

Effect of positive-energy orbitals on the configuration-interaction calculation of the H^- atom

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We present the theoretical energy eigenvalues of the 1S ground state and the $(pp)^3P^e$ state of H^- calculated in a simple configuration-interaction procedure, using a finite set of L^2 -basis functions constructed from one-electron hydrogenic orbitals. The energy corrections, due to the electron-electron interaction between configurations with various combinations of bound (negative-energy) and continuum (positive-energy) orbitals, are examined in detail. In particular, our calculation has shown that the continuum-continuum type of configurations contribute approximately 15% and 13%, respectively, to the electron affinity of the 1S ground state and the $(pp)^3P^e$ state of H^- . In addition, our calculation has shown that the calculated oscillator strength for the transition from the 1S ground state of H^- to the lowest 1P Feshbach resonance below the $n=2$ threshold is significantly reduced (nearly 30%) by the presence of the continuum-continuum type of configurations in the ground-state wave function.

I. INTRODUCTION

A reliable estimate of multielectron interaction in any atomic structure study critically relies on the analytic structure of the electronic orbitals employed in the calculation of the two-electron Coulomb matrix. For a strongly correlated system, such as the H^- atom in its ground state, the wave function is often expanded in terms of variational basis functions with *explicit* r_{12} dependence, which describes correctly the exact electronic probability density. Among the most accurate wave functions is the one employed by Frankowski and Pekeris¹ and Freund, Huxtable, and Morgan III,² and expressed in terms of the Hylleraas coordinate with the logarithmic terms suggested by Bartlett³ and Fock.⁴ In addition, Thakkar and Smith⁵ have employed a more compact integral-transform wave function for the ground and low-lying excited states of the two-electron atoms with comparable quantitative accuracy. Applications of the high-order $1/Z$ -expansion variational perturbation approach⁶ with Hylleraas-type basis functions have also led to accurate energy eigenvalues of the ground and lower-lying states of two-electron atoms. Other variational wave functions including simple r_{12}^n terms have been tested with success in the study of the $(pp)^3P^e$ bound state of H^- by Bhatia⁷ and Drake.⁸

Macek⁹ and Lin,¹⁰ in their attempts to understand the earlier $+$ and $-$ series classification of Cooper, Fano and Prats,¹¹ have explored the use of hyperspherical coordinates to describe qualitatively the radial and angular correlation for a two-electron atom. In particular, the doubly excited states are classified in terms of a set of quantum numbers K , T , and A in addition to the usual L , S , and π .^{10,12} Starting from a group-theoretical approach, an equivalent physical interpretation of the electron correlation for two-electron atoms has also been demonstrated independently by Herrick and co-workers.¹² More recently, Feagin and Briggs¹³ have shown that the quantum numbers K , T , and A are related

to the *gerade-ungerade* symmetry of the molecular-orbital description of a diatomic molecule. In particular, the potential curves for H^- derived from the *adiabatic* hyperspherical approximation by Lin¹⁰ can be obtained by a simple scaling from the corresponding potential curves for H_2^+ .¹³

A less elaborate but more convenient quantitative approach is the application of the central field approximation with basis functions constructed from a linear combination of antisymmetrized products of *one-electron* orbital functions $u_i(\mathbf{r})$. The convergence of such an approach is generally slower due to the absence of the r_{12} term in the basis functions, but its extension to more complex atoms is relatively straightforward. The effectiveness of the central field approximation is determined largely by the ability of the product of one-electron orbital functions, employed in the calculation of the two-particle Coulomb matrix, to take into account the interaction represented by the interelectronic separation r_{12} . Within this approximation, the most commonly employed basis functions are of the Slater type with the nonlinear exponential parameters determined variationally by an appropriate *optimum* procedure. Such theoretical procedures, e.g., the multiconfiguration Hartree-Fock approach¹⁴ (MCHF) and the method of superposition of configuration¹⁵ (SOC), are often capable of leading to numerical data only slightly less accurate than the most elaborate Hylleraas-type calculations for the two-electron systems.

Within the central field approximation, a less sophisticated approach is the truncated diagonalization method¹⁶ (TDM). This simple configuration-interaction (CI) procedure is usually carried out without the optimization requirement due to its use of predetermined one-particle orbital functions. Its applications have been extended to more complex atoms with variable degrees of success.¹⁷⁻¹⁹ The main drawback of this approach in quantitative calculation is the difficulty in including the positive-energy orbitals in the basis functions for the

two-electron matrix

$$\langle u_1(\mathbf{r}_i)u_2(\mathbf{r}_j)|1/r_{ij}|u_3(\mathbf{r}_i)u_4(\mathbf{r}_j)\rangle$$

due to the long-range behavior of the Coulomb interaction.²⁰ In most of the earlier applications of this CI procedure, the basis functions are limited to the products of two bound (negative-energy) one-electron orbitals (i.e., BB-type). The combinations involving continuum (positive-energy) orbitals, including products of bound-continuum (BC-type) and continuum-continuum (CC-type) orbitals, are often excluded from the basis functions due to the numerical consideration. As a result, for some of the highly correlated systems, the use of a set of *incomplete-bound-only* basis functions is not necessarily sufficient to achieve the desirable quantitative accuracy, even when the simplicity of this approach allows for a very large number of configurations to be included in an otherwise *numerically converged* calculation with the help of fast modern computers.

This difficulty can be circumvented if one replaces the incomplete set of *bound-only* basis functions with a nearly *complete* set of finite (L^2) basis functions, which includes both bound and continuum one-electron orbitals confined in a finite radius R . The value of R should be sufficiently large to cover the estimated size of the atomic states of our interest.²¹ In a series of recent applications,²¹⁻²³ we have constructed the radial part of the one-electron orbital wave function χ , subject to a frozen-core Hartree-Fock potential,^{19,21} from a set of B splines^{21,24,25} of order k and total number N defined between two end points $r_{\min}=0$ and $r_{\max}=R$. With the *continuum* contribution (represented by the positive-energy orbitals) effectively taken into account, the applications of this simple CI procedure have led to excellent results in the calculations of energy levels, the oscillator strengths, and the radiative lifetimes of divalent atoms.^{21,22,26} Application has also been carried out with excellent agreement with the experimentally observed photoelectron angular distribution following a four-photon ionization of Mg from its ground state.²³

A detailed examination of our recent calculations has shown that the CI contribution due to the *continuum-continuum* (CC-type) configurations is generally negligible in comparison with the contribution from the bound-bound (BB-type) and bound-continuum (BC-type) configurations for most of the lower-lying atomic states in complex atoms. In order to examine quantitatively the CI contribution from continuum-continuum configurations, we have extended our calculation to the strongly correlated but loosely bound lowest (ss)¹ S^e and (pp)³ P^e states of H^- . In Sec. II, we summarize briefly the simple CI procedure in the central field approximation for a two-electron atom. Detailed breakdown of the individual contribution from various BB, BC, and CC configurations will be presented in Sec. III. The accuracy of our calculated wave functions is tested by examining the variation of the dipole length and dipole velocity oscillator strengths as well as the difference between them for transition from the ¹ S ground state of H^- to the lowest narrow ¹ P Feshbach resonance below the $n=2$

threshold as we increase the number of configurations in the CI calculation.

II. SIMPLE CONFIGURATION-INTERACTION PROCEDURE

The computational procedure employed in the simple CI calculation has been presented in detail earlier.^{19,21,22} For simplicity, we have chosen the hydrogenic one-electron orbitals for our H^- calculation. The set of finite one-electron radial functions $\chi_{\mu l}$ corresponding to an orbital angular momentum l satisfy the equation

$$h_l \chi_{\mu l} = \epsilon_{\mu l} \chi_{\mu l}, \quad (1)$$

where

$$h_l(r) = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} + \frac{1}{2} \frac{l(l+1)}{r^2}. \quad (2)$$

The function $\chi_{\mu l}$ corresponding to either negative or positive energy $\epsilon_{\mu l}$ is constructed from a set of B splines of order k and total number N confined between $r=0$ and $r=R$ following the procedure outlined earlier.²¹

Representing each two-electron configuration ($\mu l, \mu' l'$) is a configuration wave function $\Psi_{\mu l, \mu' l'}^{SL}(\mathbf{r}_1, \mathbf{r}_2)$ expressed in the LS coupling in terms of Slater determinant wave functions constructed from the one-electron hydrogenic orbitals

$$u_{\mu l m_s}(\mathbf{r}) = \frac{\chi_{\mu l}(r)}{r} Y_{lm}(\theta, \varphi) \sigma(m_s). \quad (3)$$

The Hamiltonian matrix element

$$\langle \Psi_{n_\mu l_\mu, n_\nu l_\nu}^{SL} | H | \Psi_{n_\delta l_\delta, n_\gamma l_\gamma}^{SL} \rangle$$

corresponding to a pair of configurations ($n_\mu l_\mu, n_\nu l_\nu$) and ($n_\delta l_\delta, n_\gamma l_\gamma$) is given in terms of the one-particle orbital energy eigenvalues $\epsilon_{\mu l}$ and the Coulomb matrix elements by an expression similar to Eq. (6) of Ref. 19. A straightforward diagonalization of the Hamiltonian matrix will then lead to the energy eigenvalue and the state wave function of an energy eigenstate. The theoretical oscillator strength is calculated with the procedure presented elsewhere.²⁷

Similar to our earlier calculations, the basis set consists of a number of two-electron configuration series $\mu l l'$. Each $\mu l l'$ series consists of a set of configuration wave functions $\Psi_{\mu l, \mu' l'}^{SL}$ corresponding to one electron in a fixed orbit μl and the other electron with orbital angular momentum l' but variable energy, both negative and positive, over an entire finite set of eigenfunctions of h_l given by Eq. (2). When the orbital μl is bound, a configuration series $\mu l l'$ includes only the BB and BC types of configurations. Such a configuration series is in effect equivalent to an open channel in the close-coupling calculation. The CC type of configuration is included in the $\mu l l'$ series when μl represents a positive energy orbital. In Sec. III, we present in detail the CI contribution due to the continuum-continuum configurations. The numerical accuracy of our calculation is assured by varying the values of N from 35 to 50, k from 7 to 9, and R from $170a_0$ to $230a_0$ for those B splines sets included in our

convergence test. The convergence of our numerical result as a function of increasing R confirms the effectiveness of the present procedure in circumventing the numerical difficulty discussed in Sec. I due to the use of analytic Coulomb functions for the positive-energy orbitals in a CI calculation.²⁰ For an energy convergence of 10^{-6} Ry or better, up to 90 configuration series (or approximately 1000 configurations) are included in our calculation. The present calculation is carried out on a SUN 4/260 work station.

III. RESULTS AND DISCUSSION

The energy eigenvalues for the 1S ground state of H^- , calculated with various combinations of configurations, are listed in Fig. 1. The calculated *electron affinity* (EA) is 0.0226 Ry, or approximately 41% of its expected value, when we include only the BB-type $1sns$ configurations. It increases to about 48% when the entire $1ss$ configuration series is included. A total of 0.0111 Ry in energy correction resulting from the BB-type $2pnp$ configurations (i.e., from -1.0266 to -1.0377 Ry) dominates the correlation energy. When the entire $2pp$ series is added to the $1ss$ series, EA increases to 0.0438 Ry or approximately 79% of its exact value. Contribution from a large number of BB-type configurations yields an energy of -1.0332 Ry (all BB). In theory, this result (approximately 60% of the expected value) represents the *converged* value from a TDM calculation such as the one carried out by Lipsky and co-workers.¹⁶ By expanding our basis set to include

Configurations	Energy Levels	
1sns	_____ -1.0226 Ry	
1ss	_____ -1.0266 Ry	
All BB	_____ -1.0332 Ry	BC contribution
1ss+2pnp	_____ -1.0377 Ry	
1ss+2pp	_____ -1.0438 Ry	
All BB+BC	_____ -1.0470 Ry	
All BB+BC+CC(p-wave only)	_____ -1.0521 Ry	CC contribution
All BB+BC+CC(s & p waves)	_____ -1.0533 Ry	
All BB+BC+CC	_____ -1.0554 Ry	

FIG. 1. The calculated energy eigenvalues for the 1S ground state of H^- with various combinations of configurations included in the basis functions. A detailed discussion is given in the text.

more configuration series nll' with bound nl orbitals (all BB+BC) until a convergence of 10^{-6} Ry is reached, we are able to account for approximately 85% of the electron affinity. Finally, by including the continuum-continuum basis functions with $l=l'=1$ [all BB+BC+CC (p wave only)], our calculation has shown that over 9% of the electron affinity can be attributed to the CC-type configurations from p wave alone. The numerical convergence is fairly slow as we include more CC-type configurations corresponding to larger l in our calculation. Eventually, with approximately 1000 configurations (about 90 configuration series, including some with l up to 5) and with the help of an extrapolating procedure, employed in our earlier fine-structure calculation for the He $1s4f$ states,²⁸ we obtain an EA value of 0.05540 Ry. This is very close to the most accurate value of 0.055502 Ry from the calculations with Hylleraas-type variational wave functions. In Table I, we compare some of the existing theoretical EA values. The result of the present calculation actually agrees slightly better with the exact value than the results from more elaborate MCHF (Ref. 14) and SOC (Ref. 15) calculations. The results from a few selected, numerically more convenient but quantitatively less accurate, calculations²⁹⁻³² are also listed for comparison. Similar to earlier calculations, no other 1S bound excited state is found in the present study.

Detailed breakdown of the energy contributions to the lowest $(pp)^3P^e$ state of H^- from various combinations of configurations is presented in Fig. 2. Our calculation has shown that this state is not bound if we only include the BB-type $2pnp$ configurations. A nearly identical energy eigenvalue is found when we include the entire $2pp$ configuration series. The BB-type $3dnd$ configurations or the complete $3dd$ configuration series are responsible for the largest energy corrections at 5.87×10^{-4} or 8.00×10^{-4} Ry, respectively. The calculated EA including contributions from a large number of BB-type configurations is 2.29×10^{-4} Ry, which is approximately 32% of the expected value at 7.094×10^{-4} Ry from the variational calculation by Bhatia.⁷ By including three dominant configuration series, i.e., $2pp$, $3pp$, and $3dd$, the calculated EA increases to about 73% of its expected

TABLE I. Comparison of the electron affinity (in 10^{-2} Ry) for the 1S ground state of H^- from selected theoretical calculations.

Theory	Electron affinity (10^{-2} Ry)
Present	5.540
Frankowski and Pekeris (Ref. 1)	5.5502
Freund, Huxtable, and Morgan III (Ref. 2)	5.5502
Thakkar and Smith, Jr. (Ref. 5)	5.5502
Midtald, Lyslo, and Aashamar (Ref. 6)	5.550
Froese Fischer (Ref. 14)	5.502
Weiss (Ref. 15)	5.502
Hawk and Hardcastle (Ref. 29)	5.492
Neto and Ferreira (Ref. 30)	5.490
Crance and Aymar (Ref. 31)	5.46
Wu and Tsai (Ref. 32)	5.326

Configurations	Energy Levels	
2pnp (2pp)	— -0.249632 Ry	
2pnp+3dnd	— -0.250119 Ry	
All BB	— -0.250229 Ry	
2pp+3dd	— -0.250432 Ry	BC contribution
2pp+3pp+3dd	— -0.250518 Ry	
All BB+BC	— -0.250615 Ry	CC contribution
All BB+BC+CC(d-wave only)	— -0.250658 Ry	
All BB+BC+CC	— -0.2507075 Ry	

FIG. 2. The calculated energy eigenvalues for the $(pp)^3P^e$ state of H^- with various combinations of configurations included in the basis functions. A detailed discussion is given in the text.

value. Additional BB- and BC-type configurations (all BB+BC) will increase the EA to about 87% of its expected value. Finally, with many CC-type configurations included, our calculation converges to a value of 7.075×10^{-4} Ry. The theoretical EA values from a few selected earlier calculations are listed in Table II for comparison. Our result agrees very well with the results from the variational calculations by Bhatia,⁷ Drake,⁸ and Holstien.³³ While the result of the variational perturbation calculation of Aashamar^{6,34} appears to have underestimated the electron affinity, the approximate value of 7.5×10^{-4} Ry from the adiabatic hyperspherical approximation¹⁰ is about 5.7% larger than the value of Bhatia.

In addition to the energy, we have examined the oscillator strength f of the dipole transition from the 1S ground state to the lowest 1P Feshbach resonance below

TABLE II. Comparison of the electron affinity (in 10^{-4} Ry) for the $(pp)^3P^e$ state of H^- from selected theoretical calculations.

Theory	Electron affinity (10^{-4} Ry)
Present	7.075
Bhatia (Ref. 7)	7.094
Drake (Ref. 8)	7.008
Holstien (Ref. 33)	7.020
Aashamar (Ref. 34)	6.536
Lin (Ref. 10)	7.5

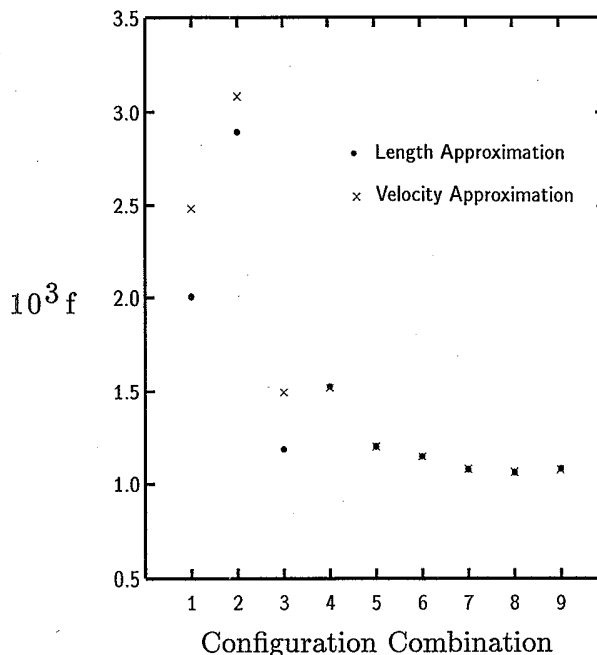


FIG. 3. The change of the calculated dipole oscillator strengths f (in 10^{-3}) in length (\bullet) and velocity (\times) approximations for the transition from the 1S ground state of H^- to the lowest 1P Feshbach resonance below the $n=2$ threshold with various configuration combinations included in the initial and final states. The configuration combinations are described in Table III.

the $n=2$ threshold. The width of this Feshbach resonance is of the order of 10^{-5} a.u., which suggests a weak coupling between the bound component of the state wave function and the $1s\epsilon p$ autoionization background channel.³⁵⁻³⁷ The change of the calculated oscillator strengths in length and velocity approximations is shown in Fig. 3 as we vary the configuration combinations included in the initial and final states listed in Table III. The f values range from 0.002 to 0.003 when the initial and final states of the transition are both limited to the BB-type configurations (e.g., combinations No. 1 and No.

TABLE III. The configuration combinations included in the initial and final states of the transition from the 1S ground state of H^- to the lowest 1P Feshbach resonance below the $n=2$ threshold. The variation of the calculated oscillator strengths is shown in Fig. 3.

Configuration combination	1S ground state	1P final state
1	$1sns + 2pnp$	$2snp + 2pns + 2pnd$
2	All BB	All BB
3	$1ss + 2pp$	$2sp + 2ps + 2pd$
4	All BB+BC	All BB+BC
5	All BB+BC+CC($l=1$)	All BB+BC
6	All BB+BC+CC($l=0-1$)	All BB+BC
7	All BB+BC+CC($l=0-2$)	All BB+BC
8	All BB+BC+CC($l=0-3$)	All BB+BC
9	All BB+BC+CC	All BB+BC+CC

2). Combination No. 3 shows that the f values decrease substantially when contributions from the BC-type configurations are included. The agreement becomes nearly perfect between the length and velocity results at approximately 1.53×10^{-3} when we exhaust the BB and BC-type configurations (combination No. 4) both in the initial and final states of the transition. The effect of the continuum-continuum type of configurations is clearly illustrated by the further decrease of the f values (e.g., combinations Nos. 5–8) when the CC-type configurations are gradually added to the initial state. The effect due to the CC-type configurations to the final state is very small. Our converged f value of approximately 1.08×10^{-3} is smaller than the previously reported value of 0.0013 from the complex-coordinate calculation by Wendoloski and Reinhardt,³⁵ which should converge to the present value if an enlarged basis is included. Our calculated energy of -0.252099 Ry for the lowest 1P Feshbach resonance below the $n=2$ threshold is in close agreement with the theoretical value of -0.252096 Ry by Wendoloski and Reinhardt³⁵ and the experimental excitation energy between 10.92 and 10.93 eV observed

by Bryant *et al.*³⁶

In summary, the present calculation has shown that the simple CI procedure with finite L^2 -basis set is capable of taking into account effectively the CI contribution from the CC-type configurations for a bound state. Applications of this approach to the bound excited states of more complex atomic systems have already been demonstrated in many of our recent structure calculations.^{21,22,26,28} The use of the complete set of the two-electron state wave functions generated from this simple CI procedure as the complete set of intermediate virtual states in a perturbation expansion has led also to recent successful theoretical calculation of the multiphoton ionization of Mg from its ground state.²³ Extension to the autoionization state embedded in the continuum is currently in progress.

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