

Partitioning technique procedure revisited: Formalism and first application to atomic problems

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Usually the partitioning technique (PT) has been studied under two aspects: (i) as a numerical tool for solving secular equations of high order, and (ii) as a theoretical method related to the infinite-order perturbation theory and the iteration–variation methods. Here it is shown that there exists a form of the PT equations which allows us to determine explicitly the spectrum and eigenstates of the Hamiltonian operator for different forms of potentials without the utilization of perturbative expansions or iterative equations of the type $E = f(E)$. As a first application of the new approach, we consider the hydrogen-atom in strong magnetic fields ($B \sim 10^9$ G).

1. Introduction

The vast majority of problems in quantum theory cannot be solved exactly. As in all theories of physics approximate methods are therefore of great importance. Perturbation theory [5,20,26], variational principle [4,24,27], generator coordinate method [8], numerical techniques [15,21,26] are some of the procedures currently in use for determining the energy eigenvalues for the one and two electron Schrödinger equation in one, two and three dimensions. However, there are in the literature other methods which, under practical standpoint, must be explored yet in order to show their possible advantages to other procedures. One of these methods is the so-called partitioning technique. In fact, during the years 1958–1965 Löwdin [16,17] was interested in the partitioning technique (PT) as a valuable procedure to determine the solution of the eigenvalue problem

$$\mathbf{H}|\Psi_l\rangle = E_l|\Psi_l\rangle \quad (1.1)$$

in quantum theory (\mathbf{H} = Hamiltonian operator, $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$).

Löwdin's studies, however, were basically restricted to the theoretical analysis in order to show the connection of the PT approach with the infinite-order perturbation

theory and the iteration–variation methods, and some applications have been made to determine upper and lower bounds for eigenvalues [2,17]. In the years 1982–1987 the PT procedure has been used [22,23] as a numerical tool for solving a secular equation of high order.

The purpose of this paper is to show that it is possible by using a new form of the PT equations to determine the eigenvalues and eigenkets of (1.1) explicitly. For this we have modified the original development of the partitioning approach in two simple aspects: (i) we have applied the partitioning technique directly to the auxiliary problem $\mathbf{H}_0|l\rangle = E_l^\circ|l\rangle$ instead of equation (1.1), and (ii) we have used as reference ket the eigenket $|\Psi_l\rangle$ of \mathbf{H} , instead of $|l\rangle$. In consequence, differently from Löwdin’s development, the reduced resolvent \mathbf{T} in our approach does not depend on \mathbf{H} , and we can obtain a set of nonlinear algebraic equations for the wave operator matrix elements w_{sl} . Hence, we can determine E_l directly in terms of w_{sl} and V_{sl} , potential matrix elements. In order to emphasize here the difference between our formulation and Löwdin’s derivation we call it the modified partitioning procedure (MPP).

This paper is organized as follows: In section 2, we present our modified partitioning procedure and we obtain the fundamental equations for the determination of the eigenvalues and eigenkets of \mathbf{H} . In section 3, as an illustration, we apply our equations to the quadratic Zeeman effect in the hydrogen-atom for magnetic fields in the range known as strong fields ($B \sim 10^9$ G). Finally, section 4 contains some concluding remarks relative to extension of our method to include many-electron systems based on the Hartree–Fock theory.

2. Modified partitioning procedure

We assume that the eigenvalues and eigenstates of \mathbf{H}_0 are known. The potential \mathbf{V} in $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$ is not necessarily small. We want to determine the eigenvalues and eigenkets of \mathbf{H} . We have, with the usual notation,

$$\mathbf{H}|\Psi_l\rangle = E_l|\Psi_l\rangle, \quad \mathbf{H}_0|l\rangle = E_l^\circ|l\rangle. \quad (2.1)$$

We introduce the self-adjoint modified projection operators \mathbf{Q} and \mathbf{P} which define certain subspaces H_a and H_b , respectively, in the total Hilbert space H , that is, they satisfy

$$\begin{aligned} \mathbf{Q}^2 &= c\mathbf{Q}, & \mathbf{Q}^+ &= \mathbf{Q}, & \mathbf{P}\mathbf{Q} &= \mathbf{Q}\mathbf{P} = 0, \\ \mathbf{P}^2 &= c\mathbf{P}, & \mathbf{P}^+ &= \mathbf{P}, & \mathbf{P} &= c - \mathbf{Q}, \end{aligned} \quad (2.2)$$

with $H = H_a \oplus H_b$.

These operators \mathbf{Q} and \mathbf{P} correspond to projection operators introduced by Löwdin [16], but with \mathbf{Q} and \mathbf{P} it is not necessary to suppose that the reference ket is normalized (for example, if $|\eta\rangle$ is the reference ket $\langle\eta|\eta\rangle = c$, we have $\mathbf{Q} = |\eta\rangle\langle\eta|$ and $\mathbf{Q}^2 = c\mathbf{Q}$).

An analysis of Löwdin's development shows that his procedure is valid for any \mathbf{H} subjected to the condition that \mathbf{H} is a self-adjoint operator bounded from below. In particular, it can be applied to $\mathbf{H} \equiv \mathbf{H}_0$. In this case, using our operators \mathbf{Q} and \mathbf{P} we can introduce the reduced resolvent \mathbf{T} by

$$\mathbf{T} = \mathbf{P}[\alpha\mathbf{Q} + \mathbf{P}(\varepsilon - \mathbf{H}_0)\mathbf{P}]^{-1}\mathbf{P}, \quad (2.3)$$

and the operator Ω by

$$\Omega = (1 + \mathbf{T}\mathbf{H}_0)\mathbf{Q}. \quad (2.4)$$

The new operators present the following properties:

$$\begin{aligned} \mathbf{T}\mathbf{Q} = \mathbf{Q}\mathbf{T} = 0, \quad \mathbf{T}\mathbf{P} = \mathbf{P}\mathbf{T} = c\mathbf{T}, \\ \Omega\mathbf{P} = 0, \quad \mathbf{Q}\Omega = c\mathbf{Q}, \end{aligned} \quad (2.5)$$

which are easily established.

From equations (2.2) and (2.5) it follows that

$$(\mathbf{H}_0 - \varepsilon)\Omega = \mathbf{Q}(\mathbf{H}_0 + \mathbf{H}_0\mathbf{T}\mathbf{H}_0 - \varepsilon)\mathbf{Q}, \quad (2.6)$$

or

$$\mathbf{H}_0\Omega = \varepsilon\Omega \quad (2.7)$$

if

$$\mathbf{Q}(\mathbf{H}_0 + \mathbf{H}_0\mathbf{T}\mathbf{H}_0 - \varepsilon)\mathbf{Q} = 0, \quad (2.8)$$

that is, Ω is an eigenoperator of \mathbf{H}_0 if ε is a root of equation (2.8). In this case, if $|\tau\rangle \in H$ and $\mathbf{Q}|\tau\rangle \neq 0$, we have that

$$|\varphi_\varepsilon\rangle = \Omega|\tau\rangle = (1 + \mathbf{T}\mathbf{H}_0)\mathbf{Q}|\tau\rangle$$

is an eigenket of \mathbf{H}_0 belonging to eigenvalue ε obtained from equation (2.8).

In order to proceed further, we define the modified projection operator \mathbf{Q} by using as reference ket $|\Psi_l\rangle$, i.e.,

$$\mathbf{Q} = |\Psi_l\rangle\langle\Psi_l|.$$

Since $|\Psi_l\rangle$ is an eigenket of \mathbf{H} , we have (see equations (2.2) and (2.3))

$$\mathbf{T}|\Psi_l\rangle = 0,$$

and as $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$, we obtain

$$\mathbf{T}\mathbf{H}_0|\Psi_l\rangle = -\mathbf{T}\mathbf{V}|\Psi_l\rangle.$$

In consequence, using (2.4), (2.7) and (2.8) we can write

$$|l\rangle = \Omega|\Psi_l\rangle/c = (1 - \mathbf{T}\mathbf{V})|\Psi_l\rangle \quad (2.9)$$

and

$$E_l = E_l^\circ + \langle \Psi_l | (1 - \mathbf{VT})\mathbf{V} | \Psi_l \rangle / \langle \Psi_l | \Psi_l \rangle, \quad (2.10)$$

where we have used that for $|\varphi_\varepsilon\rangle = |l\rangle$, $\varepsilon = E_l^\circ$ and $\mathbf{Q}^2 = c\mathbf{Q}$ with $c = \langle \Psi_l | \Psi_l \rangle$.

Introducing the modified wave operator \mathbf{w} given by

$$\mathbf{w} = (1 - \mathbf{TV})^{-1}, \quad (2.11)$$

we obtain from equations (2.9) and (2.10), respectively,

$$|\Psi_l\rangle = \mathbf{w}|l\rangle = (1 - \mathbf{TV})^{-1}|l\rangle \quad (2.12)$$

and

$$E_l = E_l^\circ + \langle l | \mathbf{V}\mathbf{w} | l \rangle / \langle l | \mathbf{w}^+ \mathbf{w} | l \rangle. \quad (2.13)$$

Equations (2.12) and (2.13) give the eigenkets (eigenvalues) $|\Psi_l\rangle$ (E_l) of \mathbf{H} in terms of the eigenkets (eigenvalues) $|l\rangle$ (E_l°) of \mathbf{H}_0 . They are the fundamental equations of the modified partitioning technique.

It is evident that $|\Psi_l\rangle$ and E_l can be determined explicitly from equations (2.12) and (2.13) if we know the modified wave operator matrix elements $w_{sl} = \langle s | \mathbf{w} | l \rangle$.

In order to determine w_{sl} , we note the relation

$$\mathbf{w} = 1 + \mathbf{TV}\mathbf{w}, \quad (2.14)$$

obtained from $(1 - \mathbf{TV})\mathbf{w} = 1$, and we consider the orthonormal complete set of eigenkets of \mathbf{H}_0 , $\{|\varphi\rangle\} \equiv \{|1\rangle, |2\rangle, \dots, |l\rangle, \dots, |s\rangle, \dots\}$. Hence, we have from (2.12), (2.13) and the completeness relation $\sum_k |k\rangle\langle k| = 1$ ($k = 1, 2, \dots$),

$$\langle s | \Psi_l \rangle = \langle s | l \rangle + \sum_{k,m} \langle s | \mathbf{T} | k \rangle \langle k | \mathbf{V} | m \rangle \langle m | \mathbf{w} | l \rangle, \quad (2.15)$$

or

$$w_{sl} = \delta_{sl} + \sum_{k,m} T_{sk} V_{km} w_{ml}. \quad (2.16)$$

To determine T_{sk} we consider the relations

$$\langle \Psi_l | = \langle l | \mathbf{w}^+ = \langle l | + \langle \Psi_l | \mathbf{VT},$$

$$\sum_k |k\rangle\langle k| = 1,$$

and

$$\mathbf{P}(E_l^\circ - \mathbf{H}_0)\mathbf{T} = \mathbf{P}.$$

It follows, after some algebraic development, that

$$(E_l^\circ - E_s^\circ)T_{sk} = \delta_{sk} - \langle s | \Psi_l \rangle \langle l | k \rangle / w_{ll}. \quad (2.17)$$

Thus, by using (2.16) we have that for $s \neq l$ (l fixed, $s = 1, 2, \dots$),

$$(E_l^\circ - E_s^\circ)w_{sl}w_{ll} - w_{ll} \sum_m V_{sm}w_{ml} + w_{sl} \sum_m V_{lm}w_{ml} = 0 \quad (2.18)$$

with

$$w_{ll} - \sum_k w_{kl}^2 = 0. \quad (2.19)$$

The number of equations in the variables w_{sl} in equations (2.18) and (2.19) is infinite. In the applications we consider a subset of $\{|\varphi\rangle\}$ with N eigenkets of \mathbf{H}_0 . Hence, the set of equations (2.18) and (2.19) has a number of equations equal to the number of variables w_{sl} . As consequence, we can determine w_{sl} and write, from equation (2.13),

$$E_l = E_l^\circ + \sum_{k=1}^N V_{lk}w_{lk}/w_{ll}, \quad (2.20)$$

which is the explicit solution of equation (1.1) for the energy value. The corresponding eigenket is written as

$$|\Psi_l\rangle = \sum_{k=1}^N w_{lk}|k\rangle. \quad (2.21)$$

Concluding this section we note that our procedure is valid for any potential \mathbf{V} (small or large) whose matrix elements V_{lk} exist. In particular, it can also be applied to systems with many electrons.

3. Application

Here, as an application, we specialize the general construction we developed in section 2 to the study of the hydrogen-atom in strong magnetic fields. As it is known [25] the electronic structure of the hydrogen-atom in a uniform magnetic field remains one of the most important and studied problems in atomic physics. So, this application can be a good test for our method. In section 3.1 we consider the case where the basis set $\{|\varphi\rangle\}$ is composed by eigenfunctions of \mathbf{H}_0 , and in section 3.2 we take for $\{|\varphi\rangle\}$ an arbitrary basis set with a parameter α to be determined.

3.1. MPP with $\{|\varphi\rangle\}$ a set of eigenfunctions of \mathbf{H}_0

We consider our set of nonlinear algebraic equations in w_{sl} , formed by relations (2.18) and (2.19), to determine the ground-state energy of the hydrogen-atom in strong magnetic fields ($B \sim 10^9$ G). In this case, we have for \mathbf{H}_0 the Hamiltonian

Table 1

Energy values ($-E$) in a.u. for the Zeeman effect in the ground-state of hydrogen-atom for different number N of basis functions (3.2) and some field strength values.

$\gamma \setminus N$	4	8	12	14	20	25
0.1	0.497518	0.497519	0.497519	0.497519	0.497519	0.497519
0.2	0.441443	0.441853	0.441981	0.442012	0.442064	0.442088
1.0	0.271236	0.273880	0.274719	0.274937	0.275287	0.275442

operator of the hydrogen-atom and for potential \mathbf{V} , in atomic units and spherical coordinates,

$$\mathbf{V} = (\gamma^2/8)r^2 \sin^2 \theta, \quad (3.1)$$

where the values of γ range from 0.1 to 1.0, and $\gamma = 1$ corresponds to $B = 2.35 \times 10^9$ [18]. For the basis set $\{|\varphi\rangle\}$, in this section, we use the eigenfunctions of the hydrogen-atom, that is (with the usual notation),

$$|\varphi\rangle = |nlm\rangle = R_{nl}(r)Y_{lm}(\theta, \phi), \quad (3.2)$$

with $n = 1, 2, \dots$, $l = 0, 1, 2, \dots, n-1$, $-l \leq m \leq l$.

In our calculations we have checked the convergence (see table 1) for the eigenvalues of E_l , by increasing the number of basis functions and comparing the obtained eigenvalues with those from a more restricted basis. For the ground-state and the values of γ in the range $0.1 \leq \gamma \leq 1.0$ we have found that only $l = 0$ and $l = 2$ are important to assure convergence. We have included in the basis set n s- and n' d-functions ($1 \leq n \leq 12$, $3 \leq n' \leq 12$). Our system of nonlinear algebraic equations has been solved by using the Newton–Raphson algorithm [7].

Our results (MPPH) for the ground-state energy using 22 basis functions are presented in table 3 as a function of γ . In this table our results are compared with those obtained by Cabib, Fabri and Fiorio (CFF) [6], Praddaude (P) [18], Brandi (B) [4], Aldrich and Greene (AG) [1], Friedrich (F) [11], Bender, Mlodinow and Papanicolau (BMP) [3], Le Guillou and Zinn-Justin (LGZJ) [12], Rösner, Wummer, Herold and Ruder (RWHR) [19], Fonte, Falsaperla, Schiffrer and Stanzial (FFSS) [10], Hajj (H) [13]. The results we have obtained using for all γ the standard hydrogen-atom wave functions can be improved by introducing, for each value γ , an optimized orbital exponent on those functions. To analyze this aspect with MPP we use in the next subsection another basis function set.

3.2. MPP with $\{|\varphi\rangle\}$ an arbitrary basis set

We consider the hydrogen-atom in strong magnetic fields but for $\{|\varphi\rangle\}$ we use the functions

$$|\varphi\rangle = |nlm\rangle = P_{nl}(r, \alpha)Y_{lm}(\theta, \phi), \quad (3.3)$$

obtained from the functions (3.2) by using the transformation $1/n \rightarrow \alpha$, where α is a variational parameter to be determined for each value of γ . The new functions (3.3), for n increasing, are less diffuse than the standard hydrogen-atom wave functions.

Equations (2.18) and (2.20) are applied directly when the set of basis functions $\{|\varphi\rangle\}$ is formed by the eigenfunctions of \mathbf{H}_0 . In other cases it is necessary to make a little mathematical development to write (2.18) and (2.20) in terms of the matrix elements of $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$. Specifically, corresponding to the relation (2.20), we obtain (note that $E_l^\circ + \sum_k V_{lk} w_{lk}/w_{ll} = \sum_k \langle l|\mathbf{H}_0 + \mathbf{V}|k\rangle w_{lk}/w_{ll} = \sum_k H_{lk} w_{lk}/w_{ll}$)

$$E_l = \sum_k H_{lk} w_{lk}/w_{ll}. \quad (3.4)$$

Similarly, we get for relation (2.18):

$$w_{sl} \sum_k H_{lk} w_{kl} + w_{ll} \sum_k H_{sk} w_{kl} = 0. \quad (3.5)$$

A direct calculation shows that, using the basis set (3.3), we have for E_l , as a functions of α ,

$$E_l = \sum_k (\alpha^2 H_{lk}^c + \alpha H_{lk}^n + (1/\alpha) H_{lk}^z) w_{lk}/w_{ll}, \quad (3.6)$$

where H_{lk}^c , H_{lk}^n and H_{lk}^z are matrix elements of the kinetic operator, electron-nucleus interaction and electron-magnetic field term of the Hamiltonian \mathbf{H} for $\alpha = 1$, respectively. With equation (3.6) we can determine for each γ an optimized value for α using the condition

$$\frac{\partial E_l}{\partial \alpha} = 0. \quad (3.7)$$

In consequence, for $\{|\varphi\rangle\}$ an arbitrary basis set, our MPP algebraic system of nonlinear equations is composed by relations (2.19), (3.5) and (3.7), and the variables are w_{lk} and α .

In the calculations with basis set (3.3) we have also analysed the convergence of the eigenvalues E_l for γ in the range $0.1 \leq \gamma \leq 1.0$. We have obtained that for this case the values of l which are important to assure convergence are also $l = 0$ and $l = 2$. In table 2 we show the energy convergence for several field strengths as a function of the number N of basis functions. We can note that for the values of γ considered it is sufficient to take only a basis with 20 functions and that the convergence turns more slow with the increase of γ . This was expected because we are close to the region $\gamma \geq 2$, where the effect of the magnetic field is dominating [18]. In this region, it is convenient to consider for the basis functions the set of solutions of the free electron in a magnetic field.

Our results (MPP α) with the basis set (3.3) are compared to others in table 3. We note that these results (MPP α) with an optimized basis set are exact numerically (see tables 2 and 3).

Table 2

Energy values ($-E$) in a.u. for the Zeeman effect in the ground-state of hydrogen-atom for different number N of basis functions (3.3) and some field strength values.

$\gamma \setminus N$	6	12	20	30	42	64
0.1	0.497526	0.497526	0.497526	0.497526	0.497526	0.497526
0.2			0.490382	0.490382	0.490382	0.490382
0.3			0.479187	0.479187	0.479187	0.479187
0.5			0.447211	0.447211	0.447211	0.447211
0.7			0.405723	0.405724	0.405724	0.405724
1.0	0.329477	0.331051	0.331167	0.331168	0.331169	0.331169

Table 3

A comparison of the ground-state energy ($-E$) in a.u. calculated with our equations, using the standard hydrogen-atom wave function (MPPH) and using the basis set optimized (MPP α), with the results of Cabib, Fabri and Fiorio (CFF) [6], Praddaude (P) [18], Brandi (B) [4], Aldrich and Greene (AG) [1], Friedrich (F) [11], Bender, Mlodinow and Papanicolau (BMP) [3], Le Guillou and Zinn-Justin (LGZJ) [12], Rösner, Wummer, Herold and Ruder (RWHR) [19], Fonte, Falsaperla, Schiffrer and Stanzial (FFSS) [10] and Hajj (H) [13].

γ	CFF	P	B	AG	F	BMP
0.1	0.49754	0.49753	0.49752	0.4975		0.497551
0.2	0.49038		0.49026			
0.3	0.47920		0.47850			
0.5	0.44724		0.44203			
0.7	0.40571		0.39332			
1.0	0.33120	0.33117	0.27551	0.3310	0.328	0.330616

γ	LGZJ	RWHR	FFSS	H	MPPH	MPP α
0.1		0.497526	0.497526	0.497526	0.49752	0.497526
0.2	0.490382			0.490382	0.49026	0.490382
0.3					0.47856	0.479187
0.5	0.447211				0.44209	0.447211
0.7					0.39848	0.405724
1.0	0.331169	0.331169	0.331169	0.331169	0.27544	0.331169

Our results indicate that the use of the modified partitioning technique can be of interest in the study of physical systems with more electrons under the presence of strong fields. In fact, this is the motivation for introducing the present treatment of this classical problem of atomic physics. Works in this direction are in progress and will be reported elsewhere.

One advantage of our method over the usual diagonalization procedure of Hamiltonian operator (UDPHO) is that whereas UDPHO is concerned with the calculation of all eigenvectors and eigenvalues of \mathbf{H} corresponding to a given expansion of $|\Psi\rangle$, our set of nonlinear algebraic equations allows us to determine a particular eigenvalue E_l and corresponding eigenvector $|\Psi_l\rangle$ of interest, since in our system of nonlinear

equations the label l is fixed. In consequence, we can choose and/or optimize a basis set for each eigenvalue E_l and eigenvector $|\Psi_l\rangle$.

With relation to the usual perturbation theory, our method presents the advantage that it does not use in its development power series expansion in \mathbf{V} , which sometimes makes it necessary to rederive the perturbation series expansions for large-order behavior, when the term \mathbf{V} increases [12,14]. On the contrary, the MPP can be applied to any (small or large) potential \mathbf{V} whose matrix elements V_{lk} exist.

4. Concluding remarks

In this paper we have reexamined the partitioning technique (PT) procedure. Specifically, we have modified the development of the PT approach in two aspects: (i) we have developed the partitioning technique directly to equation $\mathbf{H}_0|l\rangle = E_l^\circ|l\rangle$ instead of $\mathbf{H}|\Psi_l\rangle = E_l|\Psi_l\rangle$ ($\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$), and (ii) we have used as reference ket the true eigenket of \mathbf{H} instead of $|l\rangle$. Our development shows that with these modifications the PT procedure can be seen as an independent mathematical method to solve the Schrödinger equation $\mathbf{H}|\Psi_l\rangle = E_l|\Psi_l\rangle$, i.e., it leads to a system of nonlinear algebraic equations in the variables w_{sl} (modified wave operator matrix elements) and the solutions w_{sl} of this system determine explicitly E_l and $|\Psi_l\rangle$ (see equations (2.20) and (2.21)) independently of a perturbative power series expansion in \mathbf{V} or a procedure based on the relation $E = f(E)$. In this sense our development is an improved formulation of the partitioning technique procedure. As an illustration of our procedure we have applied our equations to determine the ground-state energy of the hydrogen atom in strong magnetic fields ($B \sim 10^9$ G) using two basis set $\{|\varphi\rangle\}$. The results for the ground state energy using an optimized basis set show that our set of nonlinear algebraic equations gives accurate results. In fact, our equations are general and can be applied in principle to physical systems with more electrons and for different forms of the potential (for example, they can be applied to the potentials indicated by Witwit [26]). In particular, our method can be extended to include calculations for many-body problems based on Hartree–Fock theory. For this, it is sufficient to consider $\mathbf{H}_0 = \sum_{i=1}^n \mathbf{F}(i)$, where $\mathbf{F}(i)$ is the Fock operator and $\mathbf{V} = \mathbf{H}_e - \mathbf{H}_0$ with \mathbf{H}_e the electronic Hamiltonian given by

$$\mathbf{H}_e = \sum_{i=1}^n h(i) + \sum_{i<j}^n \frac{1}{r_{ij}},$$

the first term being a sum of one-electron operators and the second term representing a two-electron operator ($n =$ number of electrons). Then, for the basis set $\{|\varphi\rangle\}$ we can consider $\{|\Phi_0\rangle, |\Phi_i^a\rangle, |\Phi_{ij}^{ab}\rangle, \dots\}$, where $|\Phi_0\rangle$ is the Hartree–Fock determinant, $|\Phi_i^a\rangle$ are singly excited determinants, $|\Phi_{ij}^{ab}\rangle$ are doubly excited determinants, etc., obtained from the reference determinant $|\Phi_0\rangle$, and equations (2.19), (2.20) are applied directly. This extension is now being worked out by the authors and the results will be published elsewhere.

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