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A Study on Coupled Clustered Method Wave Functions

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A B S T R A C T

The present investigation was carried out to study the functions of coupled clustered wave functions. The present investigation gives a brief description of the CCM wave function and the ways of performing approximations. The final form of the wave function that we shall make use of is obtained by combining these two methods in a way appropriate for a linear variational method. The effectiveness of the approximation scheme is illustrated by considering the calculation for the ground-state of the alpha-particle. From the present investigation it is concluded that the closed shell structure of the alpha-particle ground state provide an easy ground for the calculations. The alpha-particle has provided a reliable method for testing the accuracy of both the method to be used and the numerical calculation. Despite the complexity of such methods both in implementation and computer time, the J-TICI scheme was relatively easy and straight forward to apply. We managed to slightly improve the previously obtained results at no expense, provided a numerical solution of the equations is performed.

Introduction

One way of doing the construction of the trial wave function is by appropriately approximating some rather complicated, usually non-linear, parameterization. One type of such a parameterization is given by the Coupled Cluster Method (CCM). The present investigation gives a brief description of the CCM wave function. The final form of the wave function obtained by combining these two methods in a way appropriate for a linear variational method. The effectiveness of the approximation scheme is illustrated by considering the calculation for the ground-state of the alpha-particle. For this purpose the results quoted from a number of authors as well as our own. Apart from the ground-state energy, an attempt was made to examine

the calculation of the one- and two-body density distributions that can be used to provide qualitative information about the wave function. The most basic ingredient in such an approximation is the construction of the trial wave function. Another type of non-linear parameterization of the many-body wave function that is variational in nature is the Jastrow method [1, 6, 7]. The present investigation provide a brief discussion of this technique and ways of approximating it.

The Model Space

In the case of the Coupled Cluster Method (CCM) the reasoning behind the introduction of these reference states is that the set $\{|\Phi_i\rangle\}$ can act as starting functions, from which we can construct the full wave function by the action of correlation operators. A non-degenerate ground state corresponds to the case of a single reference state (D = 0) and is referred to as the 'single-reference' version of the CCM. In the case of many-body problems it is often convenient to introduce the idea of reference states. In general, a set of reference states, $\{|\Phi_i\rangle; i = 0, 1, ..., D\}$, is used, where the normality condition $\langle\Phi_i|\Phi_j\rangle = \delta_{ij}$ can be assumed to be satisfied reference states form the basis of a D-dimensional subspace of the full Hilbert space, referred to as the 'model space'.

The States of Reference

The reference state should be constructed to obey the symmetries of the exact ground state, while the correlation operators of CCM can be scalar operators that do not carry any quantum numbers. Furthermore, it is always convenient for such a state to have an analytic description, since a large part of the CCM will require calculations involving the reference function alone. When considering a many-fermion system, a non-interacting many body wave function or ground state can often be described by a Slater determinant. Such a state can serve as the reference state. It is well known that in the language of second quantization a Slater determinant can be written as

$$|\Phi_0\rangle = \prod_{i=1}^{N} a_{\nu_i}^{\dagger}|0\rangle$$

Where N is the number of particles and they $a_{\nu_i}^{\dagger}$ are Fermion creation operators that obey the usual commutation relations and are defined by their action on the vacuum state j0i. The occupied single particle states $\{|\nu_i\rangle;\ i = 1, 2, ..., N\}$ are referred to as hole states, while the set $\{|\rho_i\rangle;\ i = 1, 2, ...\}$ corresponds to states unoccupied in $|\Phi_0\rangle$ and orthogonal to the hole states $\{|\nu_i\rangle\}$, referred to as particle states. Once a reference state is provided in terms of a Slater determinant with respect to a set of hole states $\{|\nu_i\rangle\}$, a more general determinant that mixes particle and hole states is provided by Thouless theorem [8], where

$$|\Phi_0^{'}\rangle = e^{\hat{S}_1}|\Phi_0\rangle$$

The operator $\hat{S}_1$ is a one-body operator which acts on $|\Phi_0\rangle$ to produce a one-particle/one hole (1p-1h) excitation. In the notation of particle/hole states it has the explicit form

$$|\Phi_0^{'}\rangle = e^{\hat{S}_1}|\Phi_0\rangle$$

The new reference state $|\Phi_0^{'}\rangle$ is non-orthogonal to the original state $|\Phi_0\rangle$.

The exponentials Expansion

The time-independent Schrödinger equation for the ground state wave function $|\Psi_0\rangle$ is

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

Where H is a many-body Hamiltonian. As described in the previous section the exact ground state $|\Psi_0\rangle$ can be expanded in terms of a model state $|\Phi_0\rangle$ and states orthogonal to $|\Phi_0\rangle$, resulting from the dynamical correlations induced by H. Thouless theorem allows the inclusion of the simplest correlations in terms of 1p-1h excitations. A correlation operator describing a general mp-mh correlation is

$$\hat{S}_m = \frac{1}{(m!)^2} \sum_{\rho_1,\ldots,\rho_m} \sum_{\nu_1,\ldots,\nu_m} \langle \rho_1,\ldots,\rho_m|\hat{S}_m|\nu_1,\ldots,\nu_m\rangle_A a^\dagger_{\rho_1}\ldots a^\dagger_{\rho_m} a_{\nu_m}\ldots a_{\nu_1}$$

Where the subscript A denotes an antisymmetric state. As a result of the fermionic anticommutation properties

$$\{a^\dagger_{\rho_i}, a_{\nu_j}\} = \delta_{ij}\delta_{\rho\nu}, \quad \{a_{\rho_i}, a_{\nu_j}\} = 0$$

Correlation operators involving different number of particles commute with each other, i.e. $[\hat{S}_m, \hat{S}_n] = 0$. Furthermore, the successive application of the same correlation operators will result in terms involving each particle label only once. Therefore, application of the operator $(\hat{S}_m)^n$ will result in all possible terms that involve n × m distinct particle labels. In the CCM formalism the exact ground state wave function is expanded over a set of states that contains all possible correlated independent particle clusters. For example in the case of only two-body correlation operators, the expansion takes the form of

$$\begin{aligned} |\Psi_0\rangle &\simeq \left(1 + \hat{S}_2 + \frac{1}{2!}(\hat{S}_2)^2 + \frac{1}{3!}(\hat{S}_2)^3 + \ldots\right)|\Phi_0\rangle \\ &= \exp(\hat{S}_2)|\Phi_0\rangle \end{aligned}$$

Where the expansion can be written as an exponential regardless of the number of occupied states in the reference state, since all terms involved with a number of operators greater than the number of occupied states will give a zero result. When all possible cluster sizes are taken into account, an N-body ground state wave function can be constructed from the reference state as

$$\begin{aligned} |\Psi_0\rangle &= \left(\exp(\hat{S}_1)\exp(\hat{S}_2)\ldots\exp(\hat{S}_N)\right)|\Phi_0\rangle \\ &= \exp(\hat{S})|\Phi_0\rangle \ , \end{aligned}$$

where

$$\hat{S} = \sum_{i=1}^{N} \hat{S}_i \ .$$

The exponential character of equation is an important characteristic of the CCM. As a result of the commutation of the operators in the CCM exponential parameterization obeys size-extensively. A size-extensive method ensures that a calculation on a com. Pound system consisting of a number of non-interacting sub-systems yields a calculated value that is the same as that of the individual subsystem values. An important advantage of a size-extensive method is that it allows straightforward comparisons between calculations involving variable numbers of components, e.g. ionization processes or calculations using different numbers of active electrons. Lack of size-extensively implies that errors from the exact energy increase as more components enter the calculation.

Wave Function of Jastrow Variational

In order to obtain a variational wave function using CCM full wave function. This can result in the loss of structure, according to the physical problem in question. One way of significantly improving the structure of a many body wave function in the case of extended strongly interacting systems is that of Jastrow [1]. The method has been adapted for finite systems and applied to a number of light nuclei [6, 10].

Wave function of Jastrow

The TICC correlation operators take a bound of the medium to long range effects. The easiest scheme is that where Jastrow and TICI (2) are combined [9], referred to as the J-TICI2 scheme. Such formalism is similar to that of the correlated basis functions where we have a combination of linear and non-linear correlation operators acting on the wave function. In the J-TICI formalism the wave function is given by the product of a linear TICI operator (F_L) with the non-linear Jastrow factors (F_J) as The coupled cluster method can serve as a general way of unfolding the full wave function structure in terms of additive correlation operators. The fact that the wave function suitable for the linear variational problem can lead to significant decrease in the included structure. This can be enhanced by combining TICC with a Jastrow variational function. This way short range correlations are accounted for by the Jastrow factors, while

$$\begin{aligned}\Psi_{J-TICI2} &= F_J F_L \Phi_0, \\ &= \prod_{i<j} f_J(ij) \left(1 + \sum_{ij} f_{TICI2}(ij)\right) \Phi_{HO}\end{aligned}$$

Where the latter equation is the specific form mostly make use of in which a harmonic oscillator reference function, Φ_{HO}, takes care of translational invariance.

Similarities between Jastrow and Jastrow-TICI Methods

There is a close relation between these correlations and the Jastrow factors. It is observed that the application of cluster operators directly in coordinate representation can be very powerful for the description of ^{4}He. If we consider the state independent case where the Jastrow wavefunction Ψ_J is parameterized by a single Gaussian, this can be expanded as

$$\begin{aligned}\Psi_J &= \prod_{i<j}(1 - a\exp(-br_{ij}^2)\Phi_0 \\ &= (1 + a\sum_{i<j} e^{-br_{ij}^2} + a^2 \sum_{i<j}\sum_{k<l}{}' e^{-br_{ij}^2} e^{-br_{kl}^2} + \ldots \\ &\quad + a^6 e^{-(br_{12}^2+\ldots+br_{34}^2)})\Phi_0,\end{aligned}$$

Where the prime indicates that the labels k and l are distinct from i and j. If we then consider the case of VTICC (4) where the wave function has the form

$$\begin{aligned}\Psi_{VTICC(4)} &= \sum_{n_1\leq\ldots\leq n_6} \mathcal{S}[A_{n_1\ldots n_6} e^{-(b_{n_1} r_{12}^2+\ldots+b_{n_6} r_{34}^2)}]\Phi_0, \\ &= \sum_{n_1\leq\ldots\leq n_6} [A_{n_1\ldots 0}\sum_{i<j} e^{-b_{n_1} r_{ij}^2} + A_{n_1 n_2\ldots 0}\sum_{i<j}\sum_{k<l}{}' e^{-b_{n_1} r_{ij}^2} e^{-b_{n_1} r_k^2} \\ &\quad + \ldots + A_{n_1\ldots n_6} e^{-(b_{n_1} r_{12}^2+\ldots+b_{n_6} r_{34}^2)}]\Phi_0,\end{aligned}$$

We can be seen that the Jastrow wave function is similar to the VTICC form. The difference lies in the fact that each term of the VTICC form is given by a linear expansion in terms of Gaussians of different widths, while the terms of the Jastrow factor are restricted to a single Gaussian.

Table.1 Ground-state energy of ^{4}He using the Jastrow variational wave function

Potential	Correlation	No. of gaussians	Energy (MeV)
S3/MS3	SI	1	-24.4042
S3	SD	1	-25.3598
MS3	SD	1	-25.3119
S3/MS3	SI	2	-27.2136
S3	SD	2	-29.9378
MS3	SD	2	-29.7034
MT-I/III, MT-V	SI	1	-29.0604
MT-I/III	SD	1	-29.3460
MT-I/III, MT-V	SI	2	-30.8752
MT-I/III	SD	2	-32.0107

Furthermore, the coefficients $\{a, a^2, ..., a^6\}$ in the case of Jastrow wave function are non-linear, something that makes their determination much harder. This due to the fact that the linear $An_1 \ldots, n_6$ coefficients can be determined as the eigenvector of an Eigen value problem, by pre-assigning the set of non-linear widths $\{b_1 \ldots, b_6\}$. Despite the restrictions in the coefficients the Jastrow variational wave function can achieve better results than the state dependent TICI or the higher order state independent cluster expansions. This was done in [7], where an expansion up to two Gaussians was used, examining both state dependent and state independent cases for the ground state of ^{4}He. These results are shown in table 1.

Conclusions

The most general variational wave function consists of a multilinear expansion of the correlation operator. This study is particularly interested in an economic method in terms of effort that does not lack substantial accuracy. The simplest choice would be to consider a linear form for the correlation operator containing only pair correlations. When it is compared with higher order approximations this choice is rather poor. The basic principle of the CCM is that the exact wave function can be obtained by correlating a starting reference function.

It must be concluded that the closed shell structure of the alpha-particle ground state provide an easy ground for the calculations. However, our objective is not the alpha particle but the cluster description of light halo nuclei in terms of an alpha particle accompanied by a number of neutrons. Although the J-TICI scheme can be applied beyond the alpha particle it is by no means implied that an extension of this method to the open shell structure of halo nuclei will lead to any positive results. This correlation operator can be given directly in coordinate representation.

The translationally invariant coupled cluster method provides a parametrization of the correlation operator in terms of functions depending on the relative distances. It is obtained several truncated forms for the correlation operator that can be used in a variational calculation. However, a further improvement is to enrich the structure of the reference function.

One of the requirements for translational invariance is that the reference function is separable into relative and center-of-mass parts and any choice for the reference factor should respect this. The Jastrow correlation factor is such a choice. Combining the simplest approximation of the CCM, namely the TICI, with the Jastrow correlation factor leads to a variational calculation that is easily accessible both analytically and numerically, termed as the J-TICI scheme.

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