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The Wave Functions of H_2 and Symmetrical Linear H_3

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The wave functions obtained from configuration interaction treatment of H_2 (eight configurations) and H_3 (sixty-two) are examined. The relative magnitudes of the coefficients of the various terms are discussed and conclusions are drawn as to how the present functions might be simplified and improved.

Die Wellenfunktionen, die durch eine CI-Behandlung von H_2 (acht Konfigurationen) und H_3 (zweiundsechzig) gewonnen werden, werden überprüft. Die relativen Größen der Koeffizienten der verschiedenen Terme werden diskutiert und Schlußfolgerungen gezogen, wie die gegenwärtigen Funktionen vereinfacht und verbessert werden könnten.

Étude des fonctions d'onde obtenues par interaction de configurations pour H_2 (huit configurations) et H_3 (soixante deux configurations). Les grandeurs relatives des coefficients des différents termes sont examinées et l'on tire des conclusions quant à la manière dont ces fonctions pourraient être simplifiées et améliorées.

Introduction

In the previous paper the results of configuration interaction treatment of H_2 and symmetrical linear H_3 have been described. The main purpose of this paper is to discuss the form of the wave functions for the most stable configuration of H_2 and linear symmetrical H_3. Because the functions under discussion resemble most closely those recently derived by Shavitt *et al.* [1] some comparison is made with the results obtained by them in order to assess the nature and extent of some of the weaknesses of the present functions. Shavitt *et al.* employed two 1*s* orbitals and three 2*p* orbitals on each centre, the exponents of the three 2*p* orbitals on one centre being the same. Our calculations use only one 1*s* orbital on each centre and for H_3 all the 1*s* orbital exponents and all the 2*p* orbital exponents were the same. Shavitt *et al.* used different exponents for the central atom orbital from those used for the outer atom orbitals.

The recent calculations of Gianinetti *et al.* [2] are also related to the present ones; they employed 1*s*, 2*s* and three 2*p* orbitals on each centre and used different exponents for the *s* orbitals on the outer and central atoms. They examined symmetrical linear configurations only.

Hydrogen Molecule

With H_2 Shavitt *et al.* [1] obtained $D_e = 106$ kcal/mole (with $R_e = 1.402$) whereas we obtained a value a little greater than 103 (with $R_e = 1.416$). Gianinetti *et al.* [2] obtained $D_e = 106$ kcal/mole (with $R_e = 1.4165$) equal to the value obtained by Shavitt *et al.* [1]. This gives an indication of the advantage

Table 1. *Coefficients* ($\times 10^2$) *of various* AO *configurations in the* CI *function for* H_2. *These coefficients would normalise the function*

$S_A S_B$	48.8	$Z_A Z_A$	-3.5
$S_A S_A$	8.5	$Z_A Z_B$	-0.8
$S_A Z_A$	-1.3	$X_A X_A$	-2.5
$S_A Z_B$	-4.8	$X_A X_B$	-0.4

gained from allowing for in-out correlation for those dispositions when two electrons are near the same nucleus (ionic dispositions).

The eight independent coefficients of AO configurations of this CI function of H_2 at its equilibrium separation are listed in Table 1. These are derived from the figures in Tables 2 and 5 of the preceding paper.

As would be expected, the $S_A S_B$ term is largest because of the "end-to-end" correlation of the electrons. The coefficient of the ionic $S_A S_A$ term is much smaller though it is the second largest term. The simplest function that represents these is that of Coulson and Fischer [3] in which the two electrons are assigned to the orbitals $(S_A + KS_B)$ and $(S_B + KS_A)$. The constant K is a little less than 0.1. These two orbitals may be regarded as being derived from simple LCAO-MO's, end-to-end correlation having been added. Alternatively, it may be regarded as a Heitler-London function in which polarised orbitals $(S_A + KS_B)$ and $(S_B + KS_A)$ replace S_A and S_B. Polarisation can also be included, in an alternative form, by Rosen's method. This is a polarisation centred on the same nucleus rather than the other one. If both types of polarisation terms are included, to achieve greater flexibility, the orbitals become $(S_A + KS_B + K'Z_A)$ and $(S_B + KS_A - K'Z_B)$. To explain the importance of the next most important term $(S_A Z_B)$, K' must be about 0.05. The coefficient of the $S_A Z_A$ term will then be expected to be $-2 \times 0.1 \times 0.05 \times 0.488 = -0.5 \times 10^{-2}$ (obs -1.3×10^{-2}) and that of the $Z_A Z_B$ term $-0.05 \times 0.05 \times 0.488 = -0.1 \times 10^{-2}$ (-0.8×10^{-2}). This simple way of describing the molecule is therefore only satisfactory in providing a reasonable interpretation of the three largest terms ($S_A S_B$, $S_A S_A$ and $S_A Z_B$); it does not account for the coefficients of the smaller terms ($S_A Z_A$ and $Z_A Z_B$).

Fig. 1 shows graphs of S_A, S_B, Z_A and Z_B. The exponents of the S and Z-orbitals have been optimised. It is apparent that, for the Z-orbitals, the exponent is such as to place the maximum near the half-way point between the nuclei. The terms $S_A Z_A$ and $S_A Z_B$ may be considered as modifying the main part of the function ($S_A S_B$ and $S_A S_A$ terms) in respect of dispositions when one electron is near nucleus A and the other is a) between A and B, b) on the far side of A from B, and c) on the far side of B from A. The sign and magnitude of the terms are such that they particularly reduce the importance of c) as is to be expected, they increase the importance of a) as is to be expected and they increase the importance of b) which is hardly to be expected. Perhaps the difficulty lies in expecting *two* adjustable terms to introduce the required modifications into *three* types of dispositions of the two electrons. It is not necessarily possible to accommodate all three and a compromise has to be accepted. This is now in process of being investigated.

The terms $Z_A Z_A$ and $X_A X_A$ (and $Y_A Y_A$) are also of considerable importance. The sign of the coefficients shows that these allow for angular correlation of the two electrons for those situations in which two electrons are near to one nucleus. The three terms $Z_A Z_A$, $X_A X_A$ and $Y_A Y_A$ appear with approximately equal weight. This is to be expected because angular correlation is likely to be independent of orientation to a first approximation. The term $X_A X_B$ (-0.4×10^{-2}) allows for an azimuthal correlation for those dispositions in which the two electrons are near different nuclei. This is a much less important term (lower coefficient) than $X_A X_A$ because the correlation effect of charge repulsion is much less than when the two electrons are close together. Hischfelder and Linnett [4] mistakenly included $X_A X_B$ and omitted $X_A X_A$, incorrectly using the argument that the Heitler-London type terms would be likely to out-weigh ionic type terms, even in those which allow for correlation, just as they do in the main *SS* terms. This is now seen to be quite incorrect (cf. McLean, Yoshimine and Weiss [5] Rev. modern Physics) and arose from an inadequate appreciation of the effects to be achieved by the inclusion of such terms. The same behaviour can be seen in the function derived by Gianinetti *et al.* [2].

The smaller terms in the CI function can therefore be understood. They arise from two effects: – a) the need to use polarised atomic orbitals, and b) the need to take account of the effects of electron repulsion on the mutual distribution of the electrons. The first is a one-electron effect and the second a two-electron one. The major effect of b) is to force the electrons to opposite ends of the molecule. It is, however, also particularly important to include terms which operate to reduce the importance of those dispositions which place the electrons very near to one another (*e.g.* place the two electrons near one nucleus though, in this respect, the present function suffers because it contains no terms which allow for in-out correlation in ionic dispositions).

Linear H_3 *Complex*

In this paper, calculations have only been made for the symmetrical linear H_3 complex because other calculations have shown that the configuration of this type of minimum energy corresponds to the transition state for the reaction between molecular and atomic hydrogen. Conroy and Bruner [6] have concluded that the energy of this H_3 complex is 7.74 kcal/mole greater than that of $H + H_2$. The experimental value is between 7 and 10 kcal/mole [7]. However, it cannot be regarded as certain beyond all possible doubt that the closed Diophantine integration used by Conroy and Bruner gave all the integrals with the required accuracy.

The minimum energy of linear symmetrical H_3 obtained using CI functions based on a limited number of atomic orbitals are: 1*s*: -1.6106 a.u. (at $R = 1.883$ a.u.) 1*s*, 1*s*′: -1.6305 (at $R = 1.788$); 1*s*, 1*s*′, 2*p*: 1.6521 (at $R = 1.764$); 1*s*, 2*s*, 2*p*: 1.6473 (at $R = 1.792$) [2]. The energies of activation for these four treatments (relative to results obtained for similar treatments of H_2 in each case) were: 23.4, 14.0, 11.0 and 13.1 kcal/mole respectively. The present calculation (1*s*, 2*p*) gave -1.6387 (at $R = 1.771$) even though, in this calculation, the exponents for all three centres were equal to one another. The energy of activation calculated was 16.3 kcal/mole. The main reasons for the high value for the energy were the non-inclusion of in-out correlation and the employment of equal exponents at all

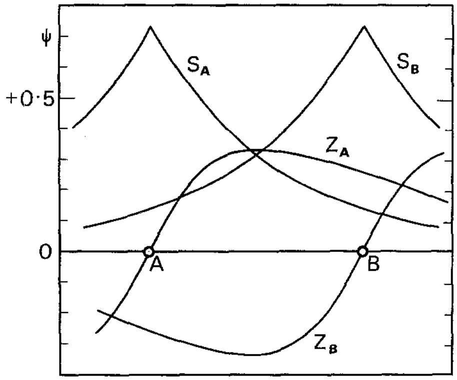

Fig. 1. Graphs of S_A, S_B, Z_A and Z_B along the HH axis for an HH separation of 1.42 a.u.

centres. Boys and Shavitt [9], using a set of functions based on the same two 1*s* orbitals at each centre, obtained -1.6119 (at $R = 1.779$) and an energy of activation of 15.4 kcal/mole. Edmiston and Kraus [10], using a Gaussian basis set, obtained -1.650 a.u. (at $R = 1.78$ a.u.). Their calculated value for the activation energy was 15 kcal/mole.

One of the objects of this stage of our calculations was to examine the form of the CI function with the object of deciding how best to make improvements. The above figures show that the present calculated energies are a little higher than some of the most recent ones but sufficiently low to suggest that it should be justifiable to make useful conclusions regarding the form of the function and the importance of the limitations placed on it. The discussion will be along similar lines to that already used with H_2 though, of course, in this case, 62 configurations are involved rather than 8 and the increased complexity renders the physical interpretation more difficult.

The scale of 2*p* orbitals is rather different in this case from what it was in H_2 because the internuclear separation is different. But again the maximum is near the mid-point between the nuclei (cf. graphs in Fig. 1 for H_2). The coefficients of various AO configurations are shown in Table 2, in which the terms are divided into six groups: A) Three *S*-orbitals; B) Two *S* and one *Z*; C) One *S* and two *Z*; D) Three *Z*; E) One *S* and two *X* (or *Y*); F) One *Z* and two *X* (or *Y*). Not all the coefficients in the table are independent because of the need for the function to be an eigenfunction of S^2.

As with H_2, the Heitler-London terms are the largest, the other *SSS* terms (ionic ones) being of the order of one-tenth of these. The coefficients cannot be explained fully using a VB-function (with ionic terms) based on the resonance: $\dot{H}\,H{-}H \leftrightarrow H{-}H\,\dot{H}$ because no terms of the type $S_A S_A S_B$ would be included. However, if the function is constructed according to the method of Coulson and Fischer, the correct form can be achieved if one of the bonding orbitals is delocalised onto the third atom. The leading determinant is

$$\|(S_A)(S_B + 0.008\, S_c)(0.16\, S_A + 0.14\, S_B + S_c)\|\,,$$

other determinants being added to make the whole function an eigenfunction of S^2 and to have the correct symmetry. With a 1-electron bond function $S_A S_A S_B$

Table 2. *Coefficients* ($\times 10^2$) *of various atomic orbital configurations in the 62 term* CI *function of* H_3. *The coefficients are those that would normalise the whole function. The order of spin functions is* $\alpha\beta\alpha$

Section A. *SSS* terms (4 independent coefficients):

$S_AS_BS_C$	41.23	$S_AS_BS_B$	5.85
$S_AS_CS_B$	20.62	$S_AS_AS_C$	3.52
$S_BS_AS_C$	20.62	$S_AS_AS_B$	3.16

Section B. *ZSS* terms (14 independent coefficients):

$Z_AS_BS_C$	−0.81	$S_AS_BZ_B$	+5.38
$Z_AS_CS_B$	−3.93	$S_BS_AZ_B$	+6.23
$S_BZ_AS_C$	+3.13	$S_AZ_BS_B$	−0.86
$Z_AS_BS_A$	−2.48	$Z_AS_AS_C$	−1.46
$Z_AS_AS_B$	−2.10	$Z_AS_CS_A$	−1.27
$S_AZ_AS_B$	+0.37	$S_AZ_AS_C$	−0.19
$Z_AS_AS_A$	+1.23	$S_AS_AZ_B$	−0.68
$Z_AS_BS_B$	−2.10	$S_BS_BZ_B$	−0.03
$Z_AS_CS_C$	+1.04	$S_AS_CZ_B$	+8.61

Section C. *SZZ* terms (13 independent coefficients):

$S_AZ_BZ_C$	+0.42	$Z_AZ_BS_B$	−0.20
$S_AZ_CZ_B$	−1.02	$Z_BZ_AS_B$	−0.97
$Z_BS_AZ_C$	+1.44	$Z_AS_BZ_B$	+0.76
$S_AZ_BZ_A$	+0.59	$S_AZ_AZ_C$	−0.47
$S_AZ_AZ_B$	−0.13	$S_AZ_CZ_A$	−0.32
$Z_AS_AZ_B$	−0.71	$Z_AS_AZ_C$	−0.15
$S_AZ_AZ_A$	−0.68	$Z_AZ_AS_B$	−1.22
$S_AZ_BZ_B$	−3.03	$Z_AZ_CS_B$	+0.53
$S_AZ_CZ_C$	−2.18	$Z_AS_BZ_C$	+1.05

Section D. *ZZZ* terms (4 independent coefficients):

$Z_AZ_CZ_B$	−0.41	$Z_AZ_AZ_C$	−0.04
$Z_AZ_AZ_B$	−0.72	$Z_AZ_BZ_B$	+0.43

Section E. *SXX* terms (13 independent coefficients):

$S_AX_AX_B$	+0.72	$S_BX_AX_B$	−0.18
$S_AX_BX_A$	+1.05	$S_BX_BX_A$	+0.35
$X_AS_AX_B$	−0.33	$X_AS_BX_B$	−0.53
$S_AX_AX_C$	+0.08	$S_BX_AX_C$	−0.00
$S_AX_CX_A$	−0.11	$X_AS_BX_C$	−0.00
$X_AS_AX_C$	+0.19		
$S_AX_BX_C$	−0.15		
$S_AX_CX_B$	+0.51		
$X_BS_AX_C$	−0.66		
$S_AX_AX_A$	−0.36	$X_AX_AS_B$	−0.88
$S_AX_BX_B$	−2.89		
$S_AX_CX_C$	−1.81		

Table 2 (continued)

Section F. *ZXX* terms (14 independent coefficients):

$Z_A X_A X_B$	-0.15	$Z_A X_B X_C$	-0.12
$Z_A X_B X_A$	-0.14	$Z_A X_C X_B$	-0.10
$X_A Z_A X_B$	-0.01	$X_B Z_A X_C$	-0.02
$Z_A X_A X_C$	$+0.04$	$Z_B X_A X_B$	-0.23
$Z_A X_C X_A$	$+0.03$	$Z_B X_B X_A$	-0.18
$X_A Z_A X_C$	$+0.02$	$X_A Z_B X_B$	-0.06
$Z_A X_A X_A$	$+0.01$	$Z_B X_A X_A$	$+0.46$
$Z_A X_B X_B$	$+0.64$	$Z_B X_B X_B$	$+1.07$
$Z_A X_C X_C$	-0.01	$Z_B X_C X_A$	-0.01

would be included but its coefficient would be too small. Again, delocalisation of one of the orbitals would achieve agreement with the coefficients in Table 2 Section A. The leading determinant is

$$\|(S_A)(0.17\, S_A + S_B)(0.13\, S_A + 0.14\, S_B + S_c)\| .$$

Because it allows for the tendency of two electrons to be near the central nucleus, the fact that the term $S_A S_B S_B$ has the largest coefficient of the ionic terms is understandable. And the coefficient of $S_A S_A S_C$ is also reasonable. However, it is surprising that the coefficient of $S_A S_A S_B$ is as large as it is, because it favours a disposition of the three electrons which tends to concentrate them towards one end of the molecule.

Some of the *SSZ* terms are important. In fact, the $S_A S_C Z_B$ term is next in importance after the Heitler-London terms. The value of its coefficient exceeds those of the ionic *SSS* terms. The contribution of these terms shows that, as in H_2, polarisation effects are important.

The *SSS* and *SSZ* terms can be examined in a variety of ways. The following seems to be a convenient though somewhat subjective one. The lobes of the Z_B orbital lie in the regions between A and B (−*ve* lobe) and between B and C (+*ve* lobe) – see Fig. 1. Similarly, the lobes of the Z_A lie in the regions outside A (−*ve*) and between A and B (+*ve*). On the basis of this feature, Table 3 is constructed from the coefficients in Table 2. In any one of the seven sets. AO configurations are considered which contain two particular *S*-orbitals, the third one being variable. For instance, set i) is based on the coefficients of $S_A S_A S_B$, $S_A S_A S_C$, $S_A S_A Z_A$, $S_A S_A Z_B$ and $S_A S_A Z_C$. The coefficients of the first are placed opposite B and C. ($S_A S_A S_A$ has a coefficient of zero.) Combinations of the *SSZ* coefficients are placed between A and B, or B and C, or above A, or below C, as these signify the regions in which the *Z*-lobes are concentrated. (The number above A is the coefficient of $S_A S_A Z_A$ with changed sign (−*ve* lobes of Z_A); between A and B the coefficient of that term minus that of the $S_A S_A Z_B$ term is listed because the negative lobe of Z_B is located there, etc.) The spins associated with the orbitals common to the set are shown on the left. The first set is constructed from configuration $S_A S_A X$.

It can be seen that the third electron concentrates in the BC bond when two electrons are near nucleus A. The probability of it lying outside C is reduced compared with the *SSS* term, though there seems to be some probability of finding

Table 3. *Analyses of SSS and SSZ functions. Two electrons are restricted to S orbitals as shown on the left of each diagram (see text). For the other electron, the coefficient of each SSS orbital is entered against each atom. It is presumed that the lobes of the* p_Z *orbitals are located between the atoms; the numbers between the atoms indicate magnitudes, remembering that between atoms two lobes contribute*

i)	+ 1.23	ii)	− 2.10	iii)	− 2.48	iv)	− 2.10
αβ A	0		− 5.85	α A	0	β A	− 3.16
	− 0.55		+ 2.07		− 2.90		− 4.13
B	+ 3.16	αβ B	0	β B	+ 5.85	α B	0
	+ 0.36		− 2.07		+ 4.57		+ 2.30
C	+ 3.52	C	+ 5.85	C	+41.23	C	+20.62
	− 1.04		+ 2.10		+ 0.81		+ 3.93

v)	− 1.27	vi)	− 0.37	vii)	+ 0.19
α A	0	α A	+ 3.16	α A	+ 3.53
	− 7.34		+ 0.49		− 0.19
B	+20.62	α B	+ 5.85	B	+41.32
	+ 7.15		+ 2.26		− 0.19
β C	+ 3.52	C	+20.62	α C	+ 3.52
	+ 1.46		− 3.12		+ 0.19

it outside A. This may be a consequence of limitations imposed by the functions used (cf. H_2 and see later), rather than representing any real effect. In set ii) the third electron is strongly excluded from the whole region near B, when the other two electrons are located near that nucleus, and is concentrated near A and C or just outside them. In set iii), the concentration on C spreads towards B, where there is an electron of opposite spin. As in i), there is some apparent probability of finding the electron outside A. In set iv), the spins associated with the two fixed orbitals are reversed compared with iii). The probability of finding the third electron near C is reduced. However, it is localised more strongly there because the electron near B has the same spin. There is some probability of finding the electron near A where there is an electron of opposite spin, but it is less than near C. Set v) is particularly interesting because, except for spin, the two "fixed" orbitals are symmetrically disposed. The electron is concentrated near B but the probability spreads markedly towards the nucleus C but not towards A – though, as in i), there is some probability of finding the electron outside A. It is interesting that the term $S_A S_C Z_B$ warrants such a high coefficient because it is making allowance for spin-polarisation (and not charge-polarisation). It might have been thought that this spin (Pauli Principle) Exclusion effect would have been achieved by the use of determinantal functions without the need for any further terms. But this is not so.

In sets vi) and vii), the two "fixed" orbitals are associated with the same spin functions. In set vi) ($S_A X S_B$), the "third" electron is spread over the region A to C though, inevitably, the probability of finding it near C is greatest. The same is true for set vii) ($S_A X S_C$) except that the "mobile" electron is strongly concentrated near B.

In Table 3, there are four locations representing the four regions covered by the lobes of the Z-orbitals. But there are only three Z-orbitals in the basis set. Therefore, the "numbers" in Table 3 for the four regions are not completely independent of one another. Probably a much better way of incorporating the polarisation effects which is achieved here by the SSZ terms would be to use *four* Gaussian functions, one for each region, instead of the *three* Z-orbitals. This is being tested.

Among the SZZ terms, the largest coefficients are associated with the $S_A Z_B Z_B$ and $S_A Z_C Z_C$ terms which introduce angular correlation ($-ve$ coefficients) into those dispositions in which two electrons are near the same centre. Including the $Z_A Z_A S_B$ term also, the coefficients are in all three instances between -0.4 and -0.6 times the coefficients of the corresponding SSS terms. The coefficients ($+ve$ signs) of the $Z_A Z_C S_B$ and $Z_A S_B Z_C$ terms show that these serve to decrease the probability of all three electrons approaching the centre of the radical (nucleus B) together. All the ZZZ terms are relatively unimportant because they combine two effects which may be regarded as corrections to the main function (polarisation and correlation). The most important term is $Z_A Z_A Z_B$, which allows for angular correlation on A and $Z_A Z_B Z_B$, which allows for angular correlation on B. The Heitler-London type term is less important.

Of the SXX terms, again those allowing for angular correlation ($-ve$ coefficient) are the most important ($S_A X_B X_B$ and $S_A X_C X_C$). The ratio of the coefficients of these and of the $X_A X_A S_B$ term to the corresponding SSS terms are -0.5, -0.5 and -0.3 respectively. Except for the last this ratio is similar to those for the SZZ terms (cf. H_2). The coefficients of the terms involving both X_A and X_C are very small because azimuthal correlation for electrons at opposite ends of this triatomic radical is of little importance. The terms containing both X_A and X_B have, on the whole, coefficients of intermediate size.

All the coefficients of the ZXX terms are small, though the ones that make some allowance for azimuthal correlation of two electrons near the same nucleus (*e.g.* $Z_A X_B X_B$ and $Z_B X_B X_B$) are the most important.

From the above discussion, it is clear that we can understand in part the form of CI functions expressed in terms of AO's which brings out the localised features. The function for H_3 given in Ref. [2] could be transformed in a similar way. It would be interesting for this to be done. This experience is being used to improve the present function by adding terms involving Gaussian functions in such a way as to make allowance for in-out correlation which has not been included here, and more effectively for the polarisation effects.

It is interesting that Michels and Harris [11] have commented on the improvement achieved by adding a $3d\sigma$ orbital on the central atom. From the above discussion, we would anticipate that the inclusion of a central $3d\sigma$ orbital along with the three $2p\sigma$ orbitals would make for some improvement because there would then be four orbitals to allow for the four regions referred to earlier when discussing the SZZ terms. The employment of four Gaussian functions along the internuclear line would probably achieve a similar result.

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