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MULTICONFIGURATION COUPLED-CLUSTER CALCULATIONS FOR EXCITED ELECTRONIC STATES: APPLICATIONS TO MODEL SYSTEMS

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A multiconfigurational coupled-cluster method previously developed in our laboratory is used to study excited states of the same spatial and spin symmetry as the ground state. Applications are made, with rather small atomic orbital basis sets, to molecular systems which are highly correlated. These small-basis calculations are viewed on model calculations whose value lies in the fact that one can also obtain the exact (full configuration interaction) energy in such cases. The results show that even though the coupled-cluster equations may have many spurious solutions, one can locate solutions corresponding to the desired excited states by using procedures similar to those utilized for ground states. To achieve this success, one should include in the reference function all of the dominant configurations of the state under consideration. Next, one should use the unique solution of the linearized coupled-cluster equations as the initial estimate to begin the solution of the non-linear coupled-cluster equations. If the solution of these non-linear equations gives rise to one or more large t amplitudes one should repeat this procedure but with the configuration corresponding to the large t amplitude included in the reference function.

1. Introduction

The coupled-cluster (CC) method [1–9] is recognized to be a powerful tool for the computational investigation of electronic properties of molecules. Within CC methods, the coupled-pair many-electron theory [2] (CP MET) is a well characterized and seemingly quite reliable approximation for the calculation of ground-state wavefunctions for systems where the Hartree–Fock single determinant is the dominant configuration. More recently, open-shell CC methods [4–9] have been developed which allow one to study systems with wavefunctions requiring multiconfigurational description. We recently applied our own coupled-cluster method [5–7], which treats multiconfiguration reference states (which we refer to as the CCMC method) to the ground states of several closed- and open-shell systems [$H_2(^1\Sigma_g^+)$, $Li(^2S)$, $HeH_2(^1A_1)$, $CH_2(^3B_1, {}^1A_1)$, and $BeH_2(^1A_1)$]. Of course, any method for the calculation of electronic properties would be of limited value if excited electronic states of the same spatial and spin symmetry as the ground state could not be obtained with reasonably similar accuracy and ease.

In this paper, we study such excited states using our CCMC method. In section 2 we briefly review our CCMC development and discuss the possibilities in which various coupled cluster methods might be expected to produce erroneous results. In section 3 the results of our CCMC calculations on the *excited* states of small atomic-orbital basis treatments of $CH_2(^1A_1)$ and $BeH_2(^1A_1)$ are presented and analyzed. We stress that in both cases, the $^1A_1$ states examined are *not* the lowest states of these symmetries. We are looking at excited states which have lower states of the same symmetry. The emphasis of this paper lies in demonstrating that our CCMC method can be used on excited electronic states in exactly the same manner as on ground states. Our test systems are chosen to illustrate and test this emphasis rather than to generate new chemical knowledge about these molecules.

2. CCMC overview

In performing CCMC calculations on excited electronic states, one must address several questions about the particular CC theory to be used. How many solutions do the coupled-cluster equations have? Do they contain the solution describing the particular excited state of interest? For a particular choice of the reference wavefunction (which must be specified in any CC theory), to which states can the coupled-cluster equations be made to converge?

To facilitate further discussion of these points, we now give a short sketch of the development of our CCMC method [5–7]. All CC methods introduce a reference wavefunction Φ^i which is viewed as a zeroth-order approximation to an ith eigenfunction ψ^i of the Schrödinger equation

$$H\psi^i = E_i\psi^i. \tag{1}$$

All CC methods use an exponential operator $\exp(T)$ to connect ψ^i to Φ^i:

$$\psi^i = e^T\Phi^i. \tag{2}$$

The operator T contains, in principle, all possible levels of orbital excitations

$$T = T_1 + T_2 + T_3 + \ldots + T_N, \tag{3}$$

where N is the number of electrons in the system. These individual operators T_j are expressed in terms of amplitudes $t_{r\alpha}$, $t_{r\alpha s\beta\ldots}$ and orbital excitation operators $e_{r\alpha}$, $e_{r\alpha s\beta\ldots}$:

$$T_1 = \sum_{r,\alpha} t_{r\alpha}e_{r\alpha},\quad T_2 = \tfrac{1}{2}\sum_{r\alpha s\beta} t_{r\alpha s\beta}e_{r\alpha s\beta},\quad \text{etc.} \tag{4}$$

The Schrödinger equation can then be rewritten as

$$\tilde{H}\Phi^i = E_i\Phi^i, \tag{5a}$$

where

$$\tilde{H} = e^{-T}He^{T} = H + [H, T] + \tfrac{1}{2}[[H, T], T] + \ldots . \tag{5b}$$

This expansion of $\tilde{H}$ truncates exactly at the fourth commutator in the closed-shell CC theory and in certain open-shell CC methods [5]. The unknown t amplitudes and the total energy E_i are calculated in the CCMC method by projecting their Schrödinger equation against the functions

$$|\Phi^i_{r\alpha s\beta\ldots}\rangle = e_{r\alpha s\beta\ldots}|\Phi^i\rangle \tag{6}$$

and $|\Phi^i\rangle$ itself:

$$\langle\Phi^i_{r\alpha s\beta\ldots}|\tilde{H}|\Phi^i\rangle = 0, \tag{7}$$

$$\langle\Phi^i|\tilde{H}|\Phi^i\rangle = E_i. \tag{8}$$

For those circumstances in which Φ^i is a multiconfigurational function written as a linear combination of orthonormal configurations $\{\chi_K\}$

$$\Phi^i = \sum_K C_K\chi_K, \tag{9}$$

the coefficients C_K can also be determined from

$$\langle\chi_L|\tilde{H}|\Phi^i\rangle = E_iC_L. \tag{10}$$

Using eq. (5b) for $\tilde{H}$ and collecting powers of the t amplitudes, allows the fundamental CC equations (7) to be rewritten in compact matrix form as

$$\mathbf{A} + \mathbf{B}t + \mathbf{C}tt + \mathbf{D}ttt + \mathbf{E}tttt = 0, \tag{11}$$

where the elements of the **A**, **B**,... matrices, for example, are

$$A_{r\alpha s\beta} = \langle\Phi_{r\alpha s\beta}|H|\Phi\rangle, \tag{12a}$$

$$B_{r\alpha s\beta,pq} = \langle\Phi_{r\alpha s\beta}|[H, e_{pq}]|\Phi\rangle, \tag{12b}$$

$$C_{r\alpha s\beta,pq,mn} = \langle\Phi_{r\alpha s\beta}|[[H, e_{pq}], e_{mn}]|\Phi\rangle, \tag{12c}$$

$$D_{r\alpha s\beta,pq,mn,ab} = \langle\Phi_{r\alpha s\beta}|[[[H, e_{pq}], e_{mn}], e_{ab}]|\Phi\rangle, \tag{12d}$$

$$E_{r\alpha s\beta,pq,mn,ab,cd} = \langle\Phi_{r\alpha s\beta}|[[[[H, e_{pq}], e_{mn}], e_{ab}], e_{cd}]|\Phi\rangle. \tag{12e}$$

These matrices are given explicitly in terms of integrals and density matrices in ref. [5]. We stress that eq. (11) is *not* an infinite series since the commutator expansion for $\tilde{H}$ truncates after the fourth term. The unknown t amplitudes can thus be determined through the solution of the system of non-linear equations given in eq. (11).

In the context of a closed-shell single-determinant reference wavefunction, Zivkovic [10] has shown that eq. (11) has at least m solutions, where m is the total number of t amplitudes. For cases referred to as "well-behaved systems" in ref. [10], these m solutions have been shown to have real energies and to be identical to the corresponding m solutions of the configuration interaction problem spanned by the $m+1$ functions $\{\Phi, T\Phi\}$. Although it is very important to know such things about the existence of solutions to the CC equations, one also needs to have a practical means of reaching the desired solution starting from some reasonable reference function Φ. Since eq. (11) is a system of m quartic equations in $\boldsymbol{t}$, there may be, according to Bezout's theorem [11], as many as 4^m solutions to these equations in cases not covered by Zivkovic's proof. Thus the coupled-cluster equations may have a lot more solutions than the corresponding CI problem, most of which are spurious. In actual (approximate) calculations, some of these spurious solutions may be real (i.e. not complex) and therefore lead to confusion when one is seeking a particular solution of the CC equations.

Although the CC equations may indeed contain many spurious solutions, we have been quite successful in obtaining ground-state wavefunctions and energies using our CCMC method [6,7]. Our success has been based largely upon using a reasonably accurate reference function Φ^i together with stable procedures for finding solutions to the CCMC equations. Because the CC equations are non-linear and because they may contain numerous spurious solutions, it is critical that we have available a reliable procedure for converging the iterative solution of eq. (11) to the desired state.

We were successful in using a Newton–Raphson (NR) procedure with an initial approximation to $\boldsymbol{t}$ obtained from the linearized CC equations $\mathbf{A}+\mathbf{B}\boldsymbol{t}=0$ for solving the $\boldsymbol{t}$ determining eq. (11). In nearly all cases, this NR procedure was found to converge to the solution nearest to the starting function Φ. (In the appendix we discuss the concept of closeness of the initial solution to the desired eigenvalue.)

We feel from experience with ground-state CCMC calculations, that one can optimize changes to converge such iterative NR procedures for excited states by following a few guidelines based on the observation that it is desirable for the expansions of the wavefunction ψ^i shown in eq. (2) and of the effective hamiltonian $\tilde{H}$ shown in eq. (5b) to be dominated by their terms which are low order in the $\boldsymbol{t}$ amplitudes. Then truncation of these expansions would be expected to yield reasonable approximations to the full CCMC solution, and the approximation could be improved by including higher-order terms.

Our prescription for achieving the dominance of the low-order $\boldsymbol{t}$-amplitude contributions involves first choosing the reference function Φ^i as close as is reasonably possible to the desired ψ^i, by placing all dominant configurations of ψ^i in the reference Φ^i. Given this choice of ϕ^i, we have good reason to expect that the $\boldsymbol{t}$ amplitudes describing further electronic interactions in the state ψ^i are small. As a result, solution of the non-linear CCMC equations can reasonably be started with the solution of the linearized version $\mathbf{A}+\mathbf{B}\boldsymbol{t}=0$. This linear set of equations has a *unique* solution which is likely to capture by itself a major part of the correlation energy difference between Φ^i and ψ^i. Indeed it has been shown that the solution of these linear equations corresponds to the summation of certain terms of the Rayleigh–Schrödinger perturbation expansions [12]. For these reasons, using the solution of the linear equations to begin the iterative NR solution of the higher-order coupled-cluster equations is most likely to lead to convergence to a final set of $\boldsymbol{t}$ amplitudes which are close to the (small and unique) $\boldsymbol{t}$ amplitudes obtained from the linear equations.

3. Illustrative model calculations

The reference wavefunctions used for all model calculations presented here are of the multiconfiguration self-consistent-field (MC SCF) type. As is well known, these functions are very convenient for achieving qualitatively correct descriptions of either ground or excited states. Moreover, use of such MC SCF wavefunctions makes certain matrix elements involving the T_1 operators in eq. (11) vanish because the generalized Brillouin theorem (GBT) $\langle\Phi^i|[H, T_1]|\Phi^i\rangle = 0$ is obeyed.

In all calculations presented here, only the single and double orbital excitation operators T_1 and T_2 have been included, and the quartic expansion of $\tilde{H}$ has been truncated at the second commutator.

If we had used $T = T_2$ alone, the expansion of $\tilde{H}$ would exactly truncate at the second commutator level. However, with $T = T_1 + T_2$, this truncation is an approximation. Because the GBT is obeyed for our class of reference wavefunction, it is likely that the amplitudes of the T_1 operators turn out to be small as a result of which this truncation of the $\tilde{H}$ expansion is reasonably justified.

3.1. $CH_2(^1A_1)$ excited state model calculations

Our calculations for the excited ($^1A_1$) state of CH_2 were performed at the geometry of the ground ($^3B_1$) state as determined by Bauschlicher and Shavitt [13] ($\theta_{HCH} = 103.4°$, $R_{CH} = 2.04$ bohr) who used a double-zeta (DZ) plus polarization basis in this geometry optimization. We employed the same double-zeta (DZ) plus polarization basis in this geometry optimization. We employed the same double-zeta basis set in our $^1A_1$-state calculations as we used earlier in our more extensive work on the $^3B_1$ state. This small basis set was used to have available the full valence configuration interaction energy in the same basis. Our CCMC method was employed earlier [6] with an extended basis set for CH_2 to study the lowest $^1A_1$ state. However, here we are simply performing a model calculation to illustrate and test our method for the first time on excited states which have lower lying states of the same symmetry, and we prefer to restrict our attention to a system for which the exact answer can be obtained.

Based upon previous calculations by ourselves [6] and others on the lowest ($1\,^1A_1$) singlet state of CH_2, two configurations $1a_1^2 2a_1^2 1b_2^2 3a_1^2$, and $1a_1^2 2a_1^2 1b_2^2 1b_1^2$ are known to be dominant. In the CCMC calculations presented here, the $1a_1$, $2a_1$ and $1b_2$ orbitals (which describe the $1s_C$ and two C–H bonds) are kept doubly occupied in all configurations. Hence in this first model calculation only one electron pair is correlated in the MC SCF and CCMC calculations.

To begin the calculations on the excited ($2\,^1A_1$) state we first obtained, via the MC SCF procedure, a two-configuration reference function: $C_1 3a_1^2 + C_2 1b_1^2$ with $C_1 = 0.35$ and $C_2 = 0.93$. The frozen orbital occupancies $1a_1^2 2a_1^2 1b_2^2$ are suppressed in this notation for the reference function. We then utilized an automated configuration selection procedure [14] to determine whether any important configurations remained outside the reference space. The excitations $3a_1 \rightarrow 4a_1$ and $3a_1^2 \rightarrow 4a_1^2$ were judged by this selection procedure to be capable of giving rise to somewhat important con-

Table 1
CCMC calculations on lowest and excited $^1A_1$ CH_2

Reference wavefunction	Level of T operators used	Energy contributions [a] (hartree)				
		E_0	E_{T_1}	$E_{T_1T_1}$	E_{T_2}	E_{tot}
lowest state ($1\,^1A_1$) $\psi_0 = 0.94384\ (3a_1^2)$ $-0.3304\ (1b_1^2)$	T_2	−38.85773			−0.009199	−38.866936
excited state ($2\,^1A_1$) $\psi_0 = 0.351004\ (3a_1^2)$	T_1	−38.761159	-0.5×10^{-4}	0.1×10^{-4}		−38.761202
$+0.93637\ (1b_1^2)$	T_2	−38.761159			−0.013937	−38.77509
excited state ($2\,^1A_1$) $\psi_0 = 0.367\ (3a_1^2)$ $+0.024\ (3a_1 4a_1)$ $-0.0512\ (4a_1^2)$ $+0.9378\ (1b_1^2)$	T_2	−38.76356			−0.011325	−38.774893
(FVCI) [b] energy (ground state)						−38.86355
(FVCI) [b] energy (excited state)						−38.775061

[a] These energy contributions are defined in eqs. (15c–e) of ref. [5].

[b] FVCI stands for full valence configuration interaction.

figurations in the wavefunction. However, inclusion of these configurations in the MC SCF calculation, as seen from table 1, changes the MC SCF energy slightly (≈ 0.002 hartree) and the CCMC energy even less, thereby indicating that the original two-configuration reference function alone gives a sufficiently good zeroth-order description of the excited state.

The data of table 1 show that the CCMC energy in which only the T_1 operators are employed is hardly improved over the MC SCF energy itself. This is, of course, because the reference MC SCF wavefunction obeys the GBT. However, the CCMC energy arising from using the T_2 operators is substantially lower than the reference MC SCF energy. Notice that both the $1\,^1A_1$ and $2\,^1A_1$ state CCMC energies (with T_2) lie slightly below the respective full valence CI energies; the CC method is not variational. However, the singlet–singlet excitation energies obtained in the full CI (2.41 eV) and CCMC (2.50 eV) calculations are very nearly identical whereas the MC SCF-based excitation energy (2.63 eV) has twice the error that the CCMC value has. Thus although the T_2 corrections to the MC SCF reference wavefunction may appear small they do improve the excitation energy considerably. As mentioned above, contributions made by T_1 are small because we use an MC SCF reference state which obeys the GBT. In fact, even when we include both T_1 and T_2 together the T_1 contributions are small.

The above analysis and the data of table 1 illustrate that our CCMC method may reliably be applied to excited states. The results obtained here are not to be viewed as relating to the actual sates of CH_2 occurring in nature. Our small atomic orbital basis severely limits the accuracy of our results. Moreover, in these CH_2 calculations the fact that we froze the $1a_1$, $2a_1$ and $1b_2$ orbital occupancies mean that we only had a single test electron pair to correlate. Therefore, the full complexity of the coupled-pair CCMC approach was not even tested in the above CH_2 calculations. To examine the performance of the CCMC method in another mode system having two "active" electron pairs, we now turn to examine the Be + H_2 → BeH_2 reaction under C_{2v} symmetry.

3.2. BeH_2 ($^1A_1$) excited state

Our calculations on the excited $2\,^1A_1$ state of BeH_2 were performed at geometries lying along a perpendicular (C_{2v}) insertion path [15] for Be(^{1}S) + $H_2(^1\Sigma_g^+) \rightarrow BeH_2$ using exactly the same atomic orbital basis as was used in our earlier work [7] and as Purvis et al. [15] used in their ground-state

Table 2
BeH_2 ($^1A_1$) first excited state

Coordinates x, y, z [a] (bohr)	T operators used	CCMC calculation				E_{FCI}
		E_0 [b] (hartree)	E_{T_2} [b] (hartree)	E_{tot} [b] (hartree)	E [c] (kcal/mole)	
A(0, ±2.54, 0.0)	T_2	−15.40332	−0.00262	−15.40594	0.94	−15.40744
B(0, ±2.08, 1.0)	T_2	−15.40886	−0.00335	−15.41223	1.13	−15.41403
C(0, ±1.62, 2.0)	T_2	−15.43515	−0.00659	−15.44174	0.63	−15.44274
D(0, ±1.39, 2.5)	T_2	−15.51571	−0.00680	−15.52250	1.25	−15.52450
E(0, ±1.275, 2.75)	T_2	−15.54447	−0.00698	−15.55145	1.58	−15.55395
F(0, ±1.16, 3.0)	T_2	−15.52857	−0.00424	−15.53271	1.57	−15.53521
G(0, ±0.93, 3.5)	T_2	−15.45307	−0.00717	−15.46024	0.94	−15.46174
H(0, ±0.70, 4.0)	T_2	−15.44513	−0.00689	−15.45202	0.75	−15.45322
I(0, ±0.70, 8.0) [d]	T_2	−15.470191	−0.00387	−15.47406	0.81	−15.47536

[a] x, $\pm y$, z are coordinates for the two H nuclei; coordinates for the Be nucleus are set (0, 0, 0).

[b] For $T = T_2$, the CCMC total energy is $E_{tot} = E_0 + E_{T_2}$, where E_{T_2} is the energy contribution from the double excitations (see ref. [6]) and E_0 is the energy of the 18-configuration reference MC SCF wavefunction.

[c] $E_{CCMC} - E_{FCI}$.

[d] Does not lie on $r/2 = 2.54 - 0.46R$; this geometry corresponds to H_2 at equilibrium with a Be atom far away.

BeH_2 calculations. We presented the results of a ground-state calculation along this same path in an earlier publication [7]. The geometries at which these calculations were performed are shown in table 2; they lie on a straight line defined by $r/2 = 2.54 - 0.46R$(in au), where r is the H–H separation and R is the distance of the Be atom to the center of the H_2. This model reaction path gives rise to challenges in both the ground- and excited-state calculations since the electronic wavefunctions require at least eight configurations to achieve qualitatively correct descriptions of the states. The geometries along this path include the fragment geometry (I) at which excited configurations for both Be(^1S) and $H_2(^1\Sigma_g^+)$ are important. At the linear (A) and transition-state (E) geometries, the excited-state reference function $\Phi^{(1)}$ must also include configurations describing the round state since $\Phi^{(1)}$ is required to be orthogonal to the ground state. The final list of configurations used in our CCMC reference function was formed by examining all configurations of $^1A_1$ symmetry constructed from the orbital space $\{2a_1, 3a_1, 4a_1, 1b_1, 1b_2 \text{ and } 2b_2\}$. A total of 18 configurations were included in our MC SCF reference function. The $1a_1$ molecular orbital is of 1s Be character throughout the reaction path; it provides a constant correlation energy contribution. Thus the $1a_1^2$ orbital occupancy is frozen in all of the calculations reported here; however, the remaining four electrons are all correlated in the MC SCF and CCMC treatments.

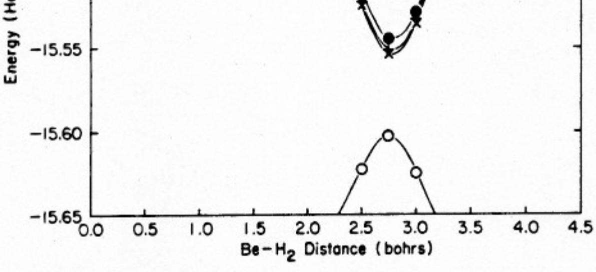

Fig. 1. BeH_2 energies along the path defined in the text. ○: full CI ground-state energy; ★: full CI excited state energy; +: CCMC excited state energy; ●: 18-configuration MC SCF excited-state energy.

The data of table 2 show that as the model excited-state reaction occurs on the excited 2^1A_1 surface, the energy contribution arising from the T_2 operator varies from 0.003 to 0.007 au (0.08 to 0.19 eV). Along this same path, the total CCMC energy (as shown in fig. 1) deviates from the full CI (with the $1a_1^2$ occupancy frozen) energy by only 0.8–1.6 kcal/mole. Thus, although the CCMC energy reasonably parallels the reference MC SCF energy, the additional correlation effects brought about by the coupled-cluster step are significant and result in excellent agreement with the full CI excited-state energy.

3.3. Concluding remarks

Examination of our numerical results demonstrates that CC calculations on excited states can be performed using a procedure similar to that used in ground-state calculations. Even though the CC equations have many spurious solutions, we have succeeded in converging to the desired excited state. Our success is related to the fact that the unique linear-CC solution incorporates the dominant terms when Φ^i contains the most important configurations.

A separate aspect of the CC equations which we have not addressed in this paper is how to explore the possibility of obtaining a solution which may not be close to the reference solution Φ^i. That is, Φ may contain only some important configurations of the desired state. In certain formalisms for which the expansions of $\tilde{H}$ and thus of energy E^i (given in eqs. (5b) and (8), respectively) are finite, it can be argued that the desired state is well represented by these expansions. However, the main difficulties of these approaches are that higher-order commutators of $\tilde{H}$ can no longer be neglected which results in a system of quartic equations from which the t-amplitudes must be determined. In addition, the effective hamiltonian $\tilde{H}$ may be non-hermitean as a result of which distinguishing the desired solution from spurious ones may not be trivial. For these reasons, we prefer the CCMC strategy described here since we know that Φ^i contains the dominant components of the wavefunction and the t amplitudes are small.

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Appendix

A measure of nearness can be introduced by using the analysis of Weinstein [16]. Let $\mathbf{H}C_i = E_i C_i$ define an eigenvalue problem corresponding to the Schrödinger equation and let (ϵ, V) represent the energy and the solution vector for a corresponding solution of the coupled-cluster equations. Let us define a distance

$$Q = (\mathbf{H} - \epsilon) V,$$

whose norm tends to zero as (ϵ, V) tend to the correct eigensolutions (E_i, C_i). Then, using the orthonormality of C_i and the expansion $V = \sum_i C_i v_i$

$$\begin{aligned} Q^+ Q &= \sum_{ij} (E_i - \epsilon)(E_j - \epsilon) C_i^+ C_j v_i v_j \\ &= \sum_i (E_i - \epsilon)^2 v_i^2, \end{aligned}$$

or

$$Q^+ Q \geqslant (E_p - \epsilon)^2,$$

or

$$|Q| \geqslant |(E_p - \epsilon)|,$$

where E_p is the closest eigenvalue to ϵ (assuming the vector V is normalized, i.e. $\sum_i v_i^2 = 1$).

The above result means that for a given initial solution (ϵ, V) there is at least one eigenvalue E_p within $|Q|$ of ϵ. It would be desirable to choose (ϵ, V) such that the circle of radius $|Q|$ encloses only the desired eigenvalue.

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