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# Nonadiabatic wavefunctions as linear expansions of correlated exponentials. A quantum Monte Carlo application to $H_2^+$ and $Ps_2$

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## Abstract

We propose to expand the nonadiabatic solution of the Schrödinger equation as a linear combination of explicitly correlated exponentials. A series of trial wavefunctions has been optimized minimizing the variance of the local energy for the  $H_2^+$  and dipositronium ( $Ps_2$ ) molecules in their ground state, without resorting to the Born–Oppenheimer approximation: the calculations have been performed using the variational Monte Carlo method. In a diffusion Monte Carlo simulation a 6-term wavefunction allowed us to compute the exact energy of the  $Ps_2$  system  $-0.51601$  hartree with a variance of  $0.00001$  hartree. © 1997 Elsevier Science B.V.

## 1. Introduction

The Born–Oppenheimer (BO) approximation [1] is of central importance in quantum chemistry, allowing the separation of nuclear motion from electronic motion. Within this approximation, solution of the electronic Schrödinger equation gives the electronic energy, which depends parametrically on the nuclear coordinates. To the chemist this gives the approximate, but nevertheless extremely useful, concept of the potential energy surface. Beyond the interpretative role, it is also the base for methods that treat the nuclear dynamics. The full treatment of the complete many body Hamiltonian is computationally extremely demanding; as a result the Born–Oppenheimer approximation is employed practically in all calculations. Only for small systems, such as the

hydrogen molecular ion and its isotopes, and the hydrogen molecule and its isotopes, has the solution of the Schrödinger equation without the BO approximation has been attempted [2], commonly employing specialized trial wavefunctions. The BO approximation is usually a good approximation, however, there are systems [2] for which it is not valid, such as the positronium molecule studied here, and so it is important to develop computational methods to treat the many body Schrödinger equation without resorting to the BO approximation.

Almost all the methods developed in the past to compute nonadiabatic wavefunctions start with the separation of the motion of the center of mass. This is usually accomplished through an involved coordinate transformation, in order to rewrite a Hamiltonian operator including only internal coordinates. However, after the separation of the center of mass, the form of the Laplacian operator is quite compli-

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cated, leading to intractable integrals. Furthermore, the choice of internal coordinate system is not unique, and there is little guidance on how to choose the most appropriate reference frame.

To avoid the problems related to the rigorous separation of the center of mass motion, Kozłowski and Adamowicz [3] suggested eliminating the kinetic energy associated to the motion of the external degrees of freedom either introducing a ‘penalty’ operator into the variational principle, or subtracting the center of mass kinetic energy from the total energy.

The problem of the solution of the complete Schrödinger equation has recently received renewed attention with the development of various methods [3]. Since, in a sense, the problem is to introduce into the trial wavefunction a ‘correlation’ between electronic and nuclear motions, it is natural to extend methods used to explicitly build the electron correlation into the electronic wavefunction.

The explicit inclusion of the interelectronic coordinates into an approximate wavefunction is an efficient and effective approach to accurately describe the electron correlation; this old and well-known method to build accurate solutions of the Schrödinger equation was used by Hylleraas [4], James and Coolidge [5] and Kolos and Wolniewicz [6] to obtain good results for two-electron systems by including the interelectronic distance  $r_{12}$  into the wavefunction. Unfortunately, it is not easy to generalize these methods to systems with more than two electrons since the resulting integrals are extremely difficult to evaluate. In 1960 Boys [7] and Singer [8] suggested using explicitly correlated Gaussian (CG) functions as this choice leads to integrals in closed form [9]. More recently various researchers have shown that these explicitly correlated Gaussian functions can give accurate results on a variety of two [10], three [11] and four [12] electron systems, provided that a careful optimization of the nonlinear parameters is performed.

These functions have been used in a number of papers to treat nonadiabatic systems [3,13,14]. Unfortunately, Gaussian functions poorly reproduce the cusp conditions [15], i.e. the behaviour of the wavefunction when two particles collide, and this has the unpleasant effect of slowing down the convergence. As a result, a large number of functions is needed to reach high accuracy, increasing the number of non-

linear parameters, and making their optimization a demanding task.

In a previous Letter [16] we proposed to expand the solution of the electronic Schrödinger equation as a linear expansion of explicitly correlated exponentials. We showed that this choice allows a good description of the cusp conditions and reduces the number of terms needed to obtain the desired accuracy by an order of magnitude, in comparison with correlated Gaussian basis sets. This expansion was applied to the hydrogen molecule and the  $\text{He}_2^+$  ion, and was shown to converge rapidly. In this letter we explore the possibility of extending the proposed functional form to a nonadiabatic description of molecular systems.

## 2. Trial wavefunction form

We propose to approximate the total wavefunction of systems with  $N$  electrons and  $M$  nuclei with the linear expansion (we consider here only rotationless states)

$$\Psi_L = \sum_{i=1}^L c_i \Phi_i, \quad (1)$$

where

$$\Phi_i = \hat{A} \left\{ \left[ \hat{O} f_i(\mathbf{r}) \exp(\mathbf{k}_i \cdot \mathbf{d}) g_i(\mathbf{R}) \right] \Theta \right\}. \quad (2)$$

In this equation  $\hat{A}$  is the antisymmetrizer operator,  $\hat{O}$  is an operator used to fix the space symmetry,  $f_i(\mathbf{r})$  is a function of the electronic ( $x, y, z$ ) and nuclear coordinates ( $X, Y, Z$ )

$$f_i(\mathbf{r}) = \prod_{j=1}^N \prod_{k=1}^M (x_j - X_k)^{\alpha_{ijk}} (y_j - Y_k)^{\beta_{ijk}} \times (z_j - Z_k)^{\gamma_{ijk}} r_{jk}^{\delta_{ijk}}, \quad (3)$$

where  $\alpha, \beta, \gamma$  and  $\delta$  are integers greater than or equal to zero.  $\mathbf{k}_i$  is the  $i$ th vector of the parameters associated to the electron–electron and electron–nucleus distances collected in the  $\mathbf{d}$  vector.  $g_i(\mathbf{R})$  is a function of the internuclear distances:  $\text{H}_2^+$  and  $\text{Ps}_2$  require different expressions, which will be presented in the next sections.  $\Theta$  is the correct spin eigenfunction for the electrons and the nuclei.

This form ensures a good description of the cusps and has the correct spin and space symmetry. However, the price one has to pay is the inability to compute analytically the matrix elements of the Hamiltonian, so a numerical method must be used to evaluate the expectation value of the energy. The variational Monte Carlo (VMC) method [17] is well suited for this purpose, the energy being estimated by averaging the local energy  $H\Psi/\Psi$  during a random walk in configuration space using a Metropolis algorithm [18] or a Langevin algorithm [19]. Thus it only requires the evaluation of the wavefunction, its gradient and its Laplacian, and these are easily computed. In this way one is completely free in the choice of the trial wavefunction and, in recent years, the VMC method has been successfully used for this task with a variety of explicitly correlated trial wavefunctions. VMC can also be used in the optimization of the parameters of the trial wavefunction, as described in detail by Umrigar [20]: the variance of the local energy is minimized instead of the energy itself since this has been proved to be numerically much more stable.

As a final remark, unlike other methods the proposed expansion, depending only on interparticle distances, allows us to avoid the problem of explicitly eliminating the coordinates of the center of mass. The conventional Cartesian coordinate system is employed in the calculations, as the total momentum of the system vanishes (the trial wavefunction depends only on the difference of the radius vectors of the particles) and the total angular momentum vanishes (the trial wavefunction is invariant under rotation of the system of particles as a whole). In conclusion, the variational Monte Carlo method automatically gives the internal energy, the translational and rotational contributions being zero.

### 3. The $H_2^+$ molecule

The purpose of this work is to explore the capabilities of the proposed expansion in treating nonadiabatic systems. As a benchmark we studied the ground state of the hydrogen molecule ion, which is a non trivial test, in spite of its apparent simplicity, and for which there are several accurate calculations with which to compare.

For this system we optimized a series of wavefunctions of the form

$$\Psi_L = \sum_i^L c_i (1 + \hat{P}_{AB}) e^{k_{i1}r_{1A} + k_{i2}r_{1B} + k_{i3}r_{AB} + k_{i4}r_{AB}^2}, \quad (4)$$

where A and B refer to the nuclei and  $\hat{P}_{AB}$  is the permutation operator for the nuclei.

As to the internuclear distance  $r_{AB}$ , for a harmonic potential the nuclear wavefunction is a Gaussian  $e^{-\alpha(r_{AB} - r_{ABe})^2}$  centered at the equilibrium geometry: expanding the exponent one gets linear and quadratic terms in  $r_{AB}$  whose parameters  $k_{i3}$  and  $k_{i4}$  are independently optimized.

For each term in Eq. (4) there are five parameters, one linear and four nonlinear. We optimized them minimizing the variance of the local energy using a fixed sample of 10000 VMC configurations, as described in Ref. [20]. The results of expansions with increasing numbers of terms are shown in Table 1 and the parameters for the 10-term wavefunction are reported in Table 2.

It can be seen that the proposed expansion is quickly convergent. A single term alone recovers 99.84% and a two-term function already recovers 99.97% of the exact energy [21], while the 10-term wavefunction has an error in the energy of the order of  $10^{-6}$  hartree. The average internuclear distance for the 10-term wavefunction is 2.06403(7) bohr in agreement with the value 2.0639 bohr computed by Bishop and Cheung [22]. For  $H_2^+$  the linear expansion (4) works exceptionally well, giving a fast convergence.

These results are even more striking if we compare them with linear expansions of explicitly corre-

Table 1  
 $H_2^+$  molecule ground state energy (hartree)

Terms	Energy	$\sigma$
1	-0.596235	0.000009
2	-0.596982	0.000006
3	-0.597006	0.000005
6	-0.597113	0.000003
10	-0.597136	0.000003
exact <sup>a</sup>	-0.597139	
70 CG <sup>b</sup>	-0.594550	
256 CG <sup>c</sup>	-0.596030	
205 CG <sup>d</sup>	-0.596901	

<sup>a</sup> Ref. [21]. <sup>b</sup> Ref. [3]. <sup>c</sup> Ref. [23]. <sup>d</sup> Ref. [2].

Table 2  
Parameters of the 10-term wavefunction for  $H_2^+$

	$c_i$	$k_{i1}$	$k_{i2}$	$k_{i3}$	$k_{i4}$
1	1.00000	-1.26032	-0.29491	5.32989	2.05532
2	-0.91967	-1.29180	-0.29922	5.45225	2.06869
3	0.02081	-1.64144	-0.00001	5.09223	2.02955
4	-0.02687	-0.20549	-1.18907	4.32025	1.87771
5	0.01078	-0.17522	-1.03804	4.48953	2.31504
6	-0.00759	-1.98603	-0.81280	8.29552	1.82583
7	0.00706	-0.44656	-1.91694	11.88243	2.25030
8	-0.00058	-0.42962	-1.22382	0.29578	2.54943
9	-0.00059	-3.22675	-0.00023	15.14346	2.25025
10	-0.00303	-1.77935	-1.81625	6.21411	2.23496

lated Gaussians: two terms of our expansion are already better than Gaussian expansions with more than 200 terms [23,2] (the result with 205 CG is better than the one with 256 terms due to different nonlinear optimization schemes). The improved quality of our basis can be explained by the fact that Gaussians poorly reproduce the cusps, while the exponentials we used can account for them. Also included in Table 1 is a result obtained by Kozłowski and Adamowicz [3] with 70 explicitly correlated Gaussians. In their paper they regretted they could not compare their results with a quantum Monte Carlo calculation, as in the literature they found only a nonadiabatic calculation on the hydrogen molecule published by Anderson and co-workers [24], but not on the hydrogen molecule ion. We would like to point out that such a comparison would be unfair to all variational methods, since they provide only an upper bound to the correct energy. On the contrary, for the hydrogen molecule and its positive ion, being nodeless systems, the quantum Monte Carlo method gives the exact answer. Instead, the variational Monte Carlo method, that we have used here, gives an upper bound to the energy, being simply an application of the Metropolis method [18] to the calculation of the expectation value of the energy of a given trial wavefunction using the variational principle. As such, the present results are directly comparable to the more common approach of using explicitly correlated Gaussians.

#### 4. The positronium molecule

Having checked the overall goodness of our *ansatz* for a nonadiabatic wavefunction, we studied the

positronium molecule  $Ps_2$ , formed by two electrons and two positrons and sometimes called 'dipositronium'. This system has been the subject of several theoretical investigations since the pioneering work of Wheeler [25] and Hylleraas and Ore [26]. More recently, the experimental observation of  $Ps^-$  ( $e^+e^-e^-$ ) has renewed the attention on systems containing positronium, and on  $Ps_2$  in particular, since this molecule has not yet been observed experimentally and so accurate computed estimates of its properties are of great importance. During the last few years, many calculations on the ground state of the positronium molecule have been attempted, whose energies range from  $-0.50043$  to  $-0.52106$  hartree (see Ref. [27] for a recent list of calculations on  $Ps_2$ ). Furthermore, a recent paper [27] reported an energy of  $-0.52106$  hartree, much lower than the previous Green's function Monte Carlo (GFMC) value [28]  $-0.51515(25)$  hartree. The space part of the ground state wavefunction of the positronium molecule is positive everywhere and for systems with this property the quantum Monte Carlo methods estimate the exact energy within statistical error.

We hope to definitively resolve the problem of the binding energy of  $Ps_2$  with the present calculations.

The four particles have the same mass and cannot be divided into fast and slow species, so for this system the Born–Oppenheimer approximation cannot be applied. The wavefunction must describe their simultaneous, mutually correlated motions: our *ansatz*, containing all interparticle distances, should be a good approximation to the ground state wavefunction.

We optimized trial wavefunctions of the form

$$\Psi_L = \sum_i^L c_i \hat{O} e^{k_{i1}r_{12} + k_{i2}r_{1a} + k_{i3}r_{1b} + k_{i4}r_{2a} + k_{i5}r_{2b} + k_{i6}r_{ab}}, \quad (5)$$

where 1 and 2 are the positive particles and a and b the negative ones.  $\hat{O}$  is the operator used to fix the correct permutational symmetry of the system [14]. In particular, one has to take into account the fact that the Hamiltonian is invariant not only with respect to the exchange of two identical particles, but also with respect to the double exchange of the two positive particles with the two negative ones.

Preliminary results were presented in our paper [29] on the stability of four-unit-charge neutral systems as the limit case of equal masses. Only a 2-term expansion was optimized without imposing the full symmetry of the system: as a consequence the VMC energy was higher and the variance larger than in the present work.

The trial wavefunctions have been optimized minimizing the variance of the local energy using 10000 configurations, and their variational energies have been estimated using a VMC program. The results are shown in Table 3 along with some reference calculations. The energies are quickly convergent, as can be seen from the comparison with a 400 Hylleraas-like trial wavefunction [30] and a 300-term correlated Gaussian expansion [2]. Our 12-term wavefunction is already 0.00014 hartree from the best variational energy. We could have improved its quality by simply adding more terms; however, it is more efficient to use optimized correlated wavefunctions as guiding functions in the diffusion Monte Carlo (DMC) method or in other similar quantum Monte Carlo simulation techniques to recover the exact energy or a good approximation to the exact energy [31]. These methods need simple, compact and easy to evaluate trial wavefunctions, so we used our 6-term wavefunction, whose parameters are reported in Table 4, in a diffusion Monte Carlo simulation of the ground state of the positronium molecule. The simulation was performed using 4000 walkers and a time step of 0.001 hartree<sup>-1</sup>. We checked, with other simulations using larger time steps, that the time step bias [31] for this value is smaller than the statistical error. As can be seen from Table 3, the diffusion Monte Carlo simulation predicts a ground state energy of  $-0.51601 \pm 0.00001$  hartree: we attribute

Table 3

Ps<sub>2</sub> molecule ground state energy (hartree)

Terms	Energy	$\sigma$
1	-0.50328	0.00001
2	-0.51438	0.00001
3	-0.51506	0.00001
6	-0.51556	0.00001
10	-0.51573	0.00001
12	-0.51586	0.00002
present work <sup>a</sup>	-0.51601	0.00001
GFMC <sup>b</sup>	-0.51515	0.00025
best variational <sup>c</sup>	-0.5160021	
400 Hylleraas <sup>d</sup>	-0.515105	
750 CG <sup>e</sup>	-0.515802	
300 CG <sup>f</sup>	-0.5159767	
300 CG <sup>g</sup>	-0.515980	
32 CG <sup>h</sup>	-0.515385	

<sup>a</sup> Diffusion Monte Carlo simulation using the 6-term expansion as trial function.

<sup>b</sup> Ref. [28]. <sup>c</sup> Ref. [32]. <sup>d</sup> Ref. [30]. <sup>e</sup> Ref. [33].

<sup>f</sup> Ref. [14]. <sup>g</sup> Ref. [34]. <sup>h</sup> Ref. [35].

the difference from the GFMC value by Lee et al. [28]  $-0.51515 \pm 0.00025$  hartree to their variance being underestimated by a factor 2–3. In any case the value  $-0.52106$  hartree by El-Gogary et al. [27] is too low and it is likely to be wrong. Discarding it, the best available variational value is  $-0.5160021$  hartree [32], in good agreement with our result. These data should conclusively define the binding energy of the dipositronium molecule as 0.0160 hartree.

As to the structure of the Ps<sub>2</sub> molecule, average values of the interparticle distances, calculated at the VMC level by the 12-term wavefunction, are reported in Table 5. Our values are slightly shorter than previous results. The e<sup>+</sup>-e<sup>-</sup> distances being

Table 4

Parameters of the 6-term wavefunction for Ps<sub>2</sub>

<i>i</i>	<i>c<sub>i</sub></i>	<i>k<sub>i1</sub></i>	<i>k<sub>i2</sub></i>	<i>k<sub>i3</sub></i>	<i>k<sub>i4</sub></i>	<i>k<sub>i5</sub></i>	<i>k<sub>i6</sub></i>
1	0.81009	-0.01167	-0.38271	-0.18135	-0.10466	-0.50774	-0.12526
2	-1.00000	-0.17564	-0.41830	-0.18135	-0.10884	-0.47718	-0.00938
3	0.08744	-0.04314	-0.27890	-0.12005	-0.73058	-0.44994	0.09631
4	0.13504	-0.14058	-0.02877	-0.55267	-0.57953	-0.05188	-0.14297
5	-0.04998	-0.06280	-0.78176	-0.60446	-0.31233	-0.22175	0.35225
6	0.07724	-0.13317	-0.48947	-0.28442	-0.56845	-0.39994	0.11026

Table 5  
Average internal distances (bohr) of the  $\text{Ps}_2$  molecule

	$\langle r_{12} \rangle = \langle r_{ab} \rangle$	$\langle r_{1a} \rangle = \langle r_{2b} \rangle$	$\langle r_{12}^2 \rangle = \langle r_{ab}^2 \rangle$	$\langle r_{1a}^2 \rangle = \langle r_{2b}^2 \rangle$
Ref. [14]	6.0252578	4.4831482	46.171736	29.010841
Ref. [27]	5.92	4.26		
Ref. [33]	5.916	4.428	43.61	27.72
Ref. [35]			45.911	28.878
present work	5.71588(28)	4.33112(44)	39.503(5)	25.837(5)

shorter than the  $e^+e^+$  and  $e^-e^-$  distances,  $\text{Ps}_2$  can be seen as a complex of two Ps systems.

## 5. Conclusions

We propose as an approximate solution of the Schrödinger equation for nonadiabatic systems a linear expansion of exponential functions of all the electron–electron, electron–nucleus and nucleus–nucleus distances. The expectation values of the energy and other properties must be estimated by a numerical method, the variational Monte Carlo method being our preferred choice.

A relatively small number of terms gives good expectation values of the energy for  $\text{H}_2^+$  and  $\text{Ps}_2$  in their ground state. In both cases the optimized wavefunctions are of high quality, as good as linear expansions of correlated Gaussians that include at least an order of magnitude of terms more. The accuracy of our optimized wavefunctions is demonstrated in the case of the  $\text{Ps}_2$  molecule: when the six-term wavefunction is used as the trial function in a diffusion Monte Carlo simulation, the statistical error of the exact energy is small, a proof of its overall goodness.

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