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The Half-Projected Hartree-Fock Method

I. Eigenvalue Formulation and Simple Applications

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A SCF method based on the solution of two eigenvalue problems, in the same manner as for the normal UHF procedure, is formulated for determining the half-projected Hartree-Fock (HPHF) function for singlet ground states of molecules, the HPHF function being defined as a linear combination of two Slater determinants containing only spin eigenfunctions with even quantum number. A computer program has been written and is described, and results are presented for two simple linear molecules. An important part of the correlation energy is obtained for these molecules.

Key words: Hartree-Fock method, half-projected ~ – Half-projected Hartree-Fock method

1. Introduction

There are many methods currently available for obtaining at least a part of the correlation energy for molecules [1–8]. However, all of these methods lose the simplicity of the restricted Hartree-Fock (RHF) formalism, and for none of them is general application straightforward.

One way of retaining this simplicity is by using the unrestricted Hartree-Fock (UHF) function which is also a single Slater determinant but the electrons of opposite spins are assigned to different spatial orbitals (DODS) [9, 10]. Such a function is not a spin eigenfunction and although it might be expected to yield an energy lower than that of the RHF function, when taken as an approximation to a singlet ground state, it generally does not do so due to the spin contamination of the function. Löwdin [11] has, therefore, suggested the projected Hartree-Fock method (PHF) in order to circumvent this problem. In this method the wavefunction, which is a spin eigenfunction, takes the form of a fixed linear combination of Slater determinants for which the coefficients depend upon the multiplicity and the number of pairs of electrons. The best orbitals are obtained, as in the RHF and UHF methods, by the variational procedure. Although some calculations have been performed with this method for small systems [12–17] it becomes intractable for larger ones owing to the large number of determinants involved.

It has recently been suggested by Smeyers and Doreste-Suarez [17] that the simpler two-determinant unrestricted function given by

$$\Psi = 2^{-1/2}(|a_1\bar{b}_1a_2\bar{b}_2\ldots a_N\bar{b}_N| + |b_1\bar{a}_1b_2\bar{a}_2\ldots b_N\bar{a}_N|) \tag{1}$$

when used as an approximation to singlet ground states, should be capable of recovering a part of the correlation energy similarly to the PHF function. The function may be shown [17] to contain only states with even spin quantum number and can be expressed as the one-determinant UHF function projected on the subspace with even spin quantum number. It is therefore referred to as the half-projected Hartree-Fock (HPHF) function.

It may also be noted [17] that changing the sign of the second Slater determinant in (1) gives a triplet, which is similarly half-projected, in that it contains only states of odd spin quantum number.

In this paper we show how the orbitals may be optimised for the function given by (1), we describe the computer program which has been written, and present the results of interest for H_2 and BH in order to illustrate the method.

2. Theory

2.1. Derivation of an Eigenvalue Formulation

In this section we give an expression for the energy of the HPHF function of Eq.(1), and show how the condition for this energy to be stationary with respect to variations in the $\{a\}$ and $\{b\}$ orbitals can be expressed as two eigenvalue equations. We assume, without loss of generality, that all the orbitals are real, and that the $\{a\}$ and $\{b\}$ each form an orthonormal set. The formulae we give are greatly simplified by assuming the orbitals to be in "corresponding" form: i.e. that they satisfy

$$\langle a_i \mid b_j \rangle = \delta_{ij} \lambda_i \tag{2}$$

The possibility of choosing orbitals to satisfy (2), in the context of normal UHF theory, was noted by Amos and Hall [10], and since the HPHF function, like the UHF, is invariant to unitary transformations among each of the orbital sets $\{a\}$ and $\{b\}$, the proof of Amos and Hall may be applied without modification, as also noted by Smeyers and Doreste-Suarez [17].

With the orbitals $\{a\}$ and $\{b\}$ chosen to satisfy Eq.(2), the norm of the wavefunction of Eq.(1) is

$$\langle \Psi \mid \Psi \rangle = 1 + D \tag{3}$$

where

$$D = \prod_{i=1}^{N} \lambda_i^2 \tag{4}$$

is the simplified expression for the determinant of the overlap matrix between the $\{a\}$ and $\{b\}$ orbitals.

We now define

$$E_1 = \sum_{i=1}^{N} \left\{ \langle a_i|h|a_i\rangle + \langle b_i|h|b_i\rangle + \tfrac{1}{2} \sum_{j=1}^{N} \left[\langle a_i a_j|g|a_i a_j\rangle - \langle a_i a_j|g|a_j a_i\rangle + \right.\right.$$
$$\left.\left. + \langle b_i b_j|g|b_i b_j\rangle - \langle b_i b_j|g|b_j b_i\rangle + 2\langle a_i b_j|g|a_i b_j\rangle \right] \right\} \tag{5}$$

which is the "unprojected" UHF energy of each Slater determinant of Eq.(1), and

$$E_2 = D \sum_{i=1}^{N} 1/\lambda_i \left\{ 2\langle a_i|h|b_i\rangle + \sum_{j=1}^{N} 1/\lambda_j \left[2\langle a_i a_j|g|b_i b_j\rangle - \langle a_i a_j|g|b_j b_i\rangle \right] \right\} \tag{6}$$

which is the cross Hamiltonian element between the two Slater determinants. For the total energy of the wave-function, we then have

$$E = \frac{\langle \Psi|\mathscr{H}|\Psi\rangle}{\langle \Psi \mid \Psi\rangle} = \frac{E_1 + E_2}{1 + D} \tag{7}$$

We now calculate the variation in the energy with respect to variations of the orbitals $\{a\}$ and $\{b\}$. Like Smeyers and Doreste-Suarez [17], we use the "generalised Brillouin's theorem", which we may derive as follows:

Owing to the invariance of Ψ to a unitary transformation among the orbitals $\{a\}$, it is sufficiently general to consider variations of the form

$$|a_i\rangle \rightarrow |a_i\rangle + \sum_{k>N} \varepsilon_{ik}|a_k\rangle \tag{8}$$

where the summation runs over all "virtual" orbitals a_k, orthogonal to every filled $\{a\}$ orbital. Under the variation (8), the change in the wave-function, to first order in the ε_{ik}, is:

$$\Psi \rightarrow \Psi + \sum_{i=1}^{N} \sum_{k>N} \varepsilon_{ik} \Psi_{ik} \tag{9}$$

where

$$\Psi_{ik} = 2^{-1/2}(|a_1\bar{b}_1 \ldots a_k\bar{b}_i \ldots a_N\bar{b}_N| + |b_1\bar{a}_1 \ldots b_i\bar{a}_k \ldots b_N\bar{a}_N|) \tag{10}$$

It is then easy to show (see McWeeny and Sutcliffe [18], pp. 33–34) that the variation in the energy is given by:

$$\frac{\partial E}{\partial \varepsilon_{ik}} = \langle \Psi|\mathscr{H}|\Psi_{ik}\rangle - E\langle \Psi \mid \Psi_{ik}\rangle \tag{11}$$

Smeyers and Doreste-Suarez [17] appear to have solved a configuration interaction problem in the functions Ψ_{ik} in order to optimise the orbitals, but we shall show here how to express the condition for energy minimum in terms of a relatively simple eigenvalue equation.

We first define the following operators:

$$R^a = \sum_{i=1}^{N} |a_i\rangle\langle a_i| \tag{12a}$$

$$R^b = \sum_{i=1}^{N} |b_i\rangle\langle b_i| \tag{12b}$$

which are operator forms of the usual (spin-less) density matrices for the $\{a\}$ and $\{b\}$ orbitals, and

$$R^{ab} = \sum_{i=1}^{N} |a_i\rangle 1/\lambda_i \langle b_i| \tag{13}$$

which arises in considering cross-terms between the two determinants. R^{ab} is not symmetric, but we may define R^{ba} as the transpose of R^{ab}.

Introducing an arbitrary basis of one-electron functions (e.g. atomic orbitals (AO)), denoted by p,q,r,s, we define

$$F^a_{pq}=h_{pq}+\sum_{r,s}[(R^a_{rs}+R^b_{rs})\langle pr|g|qs\rangle-R^a_{rs}\langle pr|g|sq\rangle] \tag{14a}$$

$$F^b_{pq}=h_{pq}+\sum_{r,s}[(R^a_{rs}+R^b_{rs})\langle pr|g|qs\rangle-R^b_{rs}\langle pr|g|sq\rangle] \tag{14b}$$

as the Hartree-Fock matrix elements arising in normal UHF theory, and the "cross-term"

$$F^{ab}_{pq}=h_{pq}+\sum_{r,s}[2R^{ab}_{rs}\langle pr|g|qs\rangle-R^{ab}_{rs}\langle pr|g|sq\rangle] \tag{15}$$

Owing to the exchange term in (15), F^{ab} is not symmetric, but, again, we may define F^{ba} as its transpose.

Using the definitions of F^a and F^{ab} above, and the methods described by McWeeny and Sutcliffe [18], the variation in the energy (Eq.(11)) can be written as follows:

$$\frac{\partial E}{\partial \varepsilon_{ik}}=\langle a_i|F^a|a_k\rangle+D/\lambda_i\langle b_i|F^{ba}|a_k\rangle+(E_2-DE)/\lambda_i\langle b_i|a_k\rangle-$$

$$-D/\lambda_i\sum_{j=1}^{N}1/\lambda_j\langle b_j|a_k\rangle\langle b_i|F^{ba}|a_j\rangle \tag{16}$$

The condition for the energy to be stationary with respect to variations in the $\{a\}$ orbitals, is then that the above expression should be zero for all filled orbitals i, and all virtual orbitals k. To reduce this condition to an eigenvalue equation, we introduce the Hermitian operator:

$$H^a=F^a+(R^{ab}+R^{ba})(E_2-DE)+D\{R^{ab}F^{ba}(1-R^{ab})+(1-R^{ba})F^{ab}R^{ba}\} \tag{17}$$

Now

$$\frac{\partial E}{\partial \varepsilon_{ik}}=\langle a_i|H^a|a_k\rangle \tag{18}$$

To prove (18), it is only necessary to make use of the following properties of R^{ab}, which follow immediately from the definition, Eq.(13):

$$R^{ab}\mid a_k\rangle=\sum_{j=1}^{N}1/\lambda_j\langle b_j\mid a_k\rangle\mid a_j\rangle \tag{19a}$$

$$R^{ba}\mid a_k\rangle=0 \tag{19b}$$

$$R^{ba}\mid a_i\rangle=1/\lambda_i\mid b_i\rangle \tag{19c}$$

Variations of the $\{b\}$ orbitals can be treated by an exactly analogous argument. Thus, letting

$$|\mathrm{b}_i\rangle\rightarrow|b_i\rangle+\sum_{k>N}\eta_{ik}\mid b_k\rangle \tag{20}$$

we have

$$\frac{\partial E}{\partial \eta_{ik}} = \langle b_i | H^b | b_k \rangle \tag{21}$$

where

$$H^b = F^b + (R^{ab} + R^{ba})(E_2 - DE) + D\{R^{ba}F^{ab}(1 - R^{ba}) + (1 - R^{ab})F^{ba}R^{ab}\} \tag{22}$$

The condition for the energy to be stationary is thus that H^a and H^b should have no matrix elements between filled and empty $\{a\}$ and $\{b\}$ orbitals respectively. Owing to invariance of Ψ under unitary transformations among the sets $\{a\}$ and $\{b\}$, we may choose "canonical" sets which completely diagonalise the operators. Thus the HPHF orbitals are found from the two eigenvalue equations:

$$\begin{aligned} H^a \mid a_i \rangle &= \varepsilon_i^a \mid a_i \rangle \\ H^b \mid b_i \rangle &= \varepsilon_i^b \mid b_i \rangle \end{aligned} \tag{23}$$

Clearly the operators H^a and H^b depend, in an even more complex way than in normal UHF theory, on the orbitals $\{a\}$ and $\{b\}$ themselves. Thus, starting from an initial guess to the orbitals, the problem must be solved in an iterative way to reach a self-consistent solution.

As with ordinary HF theory, it is not obvious that such a procedure will converge unaided. However, it is very easy to incorporate the "level-shift" method described by Hillier and Saunders [19]: this involves adding a constant to the virtual diagonal elements of the HF matrix before diagonalisation. It is easy to transfer the arguments of Ref. [19], and show that, as in HF theory, a sufficiently large level shift will guarantee convergence of the HPHF procedure described here.

Although we have used "corresponding orbitals", satisfying Eq.(2), to calculate the form of the operators in Eqs.(17) and (18), the orbitals resulting from diagonalising these operators will almost certainly not satisfy this condition. It would be possible, after each SCF iteration, to calculate the transformation required from canonical to corresponding forms, but this is unnecessary, since, in the final formulae for H^a and H^b, the corresponding orbitals only enter through the definition of R^{ab}. This operator may be calculated directly from a general basis of $\{a\}$ and $\{b\}$ orbitals:

Let

$$S_{ij}^{ab} = \langle a_i \mid b_j \rangle$$

be the overlap matrix of $\{a\}$ and $\{b\}$ orbitals in such a general basis, and $\boldsymbol{T}^{ab}$ be its inverse. Then

$$R^{ab} = \sum_{i,j=1}^{N} |a_i\rangle T_{ji}^{ab} \langle b_j| \tag{24}$$

Throughout this section we have assumed the singlet form of the wave-function, Eq.(1). In the triplet form the second Slater determinant has the opposite sign, and it is easy to see that all the formulae given here are still valid, provided we simply change the sign of D, defined in Eq.(3). Thus the method described here should be equally capable of calculating the lowest triplet state of a molecule.

Evidently the formulae given here only apply if none of the λ_i of Eq.(2) are zero, that is, if the overlap matrix between $\{a\}$ and $\{b\}$ orbitals is non-singular. If one of the λ_i is zero, the energy is given by the simpler expression

$$E=E_1+D'\langle a_p b_p|g|b_p a_p\rangle \tag{25}$$

where $\lambda_p=0$. E_1 is still given by Eq.(5), and

$$D'=\prod_{i\neq p}\lambda_i^2$$

The most likely situation in which this will happen is if a_p and b_p are localised on different atoms in a dissociated molecule, and this case the exchange integral between these orbitals will vanish. E_1 is now equal to the sum of the UHF energies of the different atoms. Thus the HPHF function for the dissociation limit of a molecule should have the same energy as the sum of the UHF energies of the separated fragments. This is an important improvement over the RHF theory (see McWeeny and Sutcliffe [18] pp. 121).

2.2. Some Properties of the Wave-Function

Of interest for calculating one-electron properties of the HPHF wave-function is the total one-electron spinless density matrix. In terms of the operators defined in Eqs.(12) and (13), this may be written

$$R^T=(1+D)^{-1}\{R^a+R^b+D(R^{ab}+R^{ba})\} \tag{26}$$

Natural orbitals (NO) are defined as the eigenfunctions of the spinless density matrix, and are useful for comparing the results of different methods of calculating electron correlation [20]. Using Eq.(26) and the definitions of Eqs.(12) and (13), it is easy to show that the NO's are linear combinations of the $\{a\}$ and $\{b\}$ corresponding orbitals: thus

$$R^T(|a_i\rangle+|b_i\rangle)=(1+D)^{-1}(1+\lambda_i+D+D/\lambda_i)(|a_i\rangle+|b_i\rangle) \tag{27a}$$

$$R^T(|a_i\rangle-|b_i\rangle)=(1+D)^{-1}(1-\lambda_i+D-D/\lambda_i)(|a_i\rangle-|b_i\rangle) \tag{27b}$$

The NO occupations are thus a function of the "splitting" between the $\{a\}$ and $\{b\}$ orbitals, measured by the overlap λ_i. In the limit where $\lambda_i=1$, these occupations become 2 and 0.

The formula for the occupations offer an interesting comparison between the HPHF and the unprojected UHF wave-functions. Amos and Hall [10] derived identical expressions for the NO's of a UHF function, to those given in Eqs.(27); however, the occupations are $1+\lambda_i$ and $1-\lambda_i$ respectively. In order to give appreciable correlation between electrons in a_i and b_i, we must have λ_i appreciably less than one. However, with $\lambda=0.9$ we have NO occupations of 1.9 and 0.1 for simple UHF. The figure of 0.1 for the orbital of small occupation is rather too high. This may be an important reason, quite separate from the problem of spin contamination, why UHF for closed-shell systems often gives the same result as RHF. For the HPHF function the occupations depend, through D, on the splittings of all the orbitals. If we assume that only one orbital is appreciably split, with

$\lambda = 0.9$, so that $D = 0.81$, we derive an occupation number of 0.0055 for the weakly occupied NO, which is more reasonable. However, the situation is less satisfactory if several orbitals are appreciably split: for example, if five orbitals in the HPHF function each have $\lambda = 0.9$, the corresponding NO occupation numbers are 0.045, which is rather high, although still not as high as the single UHF. These considerations lead us to anticipate that the HPHF wave-function may give a satisfactory description of correlation in one, or at most very few orbitals, but will not be capable of describing simultaneous correlation in many orbitals. A similar conclusion follows from considering spin contamination.

It is easy to show that the expectation value of $\mathcal{S}^2$ for the HPHF wave-function is given by

$$\frac{\langle \Psi | \mathcal{S}^2 | \Psi \rangle}{\langle \Psi \mid \Psi \rangle} = N - (1+D)^{-1} \sum_{i=1}^{N} (\lambda_i^2 + D/\lambda_i^2) \tag{28}$$

The corresponding value for simple UHF is

$$N - \sum_{i \neq 1}^{N} \lambda_i^2 \tag{29}$$

Since $\lambda_i^2 \leqslant 1$ for all i, it can be seen that the value of (28) is always less than (29), but by an amount which depends on the relative values of the λ. Returning to the two illustrative examples which we used in the previous paragraph, we can see that if only one λ is different from unity, $\mathcal{S}^2$ for the HPHF function is zero: i.e. in this case the function describes a pure singlet. With five orbitals having $\lambda = 0.9$, however, we obtain a value of $\mathcal{S}^2$ of about 0.55, indicating strong spin contamination (about 10% of quintet); the unprojected UHF value in this case is 0.95. This strongly reinforces our conclusion of the previous paragraph, since it appears that the HPHF wave function cannot describe correlation between many pairs of electrons simultaneously, without introducing an unacceptable degree of spin contamination.

3. Computational Procedure and Testing

The HPHF method described here has been programmed in FORTRAN for the Univac 1108 computer. The steps of the calculation are similar to those for a conventional UHF method, except that the overlap matrix between $\{a\}$ and $\{b\}$ orbitals must be calculated and inverted, to obtain the matrices $\boldsymbol{R}^{ab}$ and $\boldsymbol{F}^{ab}$ from Eqs.(24) and (15). To make use of the level-shift procedure [19] and to speed up the diagonalisation, the matrices $\boldsymbol{H}^a$ and $\boldsymbol{H}^b$ are calculated in the basis of trial $\{a\}$ and $\{b\}$ orbitals respectively. Both in storage requirements and in time per iteration, the calculation represents an approximately two-fold increase over simple UHF.

As trial orbitals for the first iteration, it seems reasonable to take vectors close to the RHF solution. Since the RHF vectors are themselves a solution to the HPHF equations, corresponding to a saddle-point on the energy surface, it is necessary to split the $\{a\}$ and $\{b\}$ orbitals before starting the calculation. This we do by mixing selected filled and virtual orbitals, with coefficients which have opposite signs for $\{a\}$ and $\{b\}$ sets.

The case of H_2 offers a very convenient test of the method and the programme, since for a two-electron system the HPHF function is not only a pure singlet, but is also equivalent to a two-configuration MC-SCF function [12]. Using a basis-set described previously [8], and with an initial mixing of some $1\sigma_u$ virtual orbital into the RHF $1\sigma_g$, the energy converged steadily towards the two-configuration MC-SCF value [8]. However, as well as this solution (which has the lowest energy), we found it possible to obtain three other solutions with energy lower than the RHF value, by initially mixing virtual orbitals of different symmetry into the RHF filled orbital. We shall discuss the problem of multiple solutions in a later paper.

4. Results for Boron Hydride

We shall now discuss the results obtained, at several levels of approximation including the HPHF method, for the ground state ($^1\Sigma^+$) of BH. The calculations described here have been performed using the uncontracted (9,5/4) Gaussian basis of Huzinaga [22], for which the H1*s* function was scaled by 1.2, augmented by single sets of *d*- and *p*- type polarization functions on the B and H atoms respectively, the exponents chosen for these functions being $d=0.55$ and $p=0.9$. This uncontracted basis was then contracted to (4,2,1/2,1) according to Dunning [23]. For the calculations described below all the SCF orbitals were restricted to be σ symmetry orbitals, unless otherwise indicated.

In Table 1 we compare the results of our HPHF calculations with those of other studies [24–30] and with experiment [31–32] for some spectroscopic properties of BH. It can be seen that the HPHF method compares very favourably with the more complex methods, and of course is in much better agreement with the experimental dissociation energy (*De*) than is the RHF method. Our calculated SCF error in *De* (compare near RHF limit calculation of Cade and Huo [24] is

Table 1. Total energies, dissociation energies and equilibrium internuclear distances calculated using several methods for the X $^1\Sigma^+$ state of BH

	E(hartree)	*De* (eV)	*Re* (Å)
Hartree-Fock[a]	−25.1315	2.78	1.200
Valence bond[b]	−25.1456	2.45	1.342
Large CI[c]	−25.2621	–	–
Separated pair[d]	−25.2054	3.86	1.230
Spin-optimized SCF[e]	−25.1664	3.28	1.250
Valence bond[f]	−25.1454	2.98	1.337
Optimized first-order CI[g]	−25.1798	3.27	1.276
HPHF	−25.1405	3.09	1.273
Experiment[h]	–	3.54±0.04	1.236

[a] See Ref. [24].
[b] See Ref. [25].
[c] See Ref. [26].
[d] See Ref. [27].
[e] See Ref. [28].
[f] See Ref. [29].
[g] See Ref. [30].
[h] See Refs. [31] and [32].

Table 2. Natural-orbital occupation numbers for various internuclear separations[a] calculated using the HPHF method for BH

	2σ	3σ	4σ	5σ
$R=2.41$	1.999	1.977	0.023	0.001
$R=5.0$	1.998	1.584	0.416	0.002
$R=10.0$	1.998	1.021	0.979	0.002

[a] Internuclear separations are given in bohr.

Table 3. Calculated total energies and expectation values of $\mathscr{S}^2$ for the RHF, UHF, HPUHF[a] and HPHF methods for three internuclear separations[b] for BH

	E(hartree)				$\langle\mathscr{S}^2\rangle$		
	RHF	UHF	HPUHF	HPHF	UHF	HPUHF	HPHF
$R=2.41$	−25.1243	−25.1243	−25.1243	−25.1404	0.0	0.0	0.0026
$R=5.0$	−24.9698	−25.0304	−25.0432	−25.0440	0.8948	0.0067	0.0077
$R=10.0$	−24.8373	−25.0270	−25.0271	−25.0271	1.0043	0.0088	0.0088

[a] This is a function of the HPHF type with the orbitals as determined in the UHF calculation.
[b] Internuclear separations are given in bohr.

about 0.13 eV and since this error can also probably be carried over to the HPHF calculation, our agreement with experiment would probably be even better with an improved basis set. The NO occupation numbers, given by Eq.(27), are shown, as a function of three internuclear separations (R), in Table 2. They may be compared with the results obtained from an optimised first-order wave-function (see Table 5 of Ref. [30]), the 3σ, 4σ and 5σ occupation numbers being very similar in both cases. Table 3 gives an interesting comparison of the calculated values for the total energy and $\langle\mathscr{S}^2\rangle$ for several methods as a function of R.

As has been mentioned in a previous section, it has been found that on removing the symmetry restriction, other solutions may be obtained. Over a wide range of R for BH it is possible to obtain at least one non-symmetry solution, in which the NO's are not all σ orbitals. This has been found true not only for the HPHF method but also for the UHF method. The nature of these solutions appears to change as a function of R, "σ-type" correlation being preferred at large distances (>3.5 bohr) and "π-type" correlation being preferred at shorter distances (<2.8 bohr). For all R it has been found possible to obtain both UHF and HPHF solutions lower in energy than the corresponding RHF solutions, although the UHF wave-function always has an appreciable spin contamination. One such additional solution occurs for the HPHF method at R of 2.4 bohr with an energy of −25.1451 Hartree and $\langle\mathscr{S}^2\rangle=0.0005$. The NO's with occupation numbers appreciably different from either 2 or 0 are a σ NO with occupation number of 1.910 and a π NO with occupation number of 0.090.

5. Conclusions

In the present work, we have given a simple and practicable method for the calculation of HPHF wave-functions. The computational effort required is only a factor of two greater than the simple UHF method. This simplicity may be contrasted with the extremely complicated equations arising in fully-projected methods [33]. Results have been presented for the simple molecule BH, and although the method does not appear to recover a large proportion of the total correlation energy, there is a sufficiently large improvement over RHF that the method deserves to be investigated further. These investigations, and a discussion of the problem of multiple solutions, will be presented in a subsequent paper.

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