Stability analysis of a double similarity transformed coupled cluster theory

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ABSTRACT

In this paper, we have analyzed the time series associated with the iterative scheme of a double similarity transformed coupled cluster theory. The coupled iterative scheme to solve the ground state Schrödinger equation is cast as a multivariate time-discrete map, and the solutions show the universal Feigenbaum dynamics. Using recurrence analysis, it is shown that the dynamics of the iterative process is dictated by a small subgroup of cluster operators, mostly those involving chemically active orbitals, whereas all other cluster operators with smaller amplitudes are enslaved. Using synergetics, we will indicate how the master-slave dynamics can suitably be exploited to develop a novel coupled-cluster algorithm in a much reduced dimension.

I. INTRODUCTION AND THEORY

Coupled Cluster (CC) theory is an accurate electronic structure methodology to compute the energetics and properties of small- to medium-sized atoms and molecules. CC theory, with singles, doubles, and perturbative triples excitations, the so-called CCSD(T), is known to provide very accurate results for molecules in their near-equilibrium geometry. Recently, a new iterative scheme, known as the iterative n-body excitation inclusive CCSD (iCCSDn), which takes care of the fully connected triple excitations at a computational cost less than that of CCSD(T), has been proposed. Owing to the nonlinear nature of the CC amplitude determining equations, one employs an iterative procedure to find the solutions, which are the fixed points of the iterative process. Here, we will present a posteriori analysis of the time series associated with the iterative process of iCCSDn methodology. By introducing a regularization parameter to probe the non-linearity associated with the dynamics of the iteration process, we will show that such an iteration process exhibits rich dynamical features. Furthermore, a detailed study of the dynamics would help us to establish certain inter-relationships among the different cluster operators. One may further exploit the synergy among different cluster operators to construct a novel CC iterative scheme where the effective degrees of freedom are drastically reduced. Thus, the study of the dynamics associated with the CC iteration process is important from a quantum chemistry perspective. Such a scheme to formulate an effective CC theory with significantly fewer iterables will sketchily be presented toward the end of this article. We note that such an analysis holds true for conventional CC theory as well; however, we will restrict our analysis solely to iCCSDn.

In iCCSDn, one parametrizes the wavefunction as a double exponential waveoperator \( \Omega \) acting on a reference zeroth-order wavefunction, usually taken to be the Hartree–Fock (HF) determinant,

\[
\Omega = \{ \exp(S) \} \exp(T_1 + T_2),
\]

where \( T_i \)’s are the usual CCSD excitation operators (also known as the cluster operators) and \( S \) denote the scattering operators that induce higher excitations by their action on the doubly excited determinants. \( S \) and \( T \) operators do not commute. The presence of hole \( \rightarrow \) hole (or particle \( \rightarrow \) particle) scattering in \( S \) ensures that its action on the HF determinant is trivially zero, but not on an excited determinant. The higher rank correlation effect is simulated via the contraction of \( S \) and \( T \) operators, and hence, it provides the accuracy at a cheap computational scaling. The quantity inside \( \{ \cdot \} \) denotes “normal ordering,” which ensures that the CC expansion terminates at finite power. The effective
Hamiltonian, \( G \), is constructed via two similarity transformations recursively,
\[
G = e^{-\left(T_1 + T_2\right)} W e^{\left(T_1 + T_2\right)},
\]
where
\[
W = \exp(S) - (\exp(S) - 1) \exp(S)
\]
is the first similarity transformed Hamiltonian obtained through the time-independent Wick’s theorem and the connections that depict Wick contraction. The determination of the cluster operators can be done in a coupled manner at a scaling marginally higher than CCSD. The cluster operator \( T_s \)s are responsible for inducing the dynamical correlation, whereas the \( S \) operators renormalize them through a set of local denominators by including the effects of connected triple excitations within the two-body cluster amplitudes. Thus, they are expected to be large at stretched molecular geometries. Note that the \( S \) operators do not have any direct effect on energy; however, they do indirectly contribute at high perturbative orders by renormalizing the cluster amplitudes.

Following a many-body expansion\(^{10} \) of the double similarity transformed Hamiltonian, \( G \), the amplitudes \( t_s \) (associated with \( T \) (S) and operators are obtained through a set of coupled nonlinear equations by demanding \( g_s = g_s = 0 \) upon convergence. Here, \( g \) is the amplitude associated with the tensor \( G \), and \( \mu \) (\( \alpha \)) are the collective orbital labels associated with the tensor \( T(S) \). Let us denote the orbital labels associated with \( T \) as \( \nu, \eta, \ldots \), and those associated with the scattering operator \( S \) as \( \alpha, \beta, \ldots \). In the iteration procedure, the discrete-time propagation of the vector at the \((n+1)\)th step can be represented as time-discrete maps,
\[
\begin{align*}
\xi^{(n+1)}_\mu &= \xi^{(n)}_\mu + \sum_{\nu=1}^m \frac{\partial f_\nu}{\partial \eta} \xi^{(n)}_\nu + \sum_{\beta=1}^m \frac{\partial f_\beta}{\partial \xi^{(n)}_\beta}, \\
\xi^{(n+1)}_\nu &= \xi^{(n)}_\nu + \sum_{\mu=1}^m \frac{\partial g_\mu}{\partial \eta} \xi^{(n)}_\mu + \sum_{\beta=1}^m \frac{\partial g_\beta}{\partial \xi^{(n)}_\beta}.
\end{align*}
\]

Here, \( D \) is a suitably chosen denominator, usually taken as the HF orbital energy difference associated with the orbital labels of \( \mu \) (and \( \alpha \)), and \( \eta \) is known as the damping or regularization parameter, which is sometimes used to accelerate the convergence of the iterative procedure without affecting the fixed points. Note that in control theory and system engineering, such an external parameter is known as an input, perturbation, or control parameter. Following the standard nomenclature in quantum chemistry, we will call \( \eta \) as the regularization parameter that controls the dynamics of the iteration process. Let the vector \((\vec{t}, \vec{s})\) be the fixed points of the equation such that \( t_\eta = f_\eta(\vec{t}, \vec{s}) \) and \( s_\eta = f_\eta(\vec{t}, \vec{s}) \) or, in general, \( (t_\mu, s_\nu) = f(\vec{t}, \vec{s}) \). Here, \( f_\nu \) and \( f_\mu \) are the functions having the same hole/particle tensor structure as \( g_\nu \) and \( g_\mu \), respectively, and \( f \) is the generic symbol of \( f_\nu \) and \( f_\mu \). Following Refs. 11 and 12, let us assume a small deviation around the fixed points to be \( \xi \) such that
\[
(f^{(n)}(\vec{t}), f^{(n)}(\vec{s})) = (\vec{t}, \vec{s}) + \xi^{(n)}.
\]

Hence, employing Taylor series expansion around the fixed points, we obtain
\[
(t_\mu, s_\nu) + \xi^{(n+1)}_\mu = f(\vec{t}, \vec{s}) + \sum_{\nu=1}^m \frac{\partial f_\nu}{\partial \eta} \xi^{(n)}_\nu + \sum_{\beta=1}^m \frac{\partial f_\beta}{\partial \xi^{(n)}_\beta} \xi^{(n)}_\beta + \ldots.
\]
II. RESULTS

The stability of the iterative procedure depends upon the eigenvalues of the associated stability matrix. If all the eigenvalues of the stability matrix are less than 1 (i.e., the corresponding Lyapunov exponents are negative), then the procedure converges. Thus, \( |\lambda| < 1 \) is the convergent condition for any iterative procedure. A detailed study of the highest Lyapunov exponents of each symmetry for symmetrically stretched water (bond length \( \approx 2.6741 \) bohrs, bond angle \( \approx 96.774^\circ \), and cc-pVQZ basis) is reported in Figs. 1 and 2 of the supplementary material. It is shown that the highest Lyapunov exponent (corresponding to \( A_1 \) symmetry) becomes positive at \( \eta = 0.29 \).

Near the point of equilibrium with small enough \( \eta \), the system is Lyapunov stable and the iteration converges to the same set of fixed points. In fact, there is a range of \( \eta \) for which the system takes a fewer number of steps to converge after which it increases sharply (see Fig. 3 of the supplementary material). Here, we quantify the effects of larger input disturbances, as done in control theory.

Around \( \eta = 0.2712 \), the perturbation crosses the critical value and one observes the onset of an oscillatory divergence (DIV) in the initial phase of the iteration process, followed by the generation of the period-2 cycle. \( \eta \) may be considered as a measure of the non-linearity in the system. However, a linear Lyapunov stability analysis is unable to predict the cases where the perturbation is large. For our coupled time-discrete map, the severe non-linearity results in an early onset of period-2 cycles. With the increasing value of the parameter, \( \eta \), one further observes period-2\(^n\) cycles \((n = 2, 3, \ldots)\), before the iteration becomes chaotic. Note that for such 1-parameter dynamics, a full period doubling cascade must precede chaos. The cluster amplitudes at an arbitrarily chosen \( k \)th step recur at the \((k + 2^n)\)th step for period-2\(^n\) cycle (see Figs. 4–8 of the supplementary material), and the energy obtained by evaluating the vacuum expectation value \( \langle e^{-T} \mathcal{W} e^T \rangle \) oscillates between 2\(^n\) periods. For a range of \( \eta \), it shows a period-doubling bifurcation cascade (Fig. 1). Note that also for the conventional CC theory, one observes such a period-doubling bifurcation cascade, which is shown in Fig. 9 of the supplementary material.

The range of the parameter for successive higher period cycles keeps on shrinking as a characteristic of the period-doubling bifurcation. In fact, in the limiting case, i.e., at the onset of chaos, any single parameter map follows the dynamics such that

\[
\lim_{n \to \infty} \delta = 4.6692, \quad \delta = \frac{\eta_{n+1} - \eta_n}{\eta_{n+2} - \eta_{n+1}}.
\]

Here, \( \eta_0 \) is the onset point of the period-2\(^n\) cycle. The limit of \( \delta \) is a universal constant, known as Feigenbaum constant. Despite being a multivariate map with a tensorial structure, it is indeed possible to generate all the different period cycles, as shown in Fig. 1. With a numerical algorithm based on the bisection method, we have precisely determined the onset points of different period cycles. The first eight values of \( \eta \) are shown in Table I along with the ratio \( \delta \). In the limiting case of \( n \to \infty \), the \( \delta \) computed shows excellent (error \( < 0.004\% \)) agreement with the universal value of the Feigenbaum constant. Thus, the iteration process under an perturbation, like general \( n \)-dimensional maps of 1-parameter family, shows the bifurcation doubling route to chaos, with the same geometric rate given by the Feigenbaum constant. The very high value of the first ratio demonstrates an early onset of the period-2 cycle, as otherwise predicted by the largest Lyapunov exponent. Thus, it tells us about the severe nonlinearity of the system. One should further note that the convergence to the exact value with higher period cycles is not monotonic, rather we observe an oscillating convergence.

Such a clear separation of different periodic cycles, which is the characteristic of symmetric few variable systems, indicates the presence of a set of few variables that govern the dynamics. In cases where the linear stability is lost, it is indeed possible to eliminate most of the degrees of freedom from the non-linearly interacting subsystems so that the macroscopic behavior of the system is governed by a few degrees of freedom only. Along this line, we presume that the dynamics of our system is dictated by only a few large cluster amplitudes, which are the order parameters (unstable modes) of the system that determine its macroscopic pattern.

We have further studied the dynamics with recurrence analysis. Here, each iteration was embedded as one time step. The state \( \mathbf{x}_t \) was taken as a vector comprising all the cluster amplitudes at the \( t \)th time step, \( \mathbf{x}_t = (t_1, t_2, \ldots) \), where \( t_1 \) and \( t_2 \) denote the renormalized one and two body cluster amplitudes at the \( t \)th time step, respectively. We reiterate that these operators do not contribute to energy directly; rather their effects are accounted for into the cluster operators via a set of renormalization terms. Hence, the state \( \mathbf{x}_t \) is constructed with one- and two-body cluster amplitudes only.

The distance matrix (DM, also known as the unthreshold recurrence matrix), which is a useful tool to study the phase space trajectory, is defined as

\[
\text{DM}_{ij} = \| \mathbf{x}_i - \mathbf{x}_j \|, \quad i, j = 1, \ldots, N,
\]

where \( N \) is the length of time series and \( \| \cdot \| \) is a norm. Here, the simulation was run for 4000 steps and plotted for the last \( N = 64 \) iterations.

We have plotted DM taking all the (non-zero) cluster amplitudes, here on referred to as Full-T (4938 non-zero variables), and shown for some representative \( \eta \) values (left panel of Fig. 2). To support our hypothesis stated before, we have divided the cluster amplitudes into two subsets: the largest subset, denoted as \( \{ t^2 \} \), and the smaller subset, \( \{ t^3 \} \). We have identified a set of few large cluster operators (totally 11), which have amplitudes >0.05 throughout the entire range of \( \eta \). These operators involve at least a pair of chemically active orbitals (see the supplementary material) and belong to the largest subset \( \{ t^2 \} \). Rest of the amplitudes are elements of the smaller subset \( \{ t^3 \} \). It is found that the DM for different \( \eta \), constructed with the largest subset of amplitudes, \( \{ t^2 \} \), replicates the phase space trajectory to that obtained by Full-T with excellent quantitative and qualitative accuracy. This is shown in the right panel of Fig. 2 at the same \( \eta \) values. The average variation for the largest subset, \( \{ t^2 \} \), matches with that constructed with Full-T with >93% accuracy through the entire range of \( \eta \), as shown in Fig. 3. Furthermore, the variation in the average value of the DM constructed by the full set of \( t \)-amplitudes is qualitatively replicated by the largest subset. Thus, the variation in the smaller amplitudes
is almost entirely suppressed by the largest subset, making them asymptotically negligible in the dynamics. The macroscopic pattern is solely determined by the dynamics of the large amplitudes that behave as the order parameters of the system. Their variation is independent of the microscopic sub-dynamics of the smaller amplitudes. In other words, the largest subset enslaves the smaller amplitudes. Such domination of the large subset is amplified by the non-linear terms of the CC expansion, whereas the small amplitudes effectively contribute at the linear level to provide the feedback coupling.

One may wonder whether the dynamics would repeat if the small amplitudes are set to zero. We reiterate that it is absolutely crucial that the small amplitudes provide the feedback coupling in determining the larger amplitudes, while the former set of amplitudes are determined by the latter solely. In synergetics, this is known as the circular causality. The internal dynamics of the smaller amplitudes can be considered to be frozen.

A. Recurrence quantification analysis (RQA)

The recurrence plot (RP) is a heuristic approach to quantify the epochs of a particular state to recur in a time-series and is based on its phase space trajectory. A recurrence matrix is defined as

<table>
<thead>
<tr>
<th>n</th>
<th>Period (2^n)</th>
<th>η</th>
<th>δ (% error in δ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>0.2711953</td>
<td>...</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>0.3545298</td>
<td>...</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>0.363806</td>
<td>8.983(92.4%)</td>
</tr>
<tr>
<td>4</td>
<td>16</td>
<td>0.3659015</td>
<td>4.428(5.2%)</td>
</tr>
<tr>
<td>5</td>
<td>32</td>
<td>0.366336</td>
<td>4.814(3.1%)</td>
</tr>
<tr>
<td>6</td>
<td>64</td>
<td>0.3664299</td>
<td>4.66145(0.165%)</td>
</tr>
<tr>
<td>7</td>
<td>128</td>
<td>0.3664491</td>
<td>4.67237(0.068%)</td>
</tr>
<tr>
<td>8</td>
<td>256</td>
<td>0.3664541953</td>
<td>4.66937(0.00364%)</td>
</tr>
</tbody>
</table>
\[ RP_{ij} = \Theta(\varepsilon_i - DM_{ij}), \]  

where \( \varepsilon_i \) is a suitable threshold distance and \( \Theta(\cdot) \) is the Heaviside function. Thus, if the \( DM_{ij} \) is less than the threshold, the corresponding \( RP_{ij} = 1 \), denoted by a black dot, otherwise \( RP_{ij} = 0 \) (white dot). In Recurrence Quantification Analysis (RQA), one quantifies the density of recurrence points as well as the histograms of the lengths \( l \) of the diagonal based on a suitably chosen recurrence threshold \( \varepsilon \). The recurrence threshold is the most significant quantity in RQA. It should be chosen small enough to distinguish the closely spaced trajectories but not small enough to miss out on the rich dynamics associated with the time series. We have chosen \( \varepsilon_i = 0.05 \) for all further analyses. RPs at a few selected values of \( \eta \) with \( \varepsilon = 0.05 \) is given in Fig. 4, where the left blue panels represent those constructed with the full set of \( t \)-amplitudes, while the right red panels are constructed with the largest subset. In both the cases, for a given \( \eta \), the RPs are characterized by similar continuous diagonal lines, although the RPs constructed with the largest subset (right red panels) sometimes may have denser population of the isolated black dots. RPs with a wide range of the threshold parameters and for different period cycles are presented in the supplementary material.

Recurrence analysis gives us quantitative measures of different quantities associated with the dynamics. Recurrence rate (RR), which is a measure of the density of recurrence points and signifies the probability of occurrence of a specific state, is defined as

\[ RR = \frac{1}{N^2} \sum_{ij=1}^{N} RP_{ij}. \]
Thus, higher RR corresponds to a more repetitive state space trajectory. Figure 5(a) shows the RR of our system and displays a gradual decrease from lower period cycles to higher periodic cycles and eventually to chaos. Note that the RR obtained from the time evolution of the largest subset, \( \{ t^r \} \) (red plot) follows quantitatively closely to that obtained from Full-T (blue plot). One may note that the choice of the threshold is sensitive enough to capture chaos-period transition in the islands of stability around \( \eta = 0.369 \) and \( \eta = 0.372 \), which are characterized by sudden upward spikes in the RR plot.

Deterministic periodic systems are often characterized by repeated long and continuous diagonal lines in their RPs, signifying repeated similar state evolution. The RPs corresponding to fewer period cycles have a larger number of continuous diagonal lines parallel to the Line of Identity (LOI) in a given length of the time series. Contrarily, subsequent independent values often appear as the isolated single points. Thus, the fraction of recurrence points appearing as diagonal points parallel to the LOI is considered to be a measure of determinism of the system,

\[
DET = \frac{\sum_{l=1}^{N-l_{\text{min}}} IP(l)}{\sum_{l=1}^{N} IP(l)} \quad (13)
\]

Here, \( P(l) \) is the histogram of diagonal lines of length \( l \). \( DET \) is a measure of predictability of the system. As a necessary (but not sufficient) condition, the periodic systems are characterized by a high value of \( DET \), and this has successfully been predicted quantitatively by the RQA, both with Full-T (blue) and largest subset (red) of \( T \) amplitudes [Fig. 5(d)].

A high value of maximum diagonal length \( (L_{\text{max}}) \), defined as \( L_{\text{max}} = \max(l_i; \ i = 1, 2, \ldots, N) \), is often characteristic of regular, correlated, and periodic systems. In the RQA, one may roughly interpret its inverse, known as divergence (DIV), defined

\[
DIV = \frac{1}{N} \sum_{i=1}^{N} |x_i - x_{i+1}|
\]
as $\text{DIV} = L_{\text{max}}^{-1}$, as an estimator of the Lyapunov exponent. Excluding the LOI and an appropriate Theiler window around it, the other recurrence points from the subsequent phase space vectors lead to continuous diagonal lines in the RP. Thus, the lower period cycles, with frequent recurrence of the same states, have a higher $L_{\text{max}}$ value and lower DIV. This has been quantitatively verified and shown that these two measures have identical behavior when the Full-T amplitudes and largest subset are used [Figs. 5(b) and 5(c)].

One of the important quantities that emerges from RQA is the entropy associated with the dynamics. However, studies have shown that using the Shannon entropy obtained from RP using its diagonal length histograms, given by $\text{ENTR} = -\sum_{l=1}^{N} p(l) \ln(p(l))$, where $p(l)$ is the probability distribution of the diagonal length, gives a counter-intuitive trend of entropy for period–chaos systems. It is observed that such a description often shows the decreasing value of entropy with increasing chaos and it also anti-correlates with the maximal Lyapunov exponent. A number of methods have been suggested for the calculation of entropy. Following Ref. 31, we have calculated it from the Weighted Distance Matrix (WDM), defined by

$$W_{ij} = e^{-\|\mathbf{x}_i - \mathbf{x}_j\|}.$$  

(14)

For entropy calculation, we define strength $(s_i)$ as $s_i = \sum_{j=1}^{N} W_{ij}$. The strength is used to calculate the Shannon entropy associated with the WDM through the distribution of $P(s)$.

FIG. 5. Variation in (a) RR, (b) $L_{\text{max}}$, (c) DIV, (d) DET, and (e) entropy as a function of the regularization parameter $\eta$ computed via RQA. Blue line denotes the quantities with Full-T, and red line denotes those of the largest subset. The bifurcation diagram (f) is also presented along the same horizontal scale to identify the period–period and chaos–period transition locations.
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of Chemical Physics

The basis of an effective CC theory with reduced dimensionality, which
significantly extent. Furthermore, the dimension of the largest subset
procedure. This then reduces the computational scaling to a sig-
smaller amplitudes, on the other hand, may be computed from their
process via usual numerical techniques, such as DIIS. Hundreds of
amplitudes couple in their equations to provide the feedback coupling
the corresponding cluster amplitudes, whereas the smaller ampli-
tudes is frozen, we propose a novel version of CC theory where one
considered to be frozen. All such RQA measures are found to be largely
of the time-series embedding dimension. In Subsec-
tion II B, we will show that such inter-relationship among different
sets of cluster amplitudes may be exploited to construct an effective

B. Implications to quantum chemistry

While the chaotic dynamics encountered in quantum chem-
istry methods is interesting in itself, it has immense implications to
gain insight into methods of quantum chemistry. Note that the prin-
ciples of synergetics allow us to map each of the small amplitudes as
unique functions of the larger amplitudes. In other words, one may write

\[ \mathcal{F}_k^{\delta} = \mathcal{F}_k \left( \{ t^{(1)} \} \right), \]  

where \( t^{(k)}_i \) is the \( k \)th element of the smaller subset \( \{ t^{(\delta)} \} \) and \( \mathcal{F}_k \) is the
functions of the largest subset, which determines the \( k \)th element of
the smaller subset in a function of the largest subset only. Start-
ing from a few initial iterations, one may numerically construct
these functions for each small amplitude with a suitable combina-
tion of the elements of the largest subset. The functional depend-
ence of the smaller subset on the largest subset is fixed through
the entire iteration process. That implies that one may devise an
effective CC theory where the iteration may be restricted to only a
few degrees of freedom. One may iteratively update the residues of
only the few excitations belonging to the largest subset to determine
the corresponding cluster amplitudes, whereas the smaller amplit-
uides couple in their equations to provide the feedback coupling
in the iteration process. One may further accelerate the iteration
process via usual numerical techniques, such as DIIS. Hundreds of
smaller amplitudes, on the other hand, may be computed from their
predetermined functional map without going through the iterative
procedure. This then reduces the computational scaling to a sig-
nificant extent. Furthermore, the dimension of the largest subset
\( \{ t^{(\delta)} \} \) is independent of the size of the basis set. This constitutes the
basis of an effective CC theory with reduced dimensionality, which
is currently under development and warrants a separate publication
elsewhere.

III. CONCLUSION

In summary, we have shown that the discrete-time propagation
associated with the iterative procedure of a double similarity trans-
formed CC theory shows the dynamical features of a logistic map.
The dynamics shows the usual period doubling bifurcation route to
chaos, with the universal geometric rate given by the Feigenbaum
constant. Furthermore, recurrence analysis was performed with the
state vectors comprising all the cluster amplitudes and that with
the largest subset thereof. The RQA shows an identical phase space
trajectory for these two cases. This reinforces our hypothesis that
only a few of the excitations with large amplitudes govern the iter-
ation dynamics, whereas hundreds of cluster operators with smaller
amplitudes are enslaved.

Given the fact that the internal dynamics of the smaller ampli-
tudes is frozen, we propose a novel version of CC theory where one
may restrict the iteration procedure only to determine the ampli-
tudes of the largest subset, whereas the smaller amplitudes may be
determined from their functional dependence on the largest sub-
set. Thus, the principles of synergetics are likely to pave the way to
develop a few variable effective CC theory.

SUPPLEMENTARY MATERIAL

See the supplementary material for the following:

- Largest Lyapunov exponents corresponding to different
  symmetries of symmetrically stretched \( \text{H}_2\text{O} \) molecules in the
  \( \text{cc-pVDZ} \) basis as a function of \( \eta \);
- a plot showing the number of iteration steps taken to con-
  verge to the fixed points as a function of the regularization
  parameter \( \eta \);
- representative energy vs iteration step plots and configura-
  tion space trajectories for some representative values;
- the bifurcation diagram for the conventional CCSD theory;
- a list of the cluster operators involving active orbitals with
  amplitudes \( >0.05 \), which form the largest subset;
- distance matrices for different periodic cycles with the Full-
  \( T \) and largest subset; and
- recurrence plots for different period cycles and chaos for a
  range of threshold values.

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DATA AVAILABILITY

The data that support the findings of this study are available
from the corresponding author upon reasonable request.
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