Infinite-order diagrammatic summation approach to explicitly correlated congruent transformed Hamiltonian

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A resolution of identity approach to explicitly correlated congruent transformed Hamiltonian (CTH) is presented. One of the principle challenges associated with the congruent transformation of the many-electron Hamiltonian is the generation of three, four, five, and six particle operators. Successful application of the congruent transformation requires efficient implementation of the many-particle operators. In this work, we present the resolution of identity congruent transformed Hamiltonian (RI-CTH) method to handle many-particle operators. The resolution of identity was used to project the explicitly correlated operator in a \( N \)-particle finite basis to avoid explicit computation of the many-particle operators. Single-particle states were obtained by performing Hartree-Fock calculations, which were then used for construction of many-particle states. The limitation of the finite nature of the resolution of identity was addressed by developing partial infinite order (PIOS) diagrammatic summation technique. In the PIOS method, the matrix elements of the projected congruent transformed Hamiltonian was expressed in terms of diagrammatic notation and a subset of diagrams were summed up to infinite order. The RI-CTH and RI-CTH-PIOS methods were applied to isoelectronic series of 10-electron systems (Ne, HF, H₂O, NH₃, CH₄) and results were compared with CISD and CCSD(T) calculations. One of the key results from this work is that for identical basis set, the RI-CTH-PIOS energies are lower than CISD and CCSD(T) values.

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I. Introduction

The form of the many-electron wavefunction at small electron-electron separation plays an important role in accurate determination of the ground state energy. The relationship between the Coulomb singularity in the electronic Hamiltonian and form of the many-electron wavefunction at the electron-electron coalescence point is well known and is given by the Kato cusp condition.1–2 Explicitly correlated methods improve the form of the many-electron wavefunction near the electron-electron coalescence point by incorporating explicit \( r_{12} \) dependence in the form of the wavefunction. This approach has been shown to be indispensable for high-precision calculations of ground and excited state energies in atoms and molecules and has been implemented in various methods including quantum Monte Carlo (QMC),12–16 perturbation theory (MP2-R12),17–20 coupled-cluster,21–23 configuration interaction, transcorrelated Hamiltonian,24–28 and geminal augmented MCSCF.29 One of the main challenges in efficient implementation of explicitly correlated methods is the analytical evaluation of integrals involving the \( r_{12} \) term. The electronic Hamiltonian has only one and two-particle operators, however, because of the \( r_{12} \) term in the form the wavefunction, integrals involving the Hamiltonian and explicitly correlated wavefunctions often involve three-particle and higher terms. The resolution of identity (RI) approach has been successful for efficient evaluation of many-particle integrals and has been widely adopted for implementing faster, more efficient R12-MP2,27–31 and R12-CC methods.32–34

In this article, we introduce the RI implementation of the explicitly correlated congruent transformed Hamiltonian (CTH) method.33 In the CTH method an explicitly correlated function is used, to perform congruent transformation of the electronic Hamiltonian. This approach is similar to the transcorrelated Hamiltonian method where a similarity transformation is performed on the Hamiltonian.19,20 One of the advantages of the CTH method is that the transformation preserves the Hermitian property of the Hamiltonian. As a consequence, the transformed Hamiltonian is amenable to standard variational procedures for obtaining the ground state energy.33 The transformed Hamiltonian involves up to six-particle operators and efficient implementation of these many-particle operators is crucial for application of the CTH method. This problem is addressed in the present work by introducing the RI approximation for representing the many-particle operators. The RI method is exact in the limit of the infinite number of basis functions, however, practical implementation of the RI is always approximate because of the truncation of the
basis. Here, we present a diagrammatic summation approach to include infinite-order contributions to the finite basis implementation of the RI method. We have used diagrammatic notation that is commonly used in the perturbation theory and coupled-cluster equations to represent the terms in the RI expansion. After that, we show that certain classes of diagrams can be summed up to infinite-order and the result can be expressed as an analytical expression of a renormalized two-particle operator. Because the method in its current form is applicable only to selected (as opposed to all) classes of diagrams, it is denoted as partial infinite-order summation (PIOS) method. The details of the derivation of the PIOS method are presented in section II D.

II. Theory

A. Resolution of identity

The first step in the construction of the CTH is to define an explicitly correlated two-body operator as shown below

\[ G(1, \ldots, N) = \sum_{i \neq j} g(r_{ij}) = \sum_{i \neq j} g(i, j), \quad (1) \]

where \( N \) is the number of electron in the system. The derivation presented here is independent of the choice of the two-body explicitly correlation function \( g(1, 2) \) and the specific form used in the present calculation will be discussed later. The congruent-transformed operator is defined as

\[ \tilde{\mathcal{H}} = G^1 H G \quad (2) \]
\[ \tilde{\mathcal{S}} = G^1 \mathcal{S} G \quad (3) \]

where the transformed Hamiltonian contains up to six-particle operators.\(^{35,37} \) For a given trial wavefunction \( \Psi_T \), the CTH energy is defined as

\[ E[\Psi_T, G] = \frac{\langle \Psi_T | \tilde{\mathcal{H}} | \Psi_T \rangle}{\langle \Psi_T | \tilde{\mathcal{S}} | \Psi_T \rangle}. \quad (4) \]

The congruent transformation preserves the Hermitian property of the electronic Hamiltonian and by construction the CTH energy is an upper bound to the exact ground state energy

\[ E_{\text{exact}} \leq \min_{\Psi_T} E[\Psi_T, G] \leq \min_{\Psi_T} E[\Psi_T, G = 1]. \quad (5) \]

As a consequence of the above relationship, the CTH energy is amenable to standard variational procedure and can be minimized with respect to both the trial wavefunction \( \Psi_T \) and the explicitly-correlated function \( G \). In the limit of \( G = 1 \), the CTH energy is equivalent to the expectation value of the electronic Hamiltonian. One of the challenges of implementing CTH is form of the transformed Hamiltonian. Because of the transformation, the CTH can be expressed as sum of two, three, four, five, and six-particle operators. In this work, we address this challenge by introducing a finite-basis for representing the CTH. The resolution of identity operator, in some finite basis \( M \) is defined by the following equation

\[ \mathcal{I}^{RI(M)} = \sum_k |k\rangle \langle k|. \quad (6) \]

The finite-basis representation of \( G \) is given as

\[ G^{(M)}(1, \ldots, N) = \sum_{k,k'} |\Phi_k\rangle \langle \Phi_{k'}| G |\Phi_{k'}\rangle \langle \Phi_k|, \quad (7) \]

where the superscript \( M \) in \( G^{(M)} \), represents that it is a finite-basis representation of the exact \( G \) operator. These two quantities are related to each other by the following limiting condition

\[ G = \lim_{M \to \infty} G^{(M)}. \quad (8) \]

The number of terms in Eq. (7) that contribute to the CTH energy in Eq. (4) is much less than \( M^2 \) and depend on the choice of the trial wavefunction \( \Psi_T \). If the search for the optimal trial wavefunction is restricted to the set of single Slater determinants, then as a direct consequence of Slater-Condon rules,\(^{38} \) the terms in the expansion are restricted to only singles and doubles excitation. In the following equation, the notation \( k \in S, D \) and \( G^{(S,D)} \) is used to denote that the only singles and doubles are included in the expansion

\[ E[\Phi_0, G^{(S,D)}] = \frac{\sum_{k,k' \in S, D} G_{0k} H_{kk'} G_{k'0}}{\sum_{k \in S, D} G_{0k} G_{k0}}, \quad (9) \]

where \( G_{kk'} \) and \( H_{kk'} \) are shorthand notation for matrix elements \( \langle \Phi_k | G | \Phi_{k'} \rangle \) and \( \langle \Phi_k | H | \Phi_{k'} \rangle \), respectively. The ground state energy is obtained variationally by minimizing the total energy with respect to the geminal parameters and the Slater determinant as shown below

\[ E_{\text{RI-CTH}} = \min_{\Phi_0} E[\Phi_0, G^{(S,D)}]. \quad (10) \]

B. Form of the correlation function

Although the expression in Eq. (9) is valid for any form of \( g(1, 2) \), the computational cost and ease of implementation depends on the specific choice of \( g(1, 2) \). In this work, we have used Gaussian-type geminal (GTG) functions\(^{39,40,43} \) for representing the 2-body correlation function

\[ g(r_{12}) = \sum_{k=1}^{N_k} b_k e^{-r_{12}^2/d_k^2}, \quad (11) \]

where \( b_k, d_k \) are the geminal parameters that completely define the GTG function. There are mainly two different techniques for determining the geminal parameters. In the first
method, the parameters are determined variationally by minimizing the total energy. Although this approach very accurate, it becomes computationally expensive because it involves multidimensional minimization and recomputation of the atomic orbital (AO) integrals. The second approach is to have a set of precomputed values of the geminal parameters. This approach is computationally fast, however, the challenge is to find a transferable set of parameters that can be applied to various molecules. In this work, we have developed a mixed approach where the linear geminal parameters \(b_k\) are variationally optimized during the calculation and the non-linear geminal parameters \(d_k\) are precomputed before the start of the geminal optimization. The central idea of this method is to use some appropriate characteristic length scale associated with the molecule for calculating the \(d_k\) parameters. We have used the average electron-electron separation distance as the characteristic system-dependent quantity for calculating the geminal optimization. The central ideal of this method is to find a transferable set of parameters that can be applied to various molecules. In this work, we have developed a mixed approach where the linear geminal parameters \(b_k\) are variationally optimized during the calculation and the non-linear geminal parameters \(d_k\) are precomputed before the start of the geminal optimization. The central idea of this method is to use some appropriate characteristic length scale associated with the molecule for calculating the \(d_k\) parameters. We have used the average electron-electron separation distance as the characteristic system-dependent quantity for calculating the geminal parameters. Using the reference Slater determinant \(\Phi_0\), we define the average electron-electron separation as

\[
\langle r_{12}\rangle_0 = \frac{1}{N(N-1)} \langle \Phi_0 | \sum_{i<j} r_{ij}^2 | \Phi_0 \rangle. \tag{12}
\]

The \(d_k\) parameters are selected from a set of numbers obtained by scaling \(\langle r_{12}\rangle_0\)

\[
d_k^2 \in \left[ \frac{1}{n} \langle r_{12}\rangle_0, \ldots, \frac{1}{2} \langle r_{12}\rangle_0, 2 \langle r_{12}\rangle_0, \ldots, n \langle r_{12}\rangle_0 \right]. \tag{13}
\]

The choice of \(\langle r_{12}\rangle_0\) over \(\langle r_{12}\rangle_0\) was made purely for computational convenience. The integral involving \(r_{12}\) is separable in \(x, y,\) and \(z\) components and can be integrated easily with Cartesian Gaussian-type orbitals (GTOs). Similar separation is not possible for \(\langle r_{12}\rangle_0\). The above procedure provides a fast and physically intuitive method for obtaining the non-linear geminal parameters.

After the non-linear \(d_k\) parameters were obtained using the steps described above, the linear geminal parameters \(b_k\) were optimized variationally. We have avoided recomputation of the AO integrals by postponing the inclusion of the \(b_k\) terms to the very last step of the calculation. This is shown by the following example. The expectation value of the geminal operator is defined as

\[
\langle \Phi_0 | G | \Phi_0 \rangle = \sum_{\mu \nu \lambda \sigma} P_{\mu \nu \sigma} \lambda \lambda \sigma \left( \frac{1}{2} [\mu \nu | g | \lambda \sigma] - \frac{1}{4} [\mu \sigma | g | \lambda \nu] \right) \tag{14}
\]

where \(\mu, \nu, \lambda, \sigma\) are AO indices, \(P\) is the density matrix, and the integrals are in chemist’s notation. Substituting the expression for the geminal function, Eq. (14) can be written as

\[
\langle \Phi_0 | G | \Phi_0 \rangle = \sum_k b_k \sum_{\mu \nu \lambda \sigma} P_{\mu \nu \sigma} \lambda \lambda \sigma A_{\mu \nu \lambda \sigma}^k \tag{15}
\]

\[
A_{\mu \nu \lambda \sigma}^k = \frac{1}{2} [\mu \nu | e^{-r_{12}^2/d_k^2} | \lambda \sigma] - \frac{1}{4} [\mu \sigma | e^{-r_{12}^2/d_k^2} | \lambda \nu]. \tag{16}
\]

The exact expression for the integrals can be found in Refs. 39, 44. In addition to restricting the terms in Eq. (9) to only singles and doubles, the fast evaluation of \(G_{0k}\) was used to further restrict the number of terms in the summation. We have implemented a “direct” approach in which the full \(H\) matrix is never constructed and the matrix element \(H_{i k}\) are computed as needed during the course of the calculations. The evaluation of \(H_{i k}\) is only performed when \(G_{0k} G_{0k}\) is higher than some threshold value

\[
|G_{0k} G_{0k}| > \Delta_{0k}. \tag{18}
\]

Overall, equations (13), (16), (17), and (18) represent the four key steps for efficient implementation of the RI-CTH methods.

C. Partial infinite-order summation

Up to this point, only finite expansion of the RI-CTH method has been considered. In this section, we will develop the infinite order summation approach. The main idea of this approach can be summarized in two steps. In the first step, the RI-CTH energy terms were expressed in terms of diagrammatic notations. In the next step, we used the diagrammatic summation technique to perform infinite order summation for certain classes of diagrams. Starting with Eq. (9), we define the 2-particle transition density matrix as

\[
\Gamma_{ijkl}^{\mu} = \langle \Phi_\mu | i^j j^i k | \Phi_\nu \rangle. \tag{19}
\]

Using the above expression, the numerator in the Eq. (9) can be written as

\[
G_{0m} = \sum_{ab} \sum_{ij} \langle ab | g | ij \rangle \Gamma_{abij}^{\nu m} \tag{20}
\]

where, the indices \(i, j, k, l\ldots\) are used for labeling the molecular orbitals (MOs). We have used the convention\(^{38}\) of labeling
the MOs that are occupied and unoccupied in the reference Slater determinant as $a,b,c,d...$ and $p,q,r,s...$, respectively. The overall expression of the electron-electron interaction in the RI-CTH energy is given as

$$G_{m'n'}^\text{me} G_{m'0} = \sum_{abcdijkl}^{N_{oc}} \Gamma_{abcd}^{mn} \Gamma_{ijkl}^{nm'} \Gamma_{klcd}^{mn'}$$

$$\times \langle ab|g|ij\rangle \langle ij'| \Gamma_{12}^{-1} |kl\rangle \langle kl|g|cd \rangle. \quad (21)$$

In the diagrammatic representation, the occupied MO indices $a,b,c,d$ are represented by hole lines ($\downarrow$). The general MO indices $ijkl'j'k'k'$ can be either particle ($\uparrow$) or hole ($\downarrow$) lines. For a finite RI expansion, the energy expression can be expressed in terms of finite number of diagrams. After careful analysis of the diagrams, we selected a subset of diagrams that were summed up to infinite order. The objective of performing the diagram summation is to obtain a compact renormalized operator that is more computationally tractable than the explicit infinite-order sum. The selection of diagrams for summation was based on the ease of implementation of the resulting renormalized operator. Since only a subset of diagrams (as oppose to all) were selected for summation up to infinite order, we denote this method as partial infinite-order summation (PIOS) method. The Coulomb diagrams that were summed up to infinite order in the PIOS method are presented in Figure 1. The summation of diagrams leads to the following expression

$$\sum_{\text{diagrams}} = \frac{\langle \Phi_{HF}|g(1,2)\Gamma_{12}^{-1} g(1,2)|\Phi_{HF} \rangle}{\langle \Phi_{HF}|g(1,2)g(1,2)|\Phi_{HF} \rangle}. \quad (22)$$

which is a renormalized 2-body operator. The prime over the summation in Eq. (22) is used to denote that only selected diagrams were included in the summation. Because the energy expression in Eq. (9) includes a denominator, identical procedure was also used for obtaining the denominator and the combined result is shown in Eq. (22). We define the RI-CTH-PIOS energy as

$$E_{\text{RI-CTH-PIOS}} = \tilde{E}_{\text{RI-CTH}} + E_{\text{PIOS}}, \quad (23)$$

where $E_{\text{PIOS}}$ is given by Eq. (22). The tilde on $E_{\text{RI-CTH}}$ is used to denote that RI-CTH energy should exclude diagrams that have been included in the PIOS energy calculation to prevent double counting.

D. Computational details

All the calculations were performed using $N_e = 2$ with two Gaussian-type geminal functions. The first set of geminal parameter were fixed at $h_1 = 1$ and $d_2^2 = \infty$. This choice of parameters ensured that the RI-CTH energy is always bounded from top by the Hartree-Fock energy. Hartree-Fock calculation was performed and $\langle \tau_{12}^2 \rangle_0$ was evaluated. The $\langle \tau_{12}^2 \rangle_0$ was used to construct the following trial set for the selection of the $d_2$ parameter

$$d_{\text{final}}^2 = \frac{1}{3} \langle \tau_{12}^2 \rangle_0, \frac{1}{2} \langle \tau_{12}^2 \rangle_0, \langle \tau_{12}^2 \rangle_0, 2 \langle \tau_{12}^2 \rangle_0, 3 \langle \tau_{12}^2 \rangle_0. \quad (24)$$

III. Results and conclusion

The RI-CTH method was applied for computing the ground state energy of isoelectronic 10-electron systems, Ne, HF, H2O, NH3, and CH4, and the results are presented in Table I. As expected, the RI-CTH energy is much lower than the HF energies. It was found that both CISD and CCSD(T) energies obtained using identical basis set are lower than the RI-CTH energy. This is an expected result because in the CISD calculation unconstrained optimization of the CI coefficients is performed. On the other hand, the coefficients in RI-CTH method are constrained by the functional form of the geminal function. Comparing the energies from the RI-CTH-PIOS calculations with CISD(6-31G*) and CCSD(T)(6-31G*) show that the RI-CTH-PIOS energy is consistently lower for all the 10-electron systems. We attribute this lower energy to the inclusion of diagrams that were missing in the RI-CTH method.
but were included because of the diagrammatic summation in RI-CTH-PIOS. The terms that are missing from the CISD/6-31G* calculation can be systematically included by increasing the size of the underlying 1-particle basis. To investigate this further, we have compared the RI-CTH-PIOS energies with Cisd calculation with a much larger basis set. As shown in Table I, the Cisd/cc-pV(T+d)Z are consistently lower than the RI-CTH-PIOS energy. The results in Table I indicate that the RI-CTH-PIOS method with a small basis set is able to capture part of the electron correlated energy that is only accessible to Cisd and CCSD(T) methods at larger basis sets.

In conclusion, the resolution of identity implementation of congruent transformed Hamiltonian has been presented. The congruent transformation of the many-electron Hamiltonian was performed using Gaussian-type geminal functions. The challenge of efficient optimization of the geminal function was addressed by using different strategies for optimizing linear and non-linear parameters. The linear geminal parameters were obtained variationally by minimizing the RI-CTH energy. The expectation value of the square of the electron-electron separation distance was used as the characteristic length scale for construction of the non-linear geminal parameters. One of the key results in this work is the development and application of partial infinite order summation method. Diagrammatic notation of the RI-CTH expression was introduced and the RI-CTH-PIOS calculations were performed. It was found that for identical basis functions, the RI-CTH-PIOS energies are lower than the Cisd and CCSD(T) energies for the isoelectronic 10-electron system studied in this work.

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### Table I. RI-CTH-PIOS energies for isoelectronic 10-electron systems. All the values are reported in atomic units.

| Method             | Ne | HF    | H₂O   | NH₃    | CH₄    | References                  |
|--------------------|----|-------|-------|--------|--------|----------------------------|
| HF                 |    | -128.474407 | -100.002394 | -76.009999 | -56.183815 | -40.194821 | This work |
| RI-CTH-PIOS/6-31G* |    | -128.605009 | -100.153397 | -76.165385 | -56.361897 | -40.353006 | 45 |
| CISD/6-31G*        |    | -128.623340 | -100.180709 | -76.198206 | -56.369520 | -40.431821 | 45 |
| CCSD(T)/6-31G*     |    | -128.626734 | -100.186601 | -76.205841 | -56.454729 | -40.530006 | 45 |
| Cisd/cc-pV(T+d)Z   |    | -128.791918 | -100.322996 | -76.313875 | -56.454523 | -40.424120 | 45 |
| Cisd/cc-pV(T+d)Z   |    | -128.798209 | -100.331994 | -76.324556 | -56.465536 | -40.431821 | 45 |
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