

Doubly excited ridge states of atoms

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Doubly excited ridge states of atoms are states in which two electrons reach high and comparable excitations. Our goal is to calculate sequences for some of these states by using a wave function that treats the pair of electrons as a single entity in solving the two-electron Schrödinger equation in hyperspherical coordinates: R, α, θ_{12} . For double escape of slow electrons, the so-called Wannier theory predicts that the wave function will be concentrated in the region $\alpha = \pi/4, \theta_{12} = \pi$ (that is, $\mathbf{r}_1 = -\mathbf{r}_2$) and we expect something similar for the ridge states. By expanding the Schrödinger equation around these points and retaining the first nontrivial quadratic dependences in α and θ_{12} , we seek a solution in which the form of the wave function in these two variables is analytically determined as in the Wannier theory. The R dependence of this wave function is then handled numerically and differs from the double-escape solution only in the exponential decay appropriate for bound states. For $L=0$ a polynomial in R is included, giving the proper number of nodes for the solution. Numerical eigenvalues for autoionizing ridge states are calculated and compared with available results.

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I. INTRODUCTION

The understanding of the structure and properties of doubly excited states of atoms is one of the central problems in atomic physics today. An important motivation for their study is that they are prototypes of correlated systems. Doubly excited states of H^- and He have been subjected to extensive study in the past twenty years, most of it in the language of the independent-electron model. This model regards each electron as moving in the combined field of the nucleus and the field of the other electrons. The total wave function of a doubly excited state is then taken as a product of two one-electron wave functions. A single product is normally inadequate, so that a sum of such products (each one called a configuration) is taken to represent the wave function. At high excitations, the number of products of individual electron wave functions needed increases, making this description unwieldy and unsatisfactory due to the large number of configurations that need to be superposed. Our aim in this paper is to describe a subclass of high doubly excited states in which both electrons have comparable excitation, called doubly excited ridge states [1], through an alternative procedure which employs "pair" (two-electron) quantum numbers and a wave function for the electron pair [2,3]. Experimental data available for such states are very sparse [4] and conventional numerical configuration-interaction calculations in atomic physics are usually limited to a few members of a family of such ridge states [5,6].

One modification of a multiconfiguration Hartree-Fock scheme has given energy values in the He and H^- systems out to the first ten members counting from below [7]. Another theoretical approach, which works with joint coordinates called hyperspherical coordinates of the pair of electrons, has been applied to study doubly excited states [8,9]. Even though this approach has been successful in classifying such states and studying the nature of angular and radial correlations, it suffers from limita-

tions of not being free itself from independent-electron pictures; its numerical calculations, based on an adiabatic approximation as the starting point, are restricted to low members of the family. The coupling of hyperspherical adiabatic channels beyond about 8 makes the numerical effort prohibitive [10]. A description of doubly excited states as eigenstates of a diabatical potential [11] has reported the $^1S^e$ sequence of resonant states in H^- and He. This simple procedure can be extended to high excitations with no difficulties, but its generalization for nonzero total angular momentum (L) has not been reported yet. A study [12] which liberates itself totally from the independent-electron picture was applied to the double escape of two slow electrons, which is the counterpart of our problem on the other side of the double-ionization threshold. This study and later elaborations, which are known in the field as the Wannier theory for electron correlations, provide the framework for our approach to high doubly excited states. Our goal is to derive Rydberg sequences of doubly excited states directly from the Wannier theory, extending previous studies [13]. The Schrödinger equation is analyzed with a wave function for the electron pair, and pair quantum numbers are used for the description of the correlated two-electron pair [2,14]. Rydberg sequences of $^1S^e$ and $^1,3P^o$ states are calculated and compared with similar previous calculations [3] and accurate numerical calculations where available [7,10,15].

II. TWO-ELECTRON SCHRÖDINGER EQUATION IN HYPERSPHERICAL COORDINATES

The hyperspherical coordinates are defined as

$$\begin{aligned} R &= (r_1^2 + r_2^2)^{1/2}, \\ \alpha &= \arctan(r_2/r_1), \\ \theta_{12} &= \arccos(\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2). \end{aligned} \quad (1)$$

In atomic units ($\hbar=m_e=e=1$) the Schrödinger equation for the pair is

$$\left[\frac{1}{2} \left[-\frac{1}{R^{5/2}} \frac{\partial^2}{\partial R^2} R^{5/2} + \frac{\Lambda^2 + \frac{15}{4}}{R^2} \right] + \frac{C(\alpha, \theta_{12})}{R} \right] \psi = E\psi, \quad (2)$$

where

$$C(\alpha, \theta_{12}) = -\frac{Z}{\cos\alpha} - \frac{Z}{\sin\alpha} + \frac{1}{(1 - \sin 2\alpha \cos \theta_{12})^{1/2}}, \quad (3)$$

$$\Lambda^2 = \frac{l_1^2}{\cos^2\alpha} + \frac{l_2^2}{\sin^2\alpha} - \frac{1}{\sin\alpha \cos\alpha} \frac{\partial^2}{\partial \alpha^2} \sin\alpha \cos\alpha - 4.$$

In Eq. (2) the expression in square brackets represents the kinetic energy of the electron pair. As in the single-electron problem in polar coordinates, where the kinetic-energy operator is separated into radial and centrifugal parts (both inversely proportional to the squared radial coordinate r^2), here the kinetic energy of the pair can be separated into radial and centrifugal parts, replacing r by R and l^2 by Λ^2 ; Λ is called the grand angular-momentum operator.

$C(\alpha, \theta_{12})$ in Eq. (2) allows us to see radial and angular correlation aspects independent of R . This potential has a flat saddle at $\alpha = \pi/4$, $\theta_{12} = \pi$, and drops away from $\alpha = \pi/4$, having deeping valleys at $\alpha = 0$ and $\pi/2$. The valleys correspond to very unequal excitations of the two electrons. Doubly excited ridge states (with $E < 0$), where both electrons have similar excitations can occur only if the system stays in the vicinity of the saddle point. One expects a wave function highly concentrated in this region to describe such states. This is the motivation for expanding the potential in Eq. (2) around the saddle, with

$$\beta = \frac{\pi}{4} - \alpha, \quad (4)$$

$$\gamma = \pi - \theta_{12}.$$

For states with ${}^1S^e$ symmetry, where $l_1 = l_2$, Eq. (2) simplifies to

$$\left\{ -\frac{\partial^2}{\partial R^2} - \frac{1}{R^2} \left[\frac{\partial^2}{\partial \alpha^2} + \frac{1}{4} \right] + \frac{4}{\sin^2 2\alpha \sin \theta_{12}} \left[\sin \theta_{12} \frac{\partial}{\partial \theta_{12}} \right] \right\} + 2 \frac{C(\alpha, \theta_{12})}{R} - 2E \Big] \phi(R, \alpha, \theta_{12}) = 0, \quad (5)$$

with

$$\phi(R, \alpha, \theta_{12}) = R^{5/2} \sin(2\alpha) \psi(R, \alpha, \theta_{12}). \quad (6)$$

The term $C(\alpha, \theta_{12})$ is the combined Coulomb potential of the three charges and $\phi(R, \alpha, \theta_{12})$ is a scaled version of the wave function $\psi(R, \alpha, \theta_{12})$, designed to remove first-derivative terms in R and in α in Eq. (5). We are using atomic units and first we will restrict ourselves to 1S states. Symmetry aspects of other values of total orbital

(L) and spin (S) angular momentum in the Wannier theory have been fully treated elsewhere [16], and will be incorporated into our study at the end of Sec. III. But, for studying the essential features of angular correlations between electrons, it is sufficient and advantageous to restrict ourselves first to the simplest values, $L = S = 0$. When all terms in Eq. (5) are expanded in powers of γ and β around the saddle region, we have

$$\left\{ -\frac{\partial^2}{\partial R^2} - \frac{1}{R^2} \left[\frac{\partial^2}{\partial \beta^2} + \frac{1}{4} \right] + 4(1 + 4\beta^2) \left[\frac{\partial^2}{\partial \gamma^2} + \left[\frac{1}{\gamma} - \frac{\gamma}{3} \right] \frac{\partial}{\partial \gamma} \right] \right\} - \frac{2}{R} \{ Z_0 + Z_\alpha \beta^2 - Z_\theta \gamma^2 \} + 2E \Big] \phi(R, \beta, \gamma) = 0, \quad (7)$$

with

$$\phi(R, \beta, \gamma) = R^{5/2} (1 - 2\beta^2) \psi(R, \beta, \gamma), \quad (8)$$

$$Z_0 = 2\sqrt{2} \left(Z - \frac{1}{4} \right),$$

$$Z_\alpha = 3\sqrt{2} \left(Z - \frac{1}{12} \right), \quad (9)$$

$$Z_\theta = \frac{\sqrt{2}}{16}.$$

The parameter Z_0 is an effective charge for the motion in R , whereas Z_α and Z_θ have dual roles as effective charges (because of the $1/R$ they multiply) and as harmonic-oscillator spring constants (because of the β^2 and γ^2 they multiply).

By inspecting the potential in Eq. [13], we see that it consists of a harmonic-oscillator term (γ^2/R) and an antiharmonic-oscillator term ($-\beta^2/R$) and a Coulomb form in R . Based on the ground-state wave function of the first two potentials and the zero-energy wave function of the Coulomb potential [13], the solution of Eq. (7) should be of the form

$$e^{-\sqrt{R}(A\beta^2 + B\gamma^2 + C)}. \quad (10)$$

This form is the key structure in Wannier theory describing the escaping pair and also will be adopted in the doubly excited ridge state study. The constants A , B , and C are fixed through the requirement that all terms involving $1/R$ are accounted for when Eq. (10) is substituted into Eq. (7), leaving behind only terms of higher order of smallness in $R^{-1/2}$.

III. CONSTRUCTION OF THE WAVE FUNCTION

A. ${}^1S^e$ states

As a first step in this calculation, we next consider that the wave function must include a power of $R^2(1 - 2\beta^2)$. This is a phase-space factor introduced for eliminating first derivatives in R , so that all wave functions have a multiplicative factor

$$r_1 r_2 = R^2 \cos\alpha \sin\alpha \cong R^2 (1 - 2\beta^2).$$

TABLE I. Values of energy of $1S^e$ doubly excited ridge states in H^- obtained from Eq. (17) (wave function including a polynomial in R) and Eq. (13) (nodeless wave function) compared with a similar previous calculation [3] and with accurate numerical calculations [7,15] for manifolds $\nu=4$ to 11.

ν	$-E_i$ (a.u.)				
	Eq. (17) (with nodes)	Eq. (13) (no nodes)	Ref. [3]	Ref. [15]	Ref. [10]
4	0.040 69	0.040 26	0.032 72	0.039 64	0.039 92
5	0.025 08	0.026 08	0.021 79	0.025 70	0.026 02
6	0.016 98	0.018 02	0.015 43	0.018 01	0.018 21
7	0.012 24	0.013 11	0.011 46	0.013 32	0.013 53
8	0.009 24	0.009 94	0.008 83	0.010 28	0.010 42
9	0.007 21	0.007 78	0.007 02	0.008 13	0.008 27
10	0.005 79	0.006 25	0.005 69		
11	0.004 74	0.005 13	0.004 71		

The simplest choice, therefore, for a bound state would build in the above two ingredients and an exponential falloff. On the other hand, if we consider lower-lying bound states of two-electron atoms, a reasonable zero-order wave function is

$$\exp\{-Z[(r_1+r_2)/n]\},$$

but, as is well known [17], such a function does not give binding in the negative ion H^- . One way to proceed to get this binding is to include explicitly the coordinate r_{12} through, for instance, a factor $\exp(\lambda r_{12})$, so as to introduce radial correlation between the two electrons. Translating this structure to the hyperspherical-coordinate system, we have $\exp[R(a\beta^2+b\gamma^2)]$. Combining, therefore, this structure as suggested by the lower end of the spectrum with the earlier structure suggested by Wannier theory for double escape, and, therefore, for the higher end of the spectrum, we choose as our basic ansatz:

$$\psi(R, \beta, \gamma) = [R^2(1-2\beta^2)]^{\nu-1} e^{-R/R_0} \times e^{-\sqrt{R}(A\beta^2+B\gamma^2+C)} e^{R(a\beta^2+b\gamma^2)}. \quad (11)$$

In this expression ν is a principal quantum number, conjugate to R (just as n goes with r in a one-electron problem), and R_0 is a variational parameter that gives the effective radial extent of the doubly excited state.

The coefficients A , B , C , a , and b are fixed analytically by substituting the wave function given by Eq. (11) into

the Schrödinger equation expanded around the saddle, Eq. (7) and canceling consistently all terms involving $1/R$ (including terms like β^2/R and γ^2/R) and β^2 and γ^2 , leaving behind terms in higher power of $1/R$. Several alternatives were explored and the best choice is

$$\begin{aligned} C &= 0, \\ A &= \pm i \left[\frac{3\sqrt{2}}{2} (Z - \frac{1}{2}) + \left[\frac{3\nu - 17}{2 - 4} \right] \frac{1}{R_0} \right]^{1/2}, \\ B &= \pm \frac{i}{4} \left[\frac{\sqrt{Z}}{8} + \frac{1}{2R_0} \left[\nu - \frac{5}{24} \right] \right]^{1/2}, \\ a &= \frac{1}{2R_0}, \\ b &= \frac{1}{8R_0}. \end{aligned} \quad (12)$$

For the range of R_0 , in which E has a minimum, A and B are imaginary. Using these values, we multiply by ψ^* and carry out the integration over the three hyperspherical coordinates, obtaining

$$\begin{aligned} E_\nu(R_0) &= \frac{4\nu-1}{2(4\nu+1)} \frac{1}{R_0^2} - \frac{2Z_0}{(4\nu+1)} \frac{1}{R_0} \\ &+ \frac{16 \left[\frac{9}{5} - \frac{2\nu}{3} \right]}{(4\nu-1)(4\nu+1)} \frac{1}{R_0^2}. \end{aligned} \quad (13)$$

TABLE II. The same as Table I, but for He.

ν	$-E_i$ (a.u.)				
	Eq. (17) (with nodes)	Eq. (13) (no nodes)	Ref. [3]	Ref. [15]	Ref. [10]
4	0.2215	0.2192	0.1861	0.2010	0.2012
5	0.1365	0.1421	0.1226	0.1294	0.1303
6	0.0924	0.0983	0.0863	0.0903	0.0908
7	0.0666	0.0716	0.0638	0.0638	0.0675
8	0.0503	0.0543	0.0490		
9	0.0393	0.0425	0.0388		
10	0.0315	0.0341	0.0319		
11	0.0258	0.0280			

This expression has a minimum for $R_0 \cong (2\nu - \frac{1}{2})/Z_0$.

Evaluation of this minimum for different manifolds is shown in Tables I and II, for $Z=1$ and 2, respectively. These results are compared with accurate numerical calculations [10,15] and with previous similar work [3] that did not include a and b .

These wave functions are fairly successful for calculating some of the energies of these ridge states, but the absence of nodes in the variable R makes them unsuitable for describing the whole family of states for a given L and S . This is similar to calculating the energy levels of the hydrogen atom with only the spectral sequence $1s, 2p, 3d$, etc., that is, with no nodes in r . Although the energies are correctly obtained, the wave functions do not describe the s state sequence of hydrogenic states ns . A better wave function can be built by including a polynomial in R , of degree $2(\nu-1)$, which has the proper numbers of nodes for such states.

Maintaining the same angular structure, the improved wave function is

$$\begin{aligned} \psi_\nu(R, \beta, \gamma) &= \sum_{i=1}^{2\nu-1} a(i, \nu) R^{5/2+i-1} (1-2\beta^2) \\ &\quad \times e^{-R/R_0 - \sqrt{R}(A\beta^2 + B\gamma^2 + c) + R(a\beta^2 + b\gamma^2)} \\ &= \sum_{i=1}^{2\nu-1} a(i, \nu) F(i, \nu), \end{aligned} \quad (14)$$

with

$$\begin{aligned} F(i, \nu) &= R^{5/2+i-1} (1-2\beta^2) \\ &\quad \times e^{-R/R_0 - \sqrt{R}(A\beta^2 + B\gamma^2 + C) + R(a\beta^2 + b\gamma^2)}, \end{aligned} \quad (15)$$

where A, B, C, a , and b are determined analytically, in the same way as before, to satisfy the leading $1/R$ dependences in the Schrödinger equation. For this new form $\psi_\nu(R, \beta, \gamma)$ in Eq. (14), it is not possible to get a simple variational expression for $E_\nu(R_0)$ like the one given by Eq. (13) in the previous step. For solving the eigenvalue problem

$$H\psi_\nu(R, \beta, \gamma) = E_\nu \psi_\nu(R, \beta, \gamma), \quad (16)$$

it is necessary to evaluate the $a(i, \nu)$ values in the polynomial. This is done by transforming the eigenvalue problem of Eq. (16) into a generalized eigenvalue problem, expanding $\psi_\nu(R, \beta, \gamma)$ in terms of $F(i, \nu)$, multiplying by $F^*(j, \nu)$, and integrating,

$$\begin{aligned} H\psi_\nu(R, \beta, \gamma) &= E_\nu \psi_\nu(R, \beta, \gamma), \\ \sum_{i=1}^{2\nu-1} H(j, i) a(i, \nu) &= E_\nu \sum_{i=1}^{2\nu-1} S(j, i) a(i, \nu), \end{aligned} \quad (17)$$

with

$$\begin{aligned} H(j, i) &= (F(j, \nu), HF(i, \nu)) = \int F^*(j, \nu) HF(i, \nu) d\tau, \\ S(j, i) &= (F(j, \nu), F(i, \nu)) = \int F^*(j, \nu) F(i, \nu) d\tau. \end{aligned} \quad (18)$$

Equation (17) represents a generalized eigenvalue problem, where H and S are known, and its solution will give $(2\nu-1)$ values for E_ν and their respective a_ν . The highest of these eigensolutions is the one which corresponds to the energy of the manifold with principal quantum number ν . Its corresponding eigenvector contains the coefficients for the different powers of R in the polynomial. For each manifold (ν) , E_ν is numerically minimized through the variational parameter R_0 . The result of this work is also included in Tables I and II for H^- and He, respectively.

B. $L=1$ states

In dealing with $L \neq 0$ states the complexity increases both in the structure of the wave function and in the Schrödinger equation. In this approach of working with R, β , and γ in the saddle, the increased complexity for the wave function is reduced to the introduction of a multiplicative factor $f(\beta, \gamma)$, acting on the expression given by Eq. (11). This multiplicative factor gives the symmetry characteristic of the $\{L, S, \pi\}$ state. The study of these multiplicative factors, in the context of the Wannier theory, has been done [16] for different symmetries of continuum states. Similar considerations apply for bound states because continuum and bound states share the same angular and spin behavior. For symmetries of interest to us, the factor $f(\beta, \gamma)$ is [3]

$$f(\beta, \gamma) = \begin{cases} 1 & \text{for } {}^3P^o(A=+) \\ \gamma & \text{for } {}^1P^o(A=+) \text{ and } {}^3P^e \\ \beta & \text{for } {}^1P^o(A=-) \\ \beta\gamma & \text{for } {}^1P^e \text{ and } {}^3P^o(A=-). \end{cases} \quad (19)$$

With regard to the modification of the two-electron Schrödinger equation for non- $L=0$ states, the mixing of the Euler angles with the coordinates r_1, r_2 , and θ_{12} , leads to extra terms in the Schrödinger equation (5). This extra contribution to the Schrödinger equation in the saddle region has been calculated by Wong [3] and he reduced it to an additional term C_3/R^2 in Eq. (7), with

$$\begin{aligned} C_3 &= -4(1-4\beta^2) \left[\frac{1}{\gamma^2} + \frac{1}{3} \right] \text{ for } {}^3P^e, \\ C_3 &= 4(1-2\beta+4\beta^2) \left[\left[\frac{1}{\gamma} - \frac{\gamma}{3} \right] \frac{\partial}{\partial \gamma} - 1 \right] \\ &\quad \mp 4(1+2\beta+4\beta^2) \left[\frac{1}{\gamma} + \frac{\gamma}{6} \right] \frac{\partial}{\partial \gamma} \\ &\quad \text{for } {}^1P^o(A=\pm) \text{ and } {}^3P^o(A=\mp). \end{aligned} \quad (20)$$

The extension to non- $L=0$ states can be accomplished by adding the above term, given by Eq. (20), to the two-electron Schrödinger equation [18], modifying the $L=0$ wave function by the multiplicative factor $f(\beta, \gamma)$, given by Eq. (19), and proceeding with the same methodology used in the ${}^1S^e$ calculation.

IV. RESULTS AND DISCUSSION

Sequences of ridge states calculated with these pair-basis wave functions are presented in Tables I–IV where they are compared with available results. In Fig. 1, $E^{-1/2}$ is represented as a function of ν for states $^1S^e$ and $^{1,3}P^o(A=+)$ for H^- . This graph shows that these energy values conform well with the six-dimensional Rydberg formula that has been suggested for the Wannier ridge states [19],

$$E = - \frac{[2\sqrt{2}(Z - \frac{1}{4} - \bar{\sigma})]^2}{2(\nu + \frac{3}{4} - \bar{\mu})^2}, \quad (21)$$

thereby providing a theoretical justification for this formula and a physical significance for $\bar{\sigma}$ which is seen to reflect the β^2 and γ^2 dependences in Eq. (7).

For $^1S^e$ states, we have calculated these sequences twice. The first one, with a nodeless wave function in R , is a simple calculation that gives us an analytical expression, Eq. (13), for the energy as a function of the principal quantum number (ν). Thus, the energy for doubly excited states with high ν values can be evaluated with no extra complications. This advantage is shared with Wong's calculation [3], which is similar to ours but does not include the exponential term $e^{R(a\beta^2 + b\gamma^2)}$ and has a different selection of the constants A , B , and C generating energy values less deep than ours. Our results in the second calculation, when we introduce the polynomial in R , shows

TABLE III. Values of energy for $L=1$ doubly excited ridge states in H^- obtained from equations equivalent to Eq. (13) for each symmetry and compared with previous similar calculations and accurate numerical calculations.

ν	This work	Ref. [3]	Ref. [15]	Ref. [10]
$^1P^o(A=+)$ $-E_\nu$ (a.u.)				
4	0.0352	0.0332	0.0372	0.0374
5	0.0234	0.0224	0.0246	0.0246
6	0.0165	0.0160		0.0174
7	0.0122	0.0119		0.0130
8	0.0093	0.0092		0.0101
9	0.0074	0.0073		0.0080
10	0.0059	0.0059		
$^1P^o(A=-)$ $-E_\nu$ (a.u.)				
4	0.021			
5	0.015			
6	0.012			
7	0.009	0.0104		
8	0.007	0.0081		
9	0.006	0.0067		
10	0.005	0.0055		
$^3P^o(A=+)$ $-E_\nu$ (a.u.)				
4	0.028 85	0.03251		
5	0.0193	0.02163		
6	0.0138	0.01538		
7	0.0103	0.01141		
8	0.0080	0.00881		
9	0.0064	0.00699		
10	0.0052	0.00056		
$^3P^o(A=-)$ $-E_\nu$ (a.u.)				
4	0.0242	0.03228		
5	0.0181	0.02150		
6	0.0138	0.01526		
7	0.0107	0.01132		
8	0.0084	0.00876		
9	0.0068	0.00695		
10	0.0056	0.00566		

good agreement with elaborate calculations—assumed the most accurate calculations available [7,15]. In this calculation, the energies for each manifold are obtained through the solution of the generalized eigenvalue problem, given by Eq. (17). Here we calculated the simplest cases ($L=0,1$) as a part of an attempt to provide a new basis for calculating pair ridge states. In the future, to continue with this study we must extend similar calculations to other states with higher angular momentum ($L > 1$) and we have to improve the wave function, in the same way as we did for zero angular momentum, introducing a polynomial in R as a part of the structure of the wave function. With a more reliable wave function and having extended these calculation to states $\{L,S,\pi\}$ in general, we can then expect to calculate matrix elements of the electric dipole operator between the pair wave functions to obtain transition rates between these states.

We have developed a consistent pair description of doubly excited states, as states converging to the double-ionization limit. There is fairly good agreement between

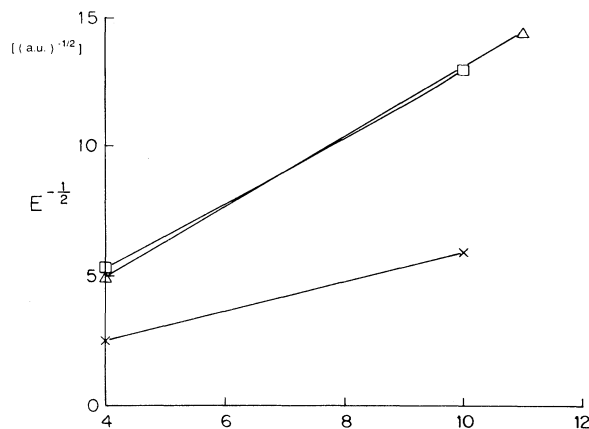


FIG. 1. The inverse of the root squares of the energy ($E^{-1/2}$) of doubly excited ridge states in H^- is represented as a function of the principal quantum number (ν) for several symmetries: [$\Delta=^1S^e$, $X=^3P^o(A=+)$, $\square=^1P^o(A=+)$].

TABLE IV. The same as Table III, but for He.

ν	This work	Ref. [3]	Ref. [7]
$^1P^o(A=+)$			
$-E_\nu$ (a.u.)			
4	0.1915	0.1887	0.1948
5	0.1274	0.1268	0.1267
6	0.0898	0.0892	0.0890
7	0.0663	0.0661	0.0659
8	0.0508	0.0508	0.0507
9	0.0401	0.0401	0.0402
10	0.0324	0.0324	0.0327
$^1P^o(A=-)$			
$-E_\nu$ (a.u.)			
4	0.113		
5	0.084		
6	0.064		
7	0.050	0.0439	
8	0.040	0.0422	
9	0.032	0.0325	
10	0.027	0.0287	
$^3P^o(A=+)$			
$-E_\nu$ (a.u.)			
4	0.1571		
5	0.1050		
6	0.0750		
7	0.0562		
8	0.0436		
9	0.0439		
10	0.0285		
$^3P^o(A=-)$			
$-E_\nu$ (a.u.)			
4	0.1316		
5	0.0987		
6	0.0749		
7	0.0580		
8	0.0459		
9	0.0370		
10	0.0304		

our results and elaborate numerical calculations at low excitations. Our study was not designed to compete in numerical accuracy with these calculations, but rather to develop a different basis based on a pair description, which becomes more appropriate at high excitations for ridge states. Conventional numerical calculations are much more quantitatively accurate at lower excitations, but cannot be readily extended to higher states because of an explosion in the number of configurations that need to be included. The pair description is adapted to describing this region near the double-ionization limit because it

explicitly builds in analytically the angular and radial correlations that dominate in this limit.

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