Ohio University

Department of Mathematics[1]

Journal of Magagula Vusi Mpendulo: Fall 2010 - 2011

Magagula Vusi Mpendulo

4 October - 8 October 2010:

Report on the article entitled "R12 Methods in Explicitly correlated Molecular electronic structure Theory"

I read the paper entitled R12 Methods in Explicitly correlated Molecular electronic structure Theory. My main aim was to understand the R12 Method. I tried to read through several times but I had quite difficulty in understanding some of the Chemistry words that were thrown at me. I have to contact the chemistry dictionary now and again in order for me to understand most of the terminology used in the paper. However, it was interesting to see how Mathematics is applied in Chemistry. I met my reaserch mates and we discussed what they understood in the paper and we shared the same theory that the the Authors are attempting to tell us that the R12 converges faster than all the other methods. I had to prepare a Presentation using latex so that I may inform the participants in the reaserch group of what I have learned from the paper. I was able to prepare the Presentation. One of group mates suggested that I read another paper by Wim Klopper entitled R12 Methods, Gaussian Geminals.I didn't have enough time to read it however, if I do, I will try to understand it and it will probably give me a better insight to R12 methods. I have to meet Dr Mohlenkamp and try to explain to him what I have read and understood from the paper.

11 October - 15 October 2010:

Report on Coupled Cluster Methods

My aim this week was to read and understand Coupled - Cluster Methods. I read the paper entitled " The Yearn to be Hermitian" by J. Bartlett etl. I read that the Coupled Cluster (CC) is a numerical technique that is used for describing many-body systems. It is mostly used as one of several quantum chemical post-HartreeFock ab initio quantum chemistry methods in the field of computational chemistry. It takes the basic HartreeFock molecular orbital method and adds back multi-electron wavefunctions to account for electron correlation. Coupled-cluster theory provides an approximate solution to the time-independent Schrodinger equation

$$H\left|\Psi_{CC}\right\rangle = E\left|\Psi_{CC}\right\rangle \tag{1}$$

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[1] Mathematics Department Ohio University, Athens, 45701, OH, US

where H is the Hamiltonian and the wavefunction is given by

$$|\Psi_{CC}\rangle = e^T |0\rangle \tag{2}$$

Note that T is the so called excitation operator. The operator is of the form:

$$T = T_1 + T_2 + T_3 + T_4 + \cdots \tag{3}$$

where T_1 is the operator of all single excitations, T_2 is the operator of all double excitations and so forth. We can conviniently represent each T_m as follows:

$$T_m = \sum_{i,j,\cdots,a,b\cdots} t_{ij}^{ab}\{a^{\varphi} b^{\varphi} \cdots ji\} \tag{4}$$

where a^{φ} and b^{φ} denote the creation and annihilation operators respectively and i, j stand for occupied and a, b for unoccupied orbitals respectively. One important thing is that when trying to find the unknown coefficients t_{ij}^{ab} is the same as approximating the solution of the wavefunction.

The types of Coupled Cluster Methods

The classification of traditional CC methods rests on the highest number of excitations allowed in the definition of T. The abbreviations for Coupled-Cluster methods usually begin with the letters "CC" (for Coupled Cluster) followed by

- S - for single excitations (singles)
- D - for double excitations (doubles)
- T - for triple excitations (triples)
- Q - for quadruple excitations (quadruples)

The terms in round brackets indicate that these terms are calculated based on perturbation theory. For example,a CCSDT(Q) approach simply means:

- A coupled-cluster method
- It includes singles,doubles and triples fully
- Quadraples are calculated with perturbation theory

We have the following types of Coupled Cluster Methods:

- CCD
- CCSD
- CCSD(T)
- CCSDT
- CCSDT(Q)
- CCSDTQ

At this point, I'm a little bit excited, I feel like I understand what I'm doing. I had problems understanding some notations and I've tried to look them up from previous references but I was not succesful. However, I still need to interpret some nice diagrams in the paper I was reading. I decided to get a book from Ohiolink and get other articles to help me understand better the CC Methods. I think understanding the basics helps to understand the bigger picture. I recommend getting a book kind of like "Quantum Chemistry for Dummies"so that we understand the basics and notations.

18 October - 22 October 2010:

Finding the Coefficients t_{ij}^{ab}

My aim for this week was to understand the pictures on the paper I'm working on. Last week I learnt that when trying to find the unknown coefficients t_{ij}^{ab} from the equation

$$T_m = \sum_{i,j,\cdots,a,b\cdots} t_{ij}^{ab}\{a^{\varphi}b^{\varphi}\cdots ji\} \tag{5}$$

is the same as approximating the solution of the wavefunction. My aim was to find out how the paper address this. I read the paper again and again but it never outlined a method they use to find those coefficients. However, I have book entitled "Recent Progress in Many - Body Theories" which seems to have solutions to this problem. I just got it few hours away and I'm yet to read it and see if I will get any kind of help. I have tried to read and understand the pictures but the Authors do not explain in detail on the criteria they use to come up with those pictures. I tried to email one of them to help me give the basics or the criteria they used but he never responded. I'm still trying to understand. However, I understood that the Hamiltonian is separated into the following parts:

$$\{H\} = \{F^{[0]}\} + \{W^{[0]}\} + \{F^{[\pm 1]}\} + \{W^{[\pm 1]}\} + \{W^{[\pm 2]}\} \tag{6}$$

$$\{H^{[0]\}} = \{F^{[0]}\} + \{W^{[0]}\} \tag{7}$$

$$\{V\} = \{F^{[\pm 1]}\} + \{W^{[\pm 1]}\} + \{W^{[\pm 2]}\} \tag{8}$$

where:

- $[\pm k]$ superscript specifies what effect the operator has in terms of particle number.

- $[0]$ means it does not change the particle number up or down.
- $[+1]$ means it introduces an excitation
- $[-1]$ means it introduces a deexcitation
- $[\pm 2]$ means it introduces two excitations or deexcitations.

I had problems trying to understand some notations and I hope I will try to address this problem by collaborating with my researchmates Ju and Yi. I have accomplished so far although it may not be that much, but a half a loaf is better than nothing. I hope some of my problems will be addressed at our weekly meeting with Dr Mohlenkamp.

25 October - 29 October 2010:

Report on Coupled Cluster Methods

My aim this week was to read and understand Coupled - Cluster Methods. Recall that I have touced upon this CC - Methods in the past few weeks and I briefly summarized it as follows:
It is a method that is mostly used as one of several quantum chemical post-HartreeFock ab initio quantum chemistry methods in the field of computational chemistry. It takes the basic HartreeFock molecular orbital method and adds back multi-electron wavefunctions to account for electron correlation. Coupled-cluster theory provides an approximate solution to the time-independent Schrodinger equation

$$H\left|\Psi_{CC}\right\rangle = E\left|\Psi_{CC}\right\rangle \tag{9}$$

where H is the Hamiltonian and the wavefunction is given by

$$\left|\Psi_{CC}\right\rangle = e^{T}\left|0\right\rangle \tag{10}$$

Note that T is the so called excitation operator. The operator is of the form:

$$T = T_1 + T_2 + T_3 + T_4 + \cdots \tag{11}$$

where T_1 is the operator of all single excitations, T_2 is the operator of all double excitations and so forth. We can conviniently represent each T_m as follows:

$$T_m = \sum_{i,j,\cdots,a,b\cdots} t_{ij}^{ab}\{a^{\varphi} b^{\varphi} \cdots ji\} \tag{12}$$

where a^{φ} and b^{φ} denote the creation and annihilation operators respectively and i, j stand for occupied and a, b for unoccupied orbitals respectively. One important thing is that when trying to find the unknown coefficients t_{ij}^{ab} is the same as approximating the solution of the wavefunction.

The types of Coupled Cluster Methods

The classification of traditional CC methods rests on the highest number of excitations allowed in the definition of T. The abbreviations for Coupled-Cluster methods usually begin with the letters “CC” (for Coupled Cluster) followed by

- S - for single excitations (singles)
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- Q - for quadruple excitations (quadruples)

The terms in round brackets indicate that these terms are calculated based on perturbation theory. For example,a CCSDT(Q) approach simply means:

- A coupled-cluster method

- It includes singles,doubles and triples fully
- Quadraples are calculated with perturbation theory

We have the following types of Coupled Cluster Methods:

- CCD
- CCSD
- CCSD(T)
- CCSDT
- CCSDT(Q)
- CCSDTQ

We are now in a position to easily understand the equations associated with the Coupled - Cluster Methods. For example,the CCSD is given by

$$|\Psi_{CCSD}\rangle = e^{T_1+T_2}\,|0\rangle \tag{13}$$

the CCSDT is given by

$$|\Psi_{CCSDT}\rangle = e^{T_1+T_2+T_3}\,|0\rangle \tag{14}$$

and the CCSDT(Q) is given by

$$\left|\Psi_{CCSDT(Q)}\right\rangle = e^{T_1+T_2+T_3+T_4}\,|0\rangle \tag{15}$$

Now, the explicit equations for cluster amplitudes, which define T , are usually obtained by projecting the connected cluster form of the electronic Schrodinger equation, that is,

$$(H_N e^T)_C\,|\Phi\rangle = \triangle E\,|\Phi\rangle \tag{16}$$

onto the excited configurations generated by T. Here, $H_N = H - \langle\Phi|H|\Phi\rangle$ is the electronic Hamiltonian in the normal-product form, $\triangle E\,|\Phi\rangle = E - \langle\Phi|H|\Phi\rangle$is the energy relative to reference energy $\langle\Phi|H|\Phi\rangle$ and subscript C indicates the connected part of a given operator expression. For example, the CCSD amplitude equations are obtained by projecting

$$(H_N e^T)_C\,|\Phi\rangle = \triangle E\,|\Phi\rangle \tag{17}$$

where $T = T1 + T2$, onto all singly and doubly excited configurations, $|\Phi_i^a\rangle$and $\left|\Phi_{ij}^{ab}\right\rangle$, respectively,

$$\left\langle\Phi_i^a\right|(H_N e^{T_1+T_2})_C\,|\Phi\rangle = 0 \tag{18}$$

$$\left\langle\Phi_{ij}^{ab}\right|(H_N e^{T_1+T_2})_C\,|\Phi\rangle = 0 \tag{19}$$

Once the system of nonlinear, energy-independent equations for cluster amplitudes is solved, we calculate the energy $\triangle E$ in the following way:

$$\triangle E = \left\langle\Phi\right|(H_N e^{T_1+T_2})_C\,|\Phi\rangle = 0 \tag{20}$$

If we solve equations 18 and 19, we determine the amplitudes t_i^a and t_{ij}^{ab}. The work presented above is extracted from an article entitled “Efficient Computer Implementation of the Renormalized Coupled Cluster Methods” by P. Piecuch and others. I have learned a lot about the coupled cluster methods and I felt it was time I looked at the methods and see how they have been solved and luckily this paper seems to shed some light on how to solve the equations in order to find those coefficients. I’m still trying to understand the notation and the formulas so that I may understand how they were able to solve the equations. One thing that I have noticed is that, there are a lot of these Coupled Cluster Methods.

1 November - 5 November 2010:

Report on Coupled Cluster Methods Continued

My aim this week was to further read the paper entitled "Efficient Computer Implementation of the Renormalized Coupled Cluster Methods" by P. Piecuch and others and try to understand how they were able to find the unknown coefficients t_{ij}^{ab} called amplitude.t_{ij}^{ab} is called double excited cluster amplitude while t_i^a is called single excited cluster amplitude. I will begin by recapturing what we achieved last week and continue to expand on that. Let me begin by summarizing what we have been reviewing in the past weeks about Coupled Cluster Methods.The ground-state wave function $|\Psi_{CC}\rangle$ of an N-electron system is represented as follows:

$$|\Psi_{CC}\rangle = e^T |\Phi\rangle \tag{21}$$

where T is the cluster operator and $|\Phi\rangle$ is the independent-particle-model reference configuration. We truncate the many-body expansion of T at a conveniently chosen excitation level. This leads to the hierarchy of the standard Coupled Cluster approximations: CCSD, when T is restricted to singly and doubly excited clusters ($T = T1 + T2$); CCSDT, when T is restricted to singly, doubly, and triply excited clusters ($T = T1+T2+T3$), CCSDTQ, when T is truncated at quadruply excited clusters ($T = T1 + T2 + T3 + T4$)etc. Now, the explicit equations for cluster amplitudes, which define T , are usually obtained by projecting the connected cluster form of the electronic Schrodinger equation, that is,

$$(H_N e^T)_C |\Phi\rangle = \triangle E |\Phi\rangle \tag{22}$$

onto the excited configurations generated by T. Here, $H_N = H - \langle\Phi|H|\Phi\rangle$ is the electronic Hamiltonian in the normal-product form, $\triangle E |\Phi\rangle = E - \langle\Phi|H|\Phi\rangle$is the energy relative to reference energy $\langle\Phi|H|\Phi\rangle$ and subscript C indicates the connected part of a given operator expression. For example, the CCSD amplitude equations are obtained by projecting

$$(H_N e^T)_C |\Phi\rangle = \triangle E |\Phi\rangle \tag{23}$$

where $T = T1 + T2$, onto all singly and doubly excited configurations, $|\Phi_i^a\rangle$and $|\Phi_{ij}^{ab}\rangle$, respectively,

$$\langle\Phi_i^a|(H_N e^{T_1+T_2})_C |\Phi\rangle = 0 \tag{24}$$

$$\langle\Phi_{ij}^{ab}|(H_N e^{T_1+T_2})_C |\Phi\rangle = 0 \tag{25}$$

Once the system of nonlinear, energy-independent equations for cluster amplitudes is solved, we calculate the energy $\triangle E$ in the following way:

$$\triangle E = \langle\Phi|(H_N e^{T_1+T_2})_C |\Phi\rangle = 0 \tag{26}$$

If we solve equations (24) and (25), we determine the amplitudes t_i^a and t_{ij}^{ab}. Next we define T_1 and T_2. We define them as follows:

$$T_1 = \sum_{i,a} t_i^a E_i^a \tag{27}$$

$$T_2 = \frac{1}{2} \sum_{ij,ab} t_{ij}^{ab} E_{ij}^{ab} \tag{28}$$

where $E_{ij}^{ab} = E_i^a E_j^b$ and E_i^a are the orbital excitation operators and $t_i^a = \langle a|t_1|i\rangle$, $t_{ij}^{ab} = \langle ab|t_2|ij\rangle$ are the spin-free singly and doubly excited cluster amplitudes respectively. The doubly excited cluster amplitudes have the following symmetry property with respect to interchanges of occupied and unoccupied orbital labels:

$$t_{ij}^{ab} = t_{ji}^{ba} \tag{29}$$

The compact form of the CCSD equations (equations (24) and (25))in terms of cluster amplitudes $t_i^a = \langle a|t_1|i\rangle$ and $t_{ij}^{ab} = \langle ab|t_2|ij\rangle$ and one- and two-electronmolecular integrals $f_q^p = \langle p|f|q\rangle$ and $v_{rs}^{pq} = \langle pq|v|rs\rangle$, corresponding to one- and two-body parts of the Hamiltonian H_N, F_N and V_N, respectively, can be written as follows:

$$D_i^a t_i^a = f_i^a + I_e^a t_i^e - I_i^{'m} t_m^a + I_e^m (2t_{mi}^{ea} - t_{im}^{ea}) + (2v_{ei}^{ma} - v_{ei}^{am}) t_m^e - v_{ei}^{mn} (2t_{mn}^{ea} - t_{mn}^{ae}) + v_{ef}^{ma} (2t_{mi}^{ef} - t_{im}^{ef}) \tag{30}$$

$$\begin{split} D_{ij}^{ab} t_{ij}^{ab} = v_{ij}^{ab} + P(ia/jb)[t_{im}^{ab} I_e^b - t_{ij}^{ae} I_j^m + \frac{1}{2} v_{ef}^{ab} c_{ij}^{ef} + \frac{1}{2} c_{mn}^{ab} I_{ij}^{mn} - t_{mj}^{ae} I_{ie}^{mb} - I_{ie}^{ma} t_{mj}^{eb} \\ + (2t_{mi}^{ea} - t_{im}^{ea}) I_{ej}^{mb} + t_i^e I_{ej}^{'ab} - t_m^a I_{ij}^{'mb}] \end{split} \tag{31}$$

The terms D_{ij}^{ab} and $D_i^a t_i^a$ are the standard MPBT denominators and in general, we have

$$D_{i\cdots}^{a\cdots} = \epsilon_i - \epsilon_a + \cdots , \tag{32}$$

where $\epsilon_p = f_q^p$ are the diagonal elements of the Fock matrix. The c_{ij}^{ab} coefficients are defined as

$$c_{ij}^{ab} = t_{ij}^{ab} + t_i^b t_j^b \tag{33}$$

and the operator $P(ia/jb)$ when acting on some expression, implies a sum of two expressions of the same type differing by a permutation of the (i, a) and (j, b) pairs and in general,

$$P(pq/rs) = 1 + (pr)(qs) \tag{34}$$

where (pq) is a transposition of indices p and q. The recursively generated intermediates I_b^a,I_j^i, $I_j^{'i}$, I_a^i,I_{kl}^{ij},I_{jb}^{ia},etc. are defined and for example, we have

$$I_a^i = f_a^i + 2v_{ae}^{im} t_m^e - v_{ea}^{im} t_m^e \tag{35}$$

The CCSD equations are solved iteratively. The algorithm used to solve this equation is explained in the paper but that is a topic for another day. At this point, I'm quite in a better position but while writing this report, I'm stuck on how they were able to get the compact form of equations from equations (24) and (25) respectively. I have learnt quite a lot of ideas and most of them were new to me. I hope that before the end of the week, I will be enlightened on the transition from equation 24 and 25 to the compact form.

8 November - 15 November 2010:

End of Quarter Report - Fall 2010 - 2011

For this week, we present what we have achieved over the quarter in our group meeting and we also report what aricles we have read and a summary of the content of those articles. Below, I'm presenting a summary of articles I've read for the whole quarter.

R12 Methods in Explicitly Correlated Molecular Electronic Structure Theory

This article, [1], a brief review of major developments in the field of Quantum Chemistry are presented. The authors surveyed older methods which led to the present CCSDR12 Method. Major developments in the field are reviewed and they make recommendations for future directions. The authors also show that the modern CCSDR12 methods can deliver high accuracy dramatically faster than by using conventional methods and it is compared with the commonly used extrapolation techniques.

The Yearn To be Hermitian

In this article [2], the authors analyze hermitian aspects which can offer improved numerical approximations, simpler computational evaluations. The authors illustrate that the Coupled Cluster Pertubation Theory (CCPT) Methods may be used as an alternative to the infinite order Coupled Cluster method. They also implement and formulate the CCPT method up to fifth order and compare thier results with the results obtained using the standard Coupled Cluster Methods.

Efficient computer implementation of the renormalized coupled-cluster methods: The R-CCSD[T], R-CCSD(T), CR-CCSD[T], and CR-CCSD(T) approaches

The details of the implementation of the renormalized (R) and completely renormalized (CR) coupled-cluster (CC) methods of the CCSD[T] and CCSD(T) types including the complete set of equations that have been used in writing efficient computer codes, memory requirements, and typical CPU timings, are detailed in this paper. These methods use recursively generated intermediates and fast matrix multiplication routines. The R-CCSD[T], R-CCSD(T), CR-CCSD[T], and CRCCSD(T) computer codes and similar codes for the standard CC methods,including the LCCD, CCD, CCSD, CCSD[T], and CCSD(T) approaches, are discussed in detail this paper and they have been implemented in a package called GAMES. The algorithm for solving the coupled cluster amplitudes is also detailed in this article [3].

The Coupled Cluster Method

The role of the Coupled Cluster Method (CCM) within modern quantum many-body theory is surveyed in this article [4], and then it is compared with other alternative microscopic formulations. The methods and each of its individual components are then discussed in detail. The authors introduce a general theoretical framework in which new key ideas to develop the Coupled Cluster theory are discussed in detail. They end the discussion with a brief review of the applications of the method to date.

Coupled - Cluster methods including noniterative corrections for Quadruple Excitations

In this article [5], the authors present a new method for treating the effects of quadruple excitations in coupled-cluster theory. In their approach,the quadruple excitation contributions are computed from a formula based on a non-Hermitian perturbation theory to justify the usual noniterative triples correction used in the coupled cluster singles and doubles method with a perturbative treatment of the triple excitations (CCSD(T)). This method discussed in this article plays a parallel role in improving energies obtained with the full coupled-cluster singles, doubles, and triples method by adding a perturbative treatment of the quadruple excitations. They also test the method for an extensive set of examples, and they show that it provides total energies that compare favorably with those obtained with the full singles, doubles, triples, and quadruples method.

New Coupled - Cluster methods with Singles, Doubles, and Noniterative Triples for high accuracy calculations of excited electronic states

In this article,[6], the authors develop the single-reference ab initio methods for high accuracy calculations of potential energy surfaces (PESs) of excited electronic states, termed the completely renormalized equation-of-motion coupled-cluster approaches with singles, doubles, and noniterative triples [CR-EOMCCSD(T)]. The authors demonstrate that the CR-EOMCCSD(T) approaches, which can be regarded as the excited-state analogs of the ground-state CR-CCSD(T) theory, provide a highly accurate description of excited states dominated by double excitations, excited states displaying a multireference character, and PESs of excited states along bond breaking coordinates with the ease of the ground-state CCSD(T) or CR-CCSD(T) calculations.

Comparison of Coupled - Cluster Methods which include the effects of connected triple excitations

In this article [9], the authors determine electron correlation energies for 14 different molecules which represent a range of chemical bonding situations. These have been determined with the coupled-cluster single, double, and triple (CCSDT) excitation model as well as with several coupled-cluster methods that include only an approximate treatment of connected triple excitations, that is, the CCSDT-la, CCSDT-lb, CCSDT-2, CCSDT-3, CCSDT-4, and the CCSD(T) method. It is however noted that the 14 molecules considered in this article, the average error of the CCSD(T) method relative to CCSDT is considerably below that obtained from any of the CCSDT-x methods [9]. It is then concluded that the CCSD(T) is to be preferred over any of the other approximate methods, both because it is the least expensive and also because it is generally the most accurate approximation to CCSDT.

A comparison of the efficiency and accuracy of the Quadratic Configuration Interaction (QCISD), Coupled Cluster (CCSD),and Brueckner Coupled Cluster (BCCD) Methods

In this article,[7],the authors formulate the coupled - cluster method restricted to single and double excitations (CCSD) from a closed-shell reference function and the corresponding quadratic configuration interaction method (QCISD). They also describe in detail a simple yet effective method to accelerate convergence in Brueckner coupled-cluster (BCCD) calculations. This procedure BCCD calculations require less effort than CCSD calculations.

The second-order approximate Coupled Cluster singles and doubles model CC2

In this article [8], an approximate coupled cluster singles and doubles model is presented and is denoted CC2. The CC2 total energy is of second-order Mϕller-Plesset perturbation theory (MP2) quality. The authors derive the CC2 linear response function. A hierarchy of coupled cluster models, CCS, CC2, CCSD, CC3, CCSDT etc, is presented where CC2 and CC3 are approximate coupled duster models defined by similar approximations.

References

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