h$ orbitals. The approximate total number of $6js$ is then $22^6 \approx 1.2 \times 10^8$, which is a large number.

One option to reduce the number of entries in the tabulations is to impose the inequalities, diagrammatically shown in Fig.4 to the angular momenta of the $6j$ symbol. Such a scheme reduces the number by a factor of 24, the number of equivalent forms. Another option is to apply the four triangular conditions in Eq.3. However, as discussed in the results sections, the exact implementation of these conditions is computationally inefficient. An optimal selection of the inequalities from Eq.7 are: $j_1 \geq j_2, j_1 \geq j_3, j_1 \geq j_3$ and $j_2 \geq l_2$. These reduces the number of equivalent forms reasonably.

**B. Tagging**

Tabulation of the $6j$ symbol during computational calculations imply tagging each one with a unique integer and a scheme to evaluate the tag efficiently. The other considerations are, the tags be in a sequence and preserve the inequality conditions. A straight forward scheme is to take advantage of the three inequalities $j_1 \geq l_1, j_1 \geq j_2$ and $j_2 \geq j_2$. Tagging each $(j_1, l_1)$ pair is equivalent to indexing the elements of the lower triangular matrix and the integer tag is $2j_1(2j_1 + 1)/2 + 2l_1$. The multiplication of $j_1$ and $l_1$ by two is essential as the angular momenta are in multiples of half. Similarly, the $(j_2, l_2)$ are tagged. Further, extending the scheme, the pairs $(j_1, l_1)$ and $(j_2, l_2)$ is mapped to a single integer number, which is like a super tag of $(j_1, j_2, l_1, l_2)$ combinations. For each tag, the possible $(j_3, l_3)$ are considered. Structurally, this can visualized as a stack of matrices $(j_3, l_3)$, one for each $(j_1, j_2, l_1, l_2)$. An important point is, unlike $(j_1, l_1)$ and $(j_2, l_2)$ pairings, tagging $(j_3, l_3)$ pairs is equivalent to indexing a full matrix. This follows from the absence of inequality between $j_3$ and $l_3$. From the inequalities adopted for tagging, the maximum number of

\[ \text{FIG. 2: One of the single excitation diagram, which involves contraction of single excitation cluster operator and } V_{es} \text{, the residual Coulomb interaction. The solid and zigzag lines represent cluster operators arising from } V_{es} \text{ and } H_{PTV} \text{ respectively. In diagram (a) the cluster operator zero rank. Whereas in (b) has rank one.} \]
FIG. 3: The $\left( j_3, l_3 \right)$ pairs for a specific $\left( j_1, l_1, j_2, l_2 \right)$ combination is like a stack, each slot in one of the stacks represents one unique $\left( j_1, l_1, j_2, l_2, j_3, l_3 \right)$ combination or 6j.

$\left( j_3, l_3 \right)$ pairs is $\left( 2j_1 + 1 \right) \left( 2j_1 + 1 \right)$. When the 6j are stored in a one dimensional array, to retrieve one 6j, skip the locations of previous $\left( j_1, l_1, j_2, l_2, j_3, l_3 \right)$ combinations and then from $\left( j_3, l_3 \right)$ evaluate the offset within the stack.

C. Efficiency

A rough estimate of the efficiency of the tabulation and retrieval, compared to the actual calculation is to compare the number of binary operations in the two schemes. This include arithmetic and boolean binary operations. The number of binary operations to calculate 6j symbol from is estimated from Eq. 4. The number of binary operations required to calculate each $\Delta(abc)$ is thirteen. In total, to evaluate the product of the four $\Delta(abc)$ require fifty six binary operations arithmetic operations. Then the, for one $t$, the number calculation of $f(t)$ require twenty four binary operations. Considering the summation over $t$, the total number of binary operations is $\approx 56 + 28 \times (\sigma + 1)$, where $\sigma$ is the number of values $t$ can have. This is without the binary operations to calculate the factorials, the assumption is these are precalculated. In comparison, for the scheme outlined to store and retrieve 6j symbols, the number of binary operations required to retrieve the 6j symbols from memory is $\approx 50$. This involves the arrangement of the six $j$ symbols to satisfy the inequality conditions adopted and calculation of the tag. Approximately, the tabulation and retrieval of 6j symbol is like calculating without the evaluation of $f(t)$. This indicates a significant gain in performance.

V. RESULTS AND DISCUSSIONS

To quantify the relative computational efficiency, between calculating the 6j symbols from Racah formula Eq. 4 and retrieving from a tabulated list, we compare the execution time of the two schemes for calculating a set of 6j symbols. The set chosen consists of 6j symbols with all possible combinations of angular momenta upto a maximum angular momentum $j_{\text{max}}$. The number of the 6j symbols with and without the imposition of the symmetry conditions are shown in Fig. 4. The plots in the

FIG. 4: Number of possible angular momenta combinations to form a 6j symbol with a maximum angular momentum $j_{\text{max}}$. Black, maroon and tan are the number of 6j symbols when no inequality, selected inequality and all inequalities are imposed to the angular momenta.

Fig. 5 shows the plots of computation time for the values of $j_{\text{max}}$ ranging from 4 to 10. The inset plots in Fig. 5 is the ratio of the computation time to calculate the 6j symbols from Racah formula and retrieve from the tabulated list. The ratio has a maximum of $\sim 3.4$ around $j_{\text{max}} = 5$ and is 2.5 for the largest $j_{\text{max}} = 10$ case. There is a significant performance gain. For the largest $j_{\text{max}}$, which is relevant for the coupled cluster calculations of heavy atoms, there is performance gain of $\sim 220\%$ gain after compiler optimizations. Performance of the tabulation is

FIG. 5: Run time to calculate 6j symbols with all the possible combinations upto the maximum angular momenta $j_{\text{max}}$. The pair of curves at the bottom, connecting the * and ○ correspond to retrieval from the tabulated list. The pair at the top, $\triangle$ and $\square$ correspond to numerical calculation from the Racah expression. The red and blue curves are with and without optimizations. The inset curves shows the ratio of the two.
enhanced further when an approximate form of the triangular conditions of the $6j$ symbols in Eq.(3) are imposed. The approximate form is to ensure that the sum of the three angular momenta, which should satisfy triangular condition, is integer. For example, consider the first inequality $|j_1 - j_2| \leq J_{12} \leq j_1 + j_2$. Instead of imposing the inequality, we check if the sum $j_1 + j_2 + J_{12}$ is integer. The retrieval scheme proceeds if it is integer, otherwise it returns a zero value. This improves the efficiency of the retrieval scheme by avoiding the steps to transform the arguments. A comparison of the run time of calculating $6j$ symbols and retrieving from the tabulated values is shown in Fig.6. There is a marked improvement, retrieving from the table is more than 350% faster than the calculation. This is evident from the inset plot in Fig.6. In coupled-cluster calculations of heavy atoms, the number of times $6j$ symbol is evaluated is extremely large. For example, consider the cluster amplitude calculations of Hg with all the core orbitals and one virtual orbitals from each symmetry. At the linear level this calculation require $\approx 2.9 \times 10^8$ evaluations of $6j$ symbol. The number is higher for full scale coupled-cluster calculations and much higher in perturbed coupled-cluster calculations $\approx 7.5 \times 10^9$. In the later case, perturbed coupled-cluster, implementing the tabulation scheme provides a $\approx 30\%$ performance improvement. In other words, calculation of $6j$ symbols takes $\approx 30\%$ of the total run time of coupled-cluster calculation, with tabulation this is reduced to less than 1%.

VI. CONCLUSIONS

Tabulating the $6j$ symbols coefficients improves the efficiency of the coupled-cluster computations significantly. The reduction of binary operations in the tabulation scheme, as explained earlier, accounts for the improvement. The optimal scheme of tabulation and retrieval is to impose a restricted set of symmetry properties and approximate triangular condition. Strict implementation of the symmetry properties and triangular conditions compromises the efficiency of the tabulation scheme. In terms of evaluating the coefficients, the tabulation scheme is more than 350% faster than the actual evaluation. This translates to reducing more than 30% run time of coupled-cluster calculations.

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