

## Calculation of autoionization widths for two-electron systems

Lester Lipsky

*Department of Computer Science and Department of Physics, University of Nebraska, Lincoln, Nebraska 68588*

M. J. Conneely

*Department of Mathematical Physics, University College, Galway, Ireland*

(Received 21 January 1976)

A procedure is used which combines the truncated diagonalization method with the open-channel close-coupling approximation in the calculation of widths of autoionization states in two-electron systems. The method is capable of systematically and efficiently calculating the widths for all two-electron systems. Calculations are made for  $^1P^o$  and  $^3P^o$  helium, and  $^1P^o$  hydrogen below the  $N = 2$  threshold. In particular, it is found that the lowest member of the third series [classified as (2,3c)] has a width of  $4.61 \times 10^{-7}$  eV, four times smaller than any previous calculation. It is also shown that the (+)(-) classification used by many authors is inadequate to describe these states. Detailed comparison is made with the three- and six-state close-coupling and other calculations.

### I. INTRODUCTION

The doubly excited states of two-electron systems are fairly well understood qualitatively, but the energies and lifetimes of most of these levels are not known in detail. Although the intensities and shapes of resonances caused by the existence of such doubly excited states depend strongly on the type of process considered (e.g., electron-atom collisions, atom-atom collisions, photoionization, etc.), the characteristic widths (or, equivalently, lifetimes) and positions are virtually independent of the particular process. A general knowledge of the energies and lifetimes of these autoionization states is needed by experimentalists in order to identify the peaks and valleys seen in their electron and photon spectra.

In this paper we describe a calculation which combines the truncated diagonalization method (TDM)<sup>1</sup> and the open-channel close-coupling (CC) approximation<sup>2</sup> to evaluate the autoionization widths of all doubly excited two-electron systems. We then discuss the results of applying this method to  $^1P^o$  and  $^3P^o$  helium, and to the  $^1P^o$  configuration for the hydrogen negative ion. Preliminary results for the widths were first presented in Ref. 3. The energies and wave functions for all two-electron systems with nuclear charge less than or equal to 5 have been discussed and tabulated elsewhere.<sup>4</sup>

Although there have been many calculations made on various systems which have been relatively successful, they are not well suited for general use because either they fail in their attempts to calculate narrow resonances, or they are very difficult and costly to use (e.g., the close-coupling method), or because they become

increasingly difficult to apply to higher members of any series. In this paper we see that previous works have failed to predict correctly the positions and/or widths of the second and third Rydberg series in  $^1P^o$  helium because not enough configurations (e.g., the  $3dkf$ ) have been included. In effect, the angular correlations between electrons have not been sufficiently accounted for. The width of the lowest member of the third series [previously classified as  $2p3d$ , but here called (2,3c) because it is 60%  $sp$ ] is too narrow to be calculated without careful numerical analysis of the procedure. We find this width to be  $4.608 \times 10^{-7}$  eV, about  $\frac{1}{4}$  the width reported by Burke and McVicar.<sup>5</sup> It is known that generally the widths calculated in the close-coupling approximation are highly dependent on the step size used, especially for narrow resonances; thus a numerical study of this dependence should be made, especially with the  $3dkf$  channel included.

### II. METHOD

Consider the problem of an electron elastically scattering off an atomic system of one electron and a nucleus with charge  $Z$ . In the static exchange approximation<sup>2</sup> (which is the same as the close-coupling approximation with only one channel), the wave functions satisfy the conditions:

$$\langle \psi_E | H | \psi_{E'} \rangle = E \delta(E - E'), \quad (1a)$$

$$H = \frac{1}{2m_e} (P_1^2 + P_2^2) - Ze^2 \left( \frac{1}{r_1} + \frac{1}{r_2} \right) + \frac{e^2}{r_{12}}, \quad (1b)$$

where

$$\psi_E(1, 2) = C [R_{1s}(1)F_E(2)Y_l^m(2) \pm R_{1s}(2)F_E(1)Y_l^m(1)] \quad (2)$$

and  $R_{1s}$  is the hydrogenic  $1s$  wave function for charge  $Z$ . The  $F_E$ 's are the continuum functions satisfying the differential equation

$$\frac{\hbar^2}{2m_e} \left( \gamma^{-2} \frac{d}{dr} \gamma^2 \frac{d}{dr} + k^2 - \frac{2m_e}{\hbar^2} Y_0(1s, 1s | \gamma) \right) F_E \\ \mp \left( E_0 - \frac{\hbar^2 k^2}{2m_e} \delta_{i_0} \langle 1s | F_E \rangle + Y_i(1s, F_E | \gamma) \right) R_{1s} = 0. \quad (3)$$

The  $Y$ 's are the usual Slater integrals over  $1/\gamma_{12}$ , which are defined below in Eq. (10).

Solving Eq. (3) for all energies is equivalent to finding the eigenfunctions of the operator  $PHP$  for the projection operator  $P$  given by O'Malley, and co-workers.<sup>6,7</sup> Briefly,  $P$  is the operator which projects all two-electron functions onto the subspace in which one of the electrons is in the  $1s$  state with nuclear charge  $Z$ . Such an operator is Hermitian and idempotent ( $P^2 = P$ ), and is called a "projection operator." The  $\psi_E$ 's which satisfy Eqs. (2) and (3) have the property that  $P\psi_E = \psi_E$  and, because Eq. (3) is derived from a variational principle, are eigenfunctions of  $PHP$ . If one includes the possible bound-state solutions of Eqs. (3), then these  $\psi_E$ 's are all the nonzero eigenfunctions of  $PHP$ .

The projection operator  $Q = I - P$  defines the Hamiltonian  $QHQ$ , whose eigenvalues can be interpreted as the energy positions of doubly excited states of the two-electron system. Many authors<sup>1,4,7-9,11</sup> have solved for approximate eigenfunctions of  $QHQ$  by variational methods. We, in particular, have used the truncated diagonalization method (TDM)<sup>1,3,4</sup> with no  $|1snl\rangle$  configurations included. Briefly, the TDM is a particular application of the Feshbach formalism<sup>10</sup> whereby (1)  $Q$  space is defined in terms of an orthonormal set of square-integrable basis functions made from products of one-electron orbitals; (2) the basis functions are separately asymptotically orthogonal to the relevant adjacent continua. Hydrogenic functions are used here because they provide uniformly accurate information (albeit incomplete) about an entire series instead of just its lowest member(s). After all, these functions have mean radii which are proportional to  $n^2$ , just as the true functions have, whereas Sturmians for instance are proportional to  $n$ .

When  $|1snl\rangle$  configurations are not used, the TDM calculations become consistent with the Hahn, O'Malley and Spruch<sup>6,7</sup> realization of the Feshbach formalism, and the equations to be solved are simpler than they would be if such basis functions were included. We feel that no useful information is lost by deviating from the Lipsky-Russek formulation and adhering to the

more conventional one.

The TDM calculations give a discrete set of wave functions  $\phi_n$ , with energy levels  $E_n$  below the  $N=2$  threshold. The  $\phi_n$ 's satisfy the conditions

$$Q\phi_n = \phi_n, \\ \langle \phi_n | QHQ | \phi_m \rangle = E_n \delta_{nm} = \langle \phi_n | H | \phi_m \rangle, \quad (4)$$

and themselves can be written as

$$\phi_n = \sum_j a_{nj} \mathfrak{u}_j, \quad (5a)$$

where

$$\mathfrak{u}_j = (1/\sqrt{2}) [R_{n_1 l_1}(1) R_{n_2 l_2}(2) Y_{L_1 l_1}^M(\hat{1}, \hat{2}) \\ \pm R_{n_2 l_2}(1) R_{n_1 l_1}(2) Y_{L_1 l_1}^M(\hat{2}, \hat{1})], \quad (5b) \\ Y_{L_1 l_1}^M(\hat{1}, \hat{2}) = \sum_{m_1} (l_1 l_2 L | m_1 M - m_1) Y_{l_1}^{m_1}(\hat{1}) Y_{l_2}^{m_2}(\hat{2}), \quad (5c)$$

where  $(l_1 l_2 L | m_1 m_2 M)$  is the Clebsch-Gordan coefficient, and  $Y_l^m$  is the spherical harmonic defined in Rose.<sup>12</sup>

The sets of functions  $\psi_E$  and  $\phi_n$  together are the eigenfunctions of the Hamiltonian

$$H_0 = PHP + QHQ. \quad (6a)$$

The total two-electron Hamiltonian can be written as

$$H = H_0 + V, \quad (6b)$$

where

$$V = PHQ + QHP. \quad (6c)$$

In comparing with Fano,<sup>13</sup> we see that  $\psi_E$  and  $\phi_n$  satisfy his Eqs. (1a) and (1c), where the  $\phi_n$ 's are the discrete states imbedded in the continuum of the  $\psi_E$ 's. We define  $V_n(E)$  by the following integral:

$$V_n(E) = \langle \psi_E | V | \phi_n \rangle = \langle \psi_E | PHQ + QHP | \phi_n \rangle \\ = \langle \psi_E | \frac{e^2}{r_{12}} | \phi_n \rangle \\ = \int \int \psi_E^*(1, 2) \frac{e^2}{r_{12}} \phi_n(1, 2) d^3 r_1 d^3 r_2 \\ = \sum a_{nj} \mathfrak{v}_j(E) \quad (7a)$$

with

$$\mathfrak{v}_j(E) = \int \int \psi_E^*(1, 2) \frac{e^2}{r_{12}} \mathfrak{u}_j(1, 2) d^3 r_1 d^3 r_2. \quad (7b)$$

The width of the  $n$ th state can then be calculated by

$$\Gamma_n = 2\pi |V_n(E_n)|^2. \quad (8)$$

This formula is strictly true only if the  $n$ th state is well separated from all other levels. We might consider two levels to be "well separated" if the sum of their widths divided by the difference of their energies is very small in magnitude. As it turns out, this ratio is always less than 0.032 for all pairs of states quoted here, and for the two closest series (the  $b$  and  $c$  series in  $^1P^o$ ) this ratio is one-sixth as great.

Note that the  $\mathcal{U}_j$ 's are integrals over the product functions  $\mathcal{U}_j$ , whereas the  $V_n$ 's are sums of  $\mathcal{U}_j$ 's, or integrals over the actual eigenfunctions of  $QHQ$ . (Compare Fig. 1 with Figs. 2, 3, and 4 below.)

If the resonances below the  $N=3$  threshold are to be examined, then the appropriate projection operator  $\bar{P}$  to be used projects onto the  $1s$ ,  $2s$ , and  $2p$  states. The eigenfunctions  $\psi_{iE}$  of  $\bar{P}H\bar{P}$  in this case are the functions of the close-coupling three-state calculations. The eigenfunctions  $\phi_n$  of  $\bar{Q}H\bar{Q}$ , as before, can be approximated by the TDM where all configurations which include a  $1s, 2s$ , or  $2p$  function are excluded. The partial autoionization widths can be evaluated by

$$\Gamma_{in} = 2\pi |\langle \psi_{iE_n} | V | \phi_n \rangle|^2, \quad (9a)$$

where  $i$  labels the exit channel. The total width is the sum of the three widths,

$$\Gamma_n = \sum_{i=1}^3 \Gamma_{in} \quad (9b)$$

This method has several attractive features. In particular, the TDM can be used to get approximations of  $QHQ$  using an arbitrarily large basis set, with many different configurations (in this paper, for  $^1, ^3P^o$ , 83 configurations were used), with relative ease. Of course, owing to the fact that the discrete set of hydrogenic functions is incomplete, the TDM can never fully describe the radial correlations between the electrons, although the angular correlations are well accounted for. The radial correlations are important only if there is a significantly high probability that both electrons will be near the nucleus at the same time, such as in the case of the  $(1s^2)^1S$  ground state of isohelium.

### III. DESCRIPTION OF CALCULATION

The calculation of widths of autoionization states by Eq. (8) was carried out for the dozen or so lowest singlet and triplet  $P$  odd states below the  $N=2$  threshold in helium, and for the lowest  $^1P^o$  state for the hydrogen negative ion. The calculation is actually made up of three separate parts. The first part involves solving Eq. (3) numerically for  $F_E$  at several different energies.

This type of calculation has been discussed many times,<sup>2</sup> and nothing need be said about it further except that the phase shifts here agreed with the literature to within four places, and the interval step size used was small enough so that six-place stability of the wave functions  $F_E$  seemed assured.

The second step involves finding the eigenfunctions of  $QHQ$ , using the TDM. An enumeration of the 83 basis functions used here is significant. They were  $2s2p$  to  $2s10p$ ,  $3s2p$  to  $10s2p$ ,  $2p3d$  to  $2p10d$ ,  $3s3p$  to  $3s10p$ ,  $4s3p$  to  $10s3p$ ,  $3p3d$  to  $3p10d$ ,  $4p3d$  to  $10p3d$ ,  $3d4f$  to  $3d10f$ ,  $4s4p$  to  $4s6p$ ,  $5s4p$ ,  $6s4p$ ,  $4p4d$  to  $4p6d$ ,  $5p4d$ ,  $6p4d$ ,  $4d4f$  to  $4d6f$ ,  $5d4f$ ,  $6d4f$ ,  $4f5g$ ,  $4f6g$ ,  $5s5p$ ,  $5p5d$ ,  $5d5f$ ,  $5f5g$ . This represents a larger basis set than carried out in the past,<sup>1,9</sup> and is the same as that quoted by Bruch *et al.*<sup>14</sup> for  $Li^+$ , and Anania *et al.*<sup>4</sup> generally.

It is not easy to compare this calculation with the CC calculations, since the TDM is superior to the three-state CC approximation in that it contains more channels (e.g.,  $3skp$ ,  $ks3p$ ,  $3pkd$ , etc.), but is inferior in that the latter contains the equivalent of higher configurations such as  $2s11p$ , etc., including the continua (e.g.,  $2skp$ ). However, comparison of results from the two methods in which the same channels are represented, where such data is available, shows agreement of the resonant energy positions to within 0.01 eV, and in many cases the agreement is 20 times closer. This point will be discussed further in Sec. VI below.

The third step of the calculation requires bringing together the first two steps, in order to evaluate Eqs. (7) and (8), for each resonant energy considered. This involves a numerical integration of the function  $F_E$ , with each of the many different Slater integrals of the form  $Y_l(1s, n_1 l_1 | r) \times R_{n_2 l_2}(r)$ , where

$$Y_l(1s, nl | r) \equiv \frac{2l+1}{r^{l+1}} \int_0^r R_{1s}(r') R_{nl}(r') r'^{l+2} dr' + (2l+1)r^l \int_r^\infty \frac{R_{1s}(r') R_{nl}(r') dr'}{r'^{l-1}}. \quad (10)$$

The  $Y_l$ 's can be expressed analytically as products of exponentials with a finite sum of powers of  $r$ . The coefficients of the powers of  $r$  must be evaluated carefully since they in turn are made up of alternating sums of rational numbers. An indiscriminate summation could introduce large roundoff errors, which would destroy the accuracy of the entire calculation.

The three steps together take about 20 minutes of processor time on an IBM 360/65 computer for

each energy  $E$ . Most of the time is consumed in step three (step two is the same for all energies and need not be repeated). Although Eq. (8) is defined at each resonant energy, it was decided to evaluate  $V_n(E)$  and  $v_j(E)$  at three energies only: at the lowest resonance energy (which for  ${}^1P^o$  is  $E = 1.5 + 0.5 - 0.688383$  a.u.), the  $2s$  threshold ( $E = 1.5$  a.u. above the  $1s$  state), and halfway in between. The various  $V_n(E_n)$ 's were then evaluated by carrying out a quadratic interpolation. This procedure will only work if the  $V_n(E)$ 's are slowly varying functions of  $E$ , which, as we shall show below, they are indeed.

The results of these calculations are summarized in Tables I and II. The rows marked  $E$  (a.u.) come directly from the TDM calculations, while the effective quantum numbers ( $n^*$ ) are defined by the formula

$$E(\text{a.u.}) = -\frac{Z^2}{2} \frac{1}{N^2} - \frac{(Z-1)^2}{2} \frac{1}{(n^*)^2}, \quad (11)$$

where

$$N=2 \quad \text{and} \quad Z=2.$$

Both of these sets of numbers are *ab initio*, in that no experimental constants are required for their evaluation. However, in order to compare with experiment and other calculations, it was also necessary to express the energies in eV.

There are no accepted conversion factors, although the equation can be written in the form

$$E(\text{eV}) = A + (B \times E)(\text{a.u.}). \quad (12)$$

Since our main interest is to compare with Burke and McVicar,<sup>4</sup> we have used their constants, as listed in Table III. For the convenience of the reader, we have included the conversion factors as used by several other authors. Bain *et al.*<sup>16</sup> argue that the resonance position which experimentalists measure can differ from process to process because of the different reduced masses of the various systems. The different conversions can give differences of as much as 30 meV; thus it is best, whenever possible, for theoretical results to be compared in a.u.

The fourth rows of Tables I and II express the widths of each of the levels in eV. It is well known that each Rydberg series (for both  ${}^1P^o$  and  ${}^3P^o$  there are three such series) is approximately characterized by a quantum defect (the fractional part of the effective quantum number) and reduced widths ( $\Gamma_n n^{*3}$ ), as well as the type of configuration mixings of the wave functions. For  ${}^1P^o$  for instance, the series beginning with the lowest level (first, third, sixth, ninth states, etc.) follows these characterizations very closely since the quantum defects are ( $2 - 1.679743$ )

$= -0.370757, -0.181034, -0.157537$ , etc., and the reduced widths are all of the same order of magnitude (0.14726, 0.16279, 0.17610, 0.18261, 0.18616). Furthermore, the hydrogenic components of each of these states [the  $a_n$ 's of Eq. (5a)] are very similar in their configuration mixings. In these states, the coefficients of the  $2snp$ ,  $ns2p$ , and  $2pnd$  configurations are all of the same sign for each  $n$  from 3 to 10, while the  $2pnd$  configurations, although far from negligible, represent less than 20% of each state. This partly supports the Cooper-Fano-Prats<sup>17</sup> notion that these states are more or less  $2snp + ns2p$ . However, the ratio of the two configurations is not nearly 1:1, but rather 1:2. The other two series (except for the second lowest level at 62.77 eV) are even less describable by a simplistic  $\pm$  configuration, since both are 40%  $2pnd$ . It is generally unreliable to classify series by their wavefunction correlations, and so the notation  $(N, n\alpha)$  has been used, where  $N$  represents the threshold below which the state exists (the state of the inner electron—see also Fano and Macek<sup>18</sup> who treat  $N$  as an actual quantum number).  $n$  represents the quantum number of the outer electron, and orders the members of a given series, and  $\alpha = a, b, c, \dots$  labels each series for a given  $L, S$ , and  $\pi$ .  $a$  is given to the series to which the lowest level of a given configuration belongs;  $b$  is given to the series to which the lowest member not belonging to series  $a$  belongs, and so on. The last rows of Tables I and II give these classifications for  ${}^1P^o$  and  ${}^3P^o$ . Bruch *et al.*<sup>14</sup> give a complete classification for all states in  $\text{Li}^+$ , while Anania *et al.*<sup>4</sup> give complete classifications and wave functions for all isohelium systems through  $Z = 5$ , below both the  $N = 2$  and  $N = 3$  thresholds.

Since the  $b$  and  $c$  series are very close to each other for  ${}^1P^o$ , it is not possible from the use of wave function and quantum defect alone to judge which series goes with the  $(2, 3b)$  state. However, the reduced widths do. The reduced widths show clearly that  $(2, 3b)$  goes with the higher member of the doublet, giving the sequence: 0.0015458, 0.00308978, 0.0034211, 0.0035353, 0.00359816. The  $c$  series has reduced widths of  $1.6086 \times 10^{-5}$ ,  $5.27562 \times 10^{-5}$ ,  $6.7948 \times 10^{-5}$ ,  $7.1178 \times 10^{-5}$ . It is most interesting to note that the reduced widths for each of the three series differ by more than a factor of 100, there being as much as a factor of 10000 between series  $a$  and  $c$ . This is true for  ${}^3P^o$  as well as  ${}^1P^o$ . This observation, which may have general validity, has not been explained adequately, and may give some support to those who are looking for some, as yet undiscovered, symmetry property. See, however, Macek<sup>19</sup> and Lin,<sup>20</sup> who have used hyperspherical coordinates

TABLE I. Energies, widths, classifications, and configuration mixings of the 13 lowest  $IP^0$  doubly excited states below the  $N=2$  threshold in helium.  $A$  ( $n$ ) means  $A \times 10^n$ .

$n^*$	1.629 243	2.275 505	2.818 966	3.268 197	3.269 547	3.642 463	4.267 537	4.292 655	4.850 682	5.267 134	5.293 813	5.854 598	6.266 850
Energy(a.u.)	-0.688 364	-0.596 564	-0.562 920	-0.546 812	-0.546 206	-0.533 865	-0.527 455	-0.521 250	-0.518 023	-0.517 842	-0.517 842	-0.514 587	-0.512 731
Energy(eV)	60.2771	62.7750	63.6905	64.1288	64.1453	64.4811	64.6555	64.8244	64.9122	64.9171	64.9171	65.0057	65.0562
Width(eV)	3.405 (-2)	1.312 (-4)	7.267 (-3)	4.608 (-7)	8.680 (-5)	3.104 (-3)	6.788 (-7)	4.325 (-5)	1.600 (-3)	4.650 (-7)	2.383 (-5)	9.282 (-4)	2.892 (-7)
$n_1$	2	0	2	1	2	0	2	1	2	0	2	1	2
$l_1$	0	2	1	0	2	1	0	2	1	0	2	1	0
$n_2$	2	0	2	1	2	0	2	1	2	0	2	1	2
$l_2$	0	2	1	0	2	1	0	2	1	0	2	1	0
Hydrogenic components													
$\sum$	0.877 584	-0.008 186	0.189 966	0.031 536	-0.026 814	0.106 309	-0.024 188	-0.019 313	-0.071 499	0.018 462	0.014 472	-0.052 643	0.014 467
	0.647 687	0.339 183	0.647 687	-0.127 515	0.278 852	0.174 091	0.079 352	0.149 983	-0.113 193	-0.054 258	-0.098 494	-0.081 934	-0.039 711
	-0.027 488	-0.255 226	-0.382 255	0.606 806	0.201 101	0.093 437	-0.123 036	0.184 231	-0.085 164	0.042 851	-0.131 974	-0.067 473	0.019 669
	-0.013 423	-0.040 913	0.032 056	-0.361 263	-0.302 150	-0.431 337	-0.486 400	0.028 898	0.087 149	0.242 617	-0.073 482	0.022 666	0.146 397
	-0.008 476	-0.023 536	-0.006 405	0.003 797	-0.000 628	0.149 162	0.552 830	-0.335 224	0.366 295	0.230 118	0.094 849	0.178 090	0.201 450
	-0.006 072	-0.016 424	-0.006 221	-0.009 788	-0.015 011	-0.008 075	-0.097 242	0.073 286	-0.273 732	-0.649 998	0.296 015	0.220 061	-0.049 013
	-0.004 690	-0.012 679	-0.005 440	-0.007 749	-0.012 605	-0.003 029	0.006 639	-0.101 451	0.043 099	0.253 638	-0.160 220	-0.357 714	-0.603 517
	-0.003 810	-0.010 425	-0.004 805	-0.006 386	-0.010 873	-0.003 173	0.005 462	-0.009 015	0.001 782	-0.024 513	0.023 310	0.116 228	0.432 751
	-0.003 219	-0.009 018	-0.004 399	-0.005 654	-0.009 960	-0.003 346	0.005 564	-0.009 312	0.002 501	-0.004 814	0.008 206	-0.005 578	-0.086 009
$\sum$ ( $nsnp$ ) <sup>2</sup>	0.804 921	0.487 554	0.298 430	0.516 222	0.210 816	0.258 736	0.573 787	0.175 667	0.243 741	0.604 393	0.155 650	0.236 193	0.625 476
	-0.302 015	-0.623 263	0.421 354	-0.167 579	-0.090 285	0.208 056	0.086 772	-0.050 709	-0.133 310	-0.055 803	0.034 383	-0.095 785	-0.040 215
	-0.056 584	0.233 959	-0.583 756	-0.164 120	-0.454 258	0.114 446	0.121 318	-0.180 163	-0.106 071	-0.083 818	0.106 039	-0.083 887	-0.062 348
	-0.031 281	0.035 921	0.056 461	0.192 445	0.376 069	-0.658 947	0.040 449	-0.271 931	0.140 781	-0.056 390	0.172 616	0.043 093	-0.049 714
	-0.021 346	0.020 258	-0.010 089	0.001 666	-0.004 304	0.245 416	-0.208 125	0.499 454	0.559 491	0.043 725	0.053 352	0.273 897	0.003 504
	-0.016 111	0.013 961	-0.010 440	0.009 135	0.012 956	-0.012 817	0.041 067	-0.100 605	-0.442 443	0.185 862	-0.520 582	0.332 597	0.090 262
	-0.012 910	0.010 688	-0.009 408	0.007 532	0.010 668	-0.004 441	-0.005 963	0.009 349	0.071 007	-0.092 169	0.237 251	-0.573 400	0.133 531
	-0.010 774	0.008 738	-0.008 475	0.006 431	0.009 027	-0.004 858	-0.005 260	0.007 711	0.002 385	0.012 603	-0.027 946	0.190 263	-0.137 368
	-0.009 295	0.007 527	-0.007 872	0.005 851	0.008 148	-0.005 263	-0.005 389	0.007 949	0.003 620	0.004 726	-0.006 965	-0.009 946	0.034 678
$\sum$ ( $ns2p$ ) <sup>2</sup>	0.096 478	0.445 337	0.521 952	0.092 271	0.356 378	0.551 061	0.068 978	0.368 762	0.562 688	0.058 452	0.373 193	0.568 796	0.054 038
	-0.294 276	0.222 701	0.155 096	0.417 810	-0.203 976	0.069 102	-0.250 956	-0.121 349	-0.042 591	0.172 455	0.083 347	-0.030 017	0.128 046
	-0.069 020	-0.126 149	-0.389 561	-0.455 743	0.538 383	0.020 776	-0.001 270	0.111 637	-0.029 195	0.048 667	-0.039 268	-0.024 518	0.051 154
	-0.040 700	-0.022 216	0.031 644	0.080 520	-0.316 206	-0.400 559	0.470 342	0.419 027	0.104 197	-0.203 365	-0.218 232	0.043 725	-0.107 941
	-0.028 744	-0.013 384	-0.012 808	0.007 264	0.006 883	0.152 308	-0.265 327	-0.493 312	0.324 593	-0.300 183	-0.178 788	0.165 854	-0.222 967
	-0.022 155	-0.009 591	-0.012 179	-0.005 411	-0.007 755	-0.011 741	0.037 587	0.094 278	-0.268 040	0.397 447	0.571 111	0.184 442	-0.070 907
	-0.017 998	-0.007 531	-0.010 842	-0.004 879	-0.006 400	-0.005 969	0.002 914	-0.005 853	0.046 771	-0.122 226	-0.236 825	-0.340 224	0.420 534
	-0.015 165	-0.006 266	-0.009 762	-0.004 457	-0.005 393	-0.006 067	0.003 035	-0.004 615	0.003 814	0.005 525	0.024 156	0.118 025	-0.237 942
	-0.013 177	-0.005 468	-0.009 090	-0.004 240	-0.004 858	-0.006 342	0.003 163	-0.004 827	0.004 838	-0.002 671	0.004 126	-0.003 686	0.035 168
$\sum$ ( $2pnd$ ) <sup>2</sup>	0.095 064	0.066 400	0.177 422	0.388 894	0.431 650	0.189 102	0.356 041	0.455 096	0.192 955	0.336 517	0.470 933	0.194 637	0.320 108
$\sum$ (other) <sup>2</sup>	0.003 538	0.000 710	0.002 216	0.002 612	0.001 156	0.001 100	0.001 193	0.000 475	0.000 616	0.000 639	0.000 245	0.000 374	0.000 378
Classification	(2,2)a	(2,3)b	(2,3)a	(2,3)c	(2,4)b	(2,4)a	(2,4)c	(2,5)b	(2,5)a	(2,5)c	(2,6)b	(2,6)a	(2,6)c

TABLE II. Energies, widths, classifications, and configuration mixings of the 13 lowest  $3p^0$  doubly excited states below the  $N=2$  threshold in helium.  $A$  ( $\alpha$ ) means  $A \times 10^7$ .

$n^*$	1.391 344	2.449 180	2.523 220	3.209 669	3.442 112	3.566 105	4.191 338	4.438 111	4.581 634	5.183 650	5.435 566	5.589 101	6.179 755
Energy(a.u.)	-0.755 286	-0.583 354	-0.578 534	-0.548 534	-0.542 201	-0.539 317	-0.525 462	-0.525 385	-0.523 819	-0.518 608	-0.516 923	-0.516 006	-0.513 093
Energy(eV)	58.3745	63.1345	63.2657	64.0820	64.2543	64.3328	64.6281	64.7119	64.7545	64.8963	64.9421	64.9671	65.0463
Width(eV)	1.392 (-2)	4.113 (-3)	4.560 (-5)	3.301 (-6)	1.613 (-3)	1.570 (-5)	1.833 (-6)	7.682 (-4)	7.823 (-6)	1.041 (-6)	4.211 (-4)	4.469 (-6)	6.387 (-7)
$n_1$	2	0	2	1	2	0	2	1	2	0	2	1	2
$l_1$	0	2	1	0	1	0	2	1	0	1	0	2	1
$n_2$	2	0	2	1	2	0	2	1	2	0	2	1	2
$l_2$	0	2	1	0	1	0	2	1	0	1	0	2	1
$\sum (2snp)^2$	0.955 219	0.166 933	-0.026 010	-0.013 706	-0.086 246	-0.012 068	0.010 076	-0.055 301	0.007 751	0.007 504	-0.039 519	-0.005 585	0.005 814
	-0.189 989	0.535 732	-0.485 803	0.297 020	-0.194 018	-0.184 007	0.163 085	-0.110 901	0.107 735	-0.106 274	-0.075 171	-0.074 091	-0.076 634
	-0.054 713	-0.398 262	0.241 621	-0.403 157	-0.359 552	-0.243 903	0.037 059	-0.196 921	0.150 360	-0.065 166	-0.129 827	-0.104 115	-0.059 105
	-0.030 969	-0.040 607	0.011 907	0.129 275	0.558 452	0.348 147	-0.438 125	-0.124 644	0.046 574	0.154 460	-0.119 284	-0.063 532	0.069 015
	-0.021 322	-0.029 512	0.010 030	-0.001 499	-0.047 521	-0.050 609	0.284 555	0.620 202	-0.365 393	0.308 576	0.097 239	0.095 077	0.205 952
	-0.016 133	-0.021 944	0.007 162	0.000 975	0.016 135	0.004 771	-0.035 942	-0.196 035	0.148 729	-0.410 847	0.558 634	0.296 445	0.100 469
	-0.010 737	-0.017 543	0.005 535	0.000 494	0.015 105	0.004 629	0.000 787	0.017 393	-0.012 695	0.119 157	-0.363 711	-0.245 958	-0.448 673
	-0.009 206	-0.013 044	0.003 951	0.000 128	0.012 928	0.004 303	0.000 620	0.010 058	-0.003 045	-0.007 102	0.058 413	0.048 464	0.237 846
	0.953 574	0.477 186	0.295 423	0.267 660	0.489 329	0.217 340	0.302 290	0.493 273	0.192 258	0.317 718	0.495 522	0.180 163	0.325 739
	-0.169 934	0.559 930	0.594 823	-0.104 305	-0.207 724	0.201 163	-0.059 279	-0.120 411	-0.113 693	0.039 197	-0.082 212	0.076 908	0.028 471
	-0.046 925	-0.391 807	-0.331 880	0.223 661	-0.341 122	0.375 456	0.012 685	-0.192 817	-0.213 896	0.010 111	-0.128 688	0.143 308	0.012 838
	-0.026 034	-0.039 053	-0.018 356	-0.093 002	0.532 208	-0.533 524	0.219 441	-0.107 437	-0.100 206	-0.090 037	-0.108 509	0.111 594	-0.047 079
	-0.017 724	-0.028 048	-0.015 974	-0.000 312	-0.045 021	0.079 301	-0.174 624	0.581 935	0.590 251	-0.139 387	0.100 317	-0.132 287	-0.100 115
	-0.013 319	-0.020 706	-0.011 792	-0.002 071	0.015 192	-0.007 944	0.022 982	-0.184 212	-0.241 016	0.232 891	0.517 444	-0.498 510	-0.029 306
	-0.010 612	-0.016 480	-0.009 340	-0.001 514	0.014 173	-0.007 829	-0.001 473	0.016 342	0.020 853	-0.072 232	-0.339 371	0.407 638	0.241 365
	-0.008 797	-0.013 840	-0.007 822	-0.001 193	0.012 801	-0.007 382	-0.001 309	0.009 427	0.005 160	0.005 594	0.054 628	-0.080 424	-0.137 683
	-0.007 525	-0.012 190	-0.006 892	-0.001 028	0.012 077	-0.007 155	-0.001 280	0.010 155	0.005 744	0.001 208	0.008 284	-0.002 993	0.022 203
	0.032 495	0.470 386	0.464 886	0.069 562	0.445 526	0.472 600	0.082 857	0.436 261	0.475 698	0.088 659	0.431 130	0.477 563	0.091 780
	-0.105 595	0.134 020	-0.395 058	-0.537 663	-0.061 621	-0.099 488	-0.309 264	-0.036 906	0.051 415	0.206 523	-0.025 498	-0.033 384	0.151 039
	-0.032 275	-0.171 952	0.284 075	0.584 014	-0.089 144	-0.306 385	-0.052 971	-0.055 896	0.159 502	0.097 524	-0.038 640	-0.102 614	0.090 052
	-0.018 730	-0.018 088	0.021 252	-0.167 995	0.225 369	0.448 810	0.608 685	-0.014 413	0.095 861	-0.221 559	-0.025 287	-0.096 461	-0.101 711
	-0.013 070	-0.013 997	0.018 117	0.002 444	-0.022 390	-0.063 817	-0.376 514	0.239 939	-0.503 286	-0.416 642	0.057 488	0.101 708	-0.282 449
	-0.009 972	-0.010 680	0.013 761	-0.000 777	0.006 968	0.009 221	0.046 751	-0.084 238	0.201 951	0.541 812	0.208 371	0.451 750	-0.131 760
	-0.008 026	-0.008 672	0.011 132	-0.000 265	0.006 777	0.008 857	-0.000 713	0.007 475	-0.019 334	-0.150 998	-0.150 397	-0.345 797	0.587 982
	-0.006 702	-0.007 382	0.009 465	-0.000 018	0.006 258	0.008 318	-0.000 526	0.004 295	-0.006 016	0.008 922	0.025 068	0.069 589	-0.309 284
	-0.005 764	-0.006 565	0.008 433	0.000 100	0.005 989	0.008 087	-0.000 447	0.004 719	-0.006 629	0.000 517	0.003 683	0.004 191	0.045 195
	0.012 956	0.048 339	0.238 023	0.658 384	0.063 206	0.309 571	0.612 896	0.069 457	0.331 832	0.592 595	0.072 767	0.342 163	0.581 827
$\sum (2pnd)^2$	0.000 975	0.004 089	0.001 668	0.004 394	0.001 939	0.000 490	0.001 957	0.001 008	0.000 211	0.001 028	0.000 581	0.000 111	0.000 603
$\sum$ (other) <sup>2</sup>	(2, 2)a	(2, 3)a	(2, 3)b	(2, 3)c	(2, 4)a	(2, 4) <sup>b</sup>	(2, 4)c	(2, 5)a	(2, 5)b	(2, 5)c	(2, 6)a	(2, 6)b	(2, 6)c
Classification	(2, 2)a	(2, 3)a	(2, 3)b	(2, 3)c	(2, 4)a	(2, 4) <sup>b</sup>	(2, 4)c	(2, 5)a	(2, 5)b	(2, 5)c	(2, 6)a	(2, 6)b	(2, 6)c

TABLE III. Constants for conversion from a.u. to eV as chosen by various authors. See Eq. (12).

Authors	A	B	Value of $-0.5$ a.u. in eV
Lipsky and Russek <sup>a</sup>	78.983	27.210	65.378
Burke and McVicar <sup>b</sup>	79.0078	27.2106	65.4025
Bhatia and Temkin <sup>c</sup> (electron-atom)	79.015 14	27.211 65	65.4093
Bhatia and Temkin <sup>c</sup> (photon-atom)	79.004 39	27.207 95	65.4004
NBS (1973) <sup>d</sup>	79.0058	27.2116	65.4000

<sup>a</sup> Reference 1 data taken from C. E. Moore, *Atomic Energy Levels*, Nat. Bur. Stand. (U.S.), Cir. 467 (U.S. GPO, Washington, 1949).

<sup>b</sup> Reference 5.

<sup>c</sup> Reference 8 (1975); authors claim that conversion depends on process.

<sup>d</sup> Reference 15.

to approximately separate the Hamiltonian. The resulting equations, when decoupled, produce potential curves for each series which support the hierarchy of widths.

#### IV. ENERGY DEPENDENCY OF $\mathcal{U}_j(E)$ AND $V_n(E)$

In the previous section it was mentioned that only three energies were used to evaluate Eqs. (7) and (8) for all energies, by quadratic interpolation. To test the smoothness of these integrals, the calculations were actually carried out for many energies between  $E = 0.15$  and 10 Ry. The value of  $\mathcal{U}_j(E)(2\pi k)^{1/2}$  for the lowest  $j$ 's are plotted in Fig. 1. We see that in the range of interest (between 2.6 and 3 Ry) they are all slowly varying and of the same order of magnitude. This fact shows that even a simple model will give more or less correct results for the  $a$  series, since the corre-

sponding  $V_n(E)$  will be more or less a positive weighted average of these curves, owing to the fact that all configurations have the same relative sign. Furthermore, even the poorest of calculations will show that the other series are much narrower than the  $a$  series, since the  $\mathcal{U}$ 's will subtract from each other. However, the super-narrowness of the  $c$  series must depend most heavily on a precise knowledge of the wave functions. This point will be discussed in more detail below, when comparison is made with other calculations.

It is of interest to see how the  $V_n(E)$ 's [Eq. (7a)] behave, since not only do they determine the widths, but they also can be used to evaluate  $\Delta$ , the shift due to coupling to the continuum. From Fano<sup>13</sup> or Feshbach<sup>6,7,10</sup> it can be shown that

$$\Delta_n = P \int \frac{|V_n(E)|^2}{E - E_n} dE \quad (13)$$

where  $P$  stands for the principal value of the integral, and the integration is over all  $E$ , including a sum over discrete states of  $PHP$ , if any. We have not evaluated the shifts, but from Eq. (13) and Figs. 2-5 it can be seen that  $\Delta_n$  and  $\Gamma_n$  are of the same order of magnitude.

The  $V_n(E)$ 's times  $(2\pi k)^{1/2}$  for the three lowest  $a$ -series states are plotted in Fig. 2. It is clear that these are also smooth functions of  $E$ . Furthermore, they behave much better near the origin than the  $\mathcal{U}_j$ 's.

The three lowest  $b$ -series states are plotted in Fig. 3. Here too, their behavior near the origin seems regular. Note, however, that these curves reach their peaks below the resonance region rather than above and are a factor of 10 smaller than the  $a$ -series curves for all energies.

Figure 4 shows a different behavior for the  $c$  series. Here, the curves reach their minima

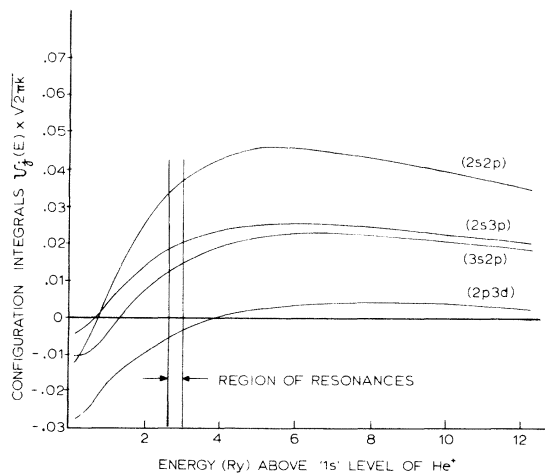


FIG. 1. Dependence of  $\mathcal{U}_j(2\pi k)^{1/2}$  on Energy (in rydbergs), for the four product functions  $2s2p$ ,  $2s3p$ ,  $3s2p$ , and  $2p3d$  in  $1P^0$  helium. The  $\mathcal{U}_j$ 's are defined in Eq. (7b).

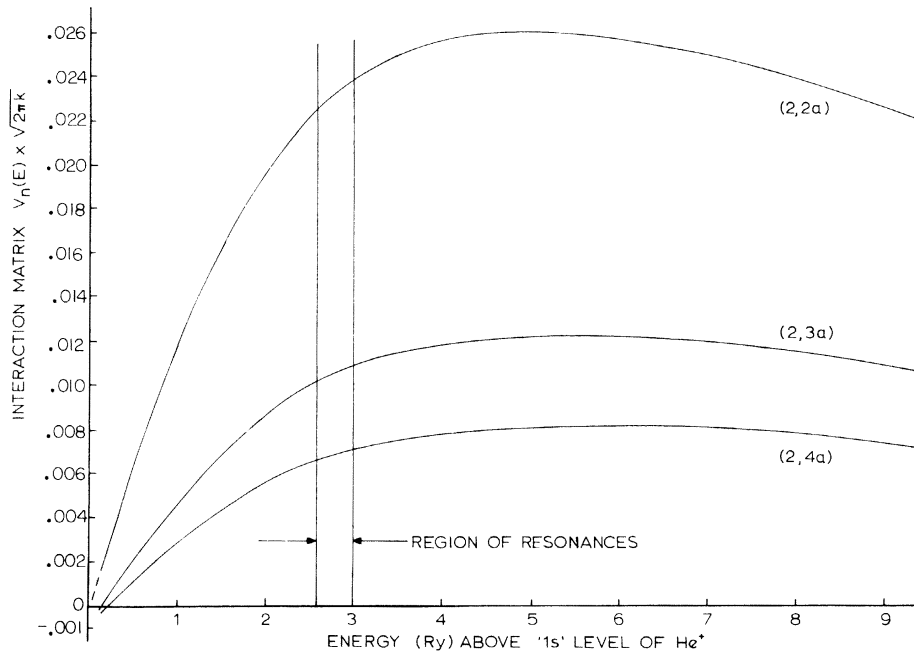


FIG. 2. Dependence of the interaction matrices  $V_n(E)(2\pi k)^{1/2}$  as a function of energy (Ry), for the three lowest  $a$ -series doubly excited states in  $1P^0$  helium. The  $V_n$ 's are defined by Eq. (7a).

near the range of interest, rather than maxima as with the other two series. Except near the origin, these curves are an order of magnitude smaller than the  $b$ -series curves. This behavior may be inaccurate, indicating that either more configurations are needed to evaluate  $V_n(E)$  far from the range of validity (2.6 to 3 Ry), or that even more care must be taken in the numerical procedures, or both. In any case, the  $V_n$ 's are still very accurate at the energies appropriate to this paper.

In Fig. 5, the width functions  $\Gamma_n(E)$ , expressed

in eV, are plotted against electron energy expressed in rydbergs for the six lowest states in  $1P^0$  He. The width functions are defined by

$$\Gamma_n(E) = 2\pi |V_n(E)|^2,$$

and are the squares of those functions plotted in Figs. 2 to 4 divided by  $\sqrt{E}$ . Note that the ordinate axis has a logarithmic scale, and that the different series differ by over a factor of 10 throughout the entire energy range above 1 Ry. Also note that there is no evidence of  $E^{-1/2}$  behavior even for energies as low as 0.1 Ry. The width of each

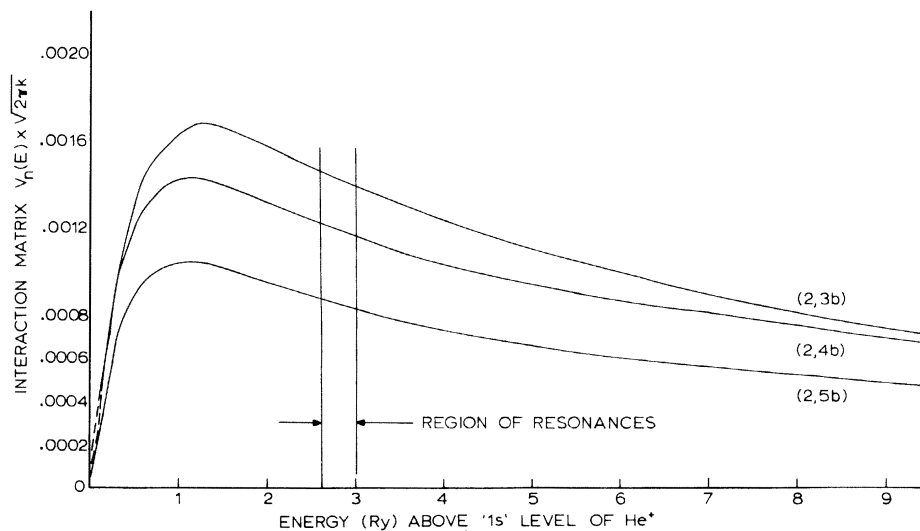


FIG. 3. Dependence of the interaction matrices  $V_n(E)(2\pi k)^{1/2}$  as a function of energy (Ry), for the three lowest  $b$ -series doubly excited states in  $1P^0$  helium. The  $V_n$ 's are defined by Eq. (7a).



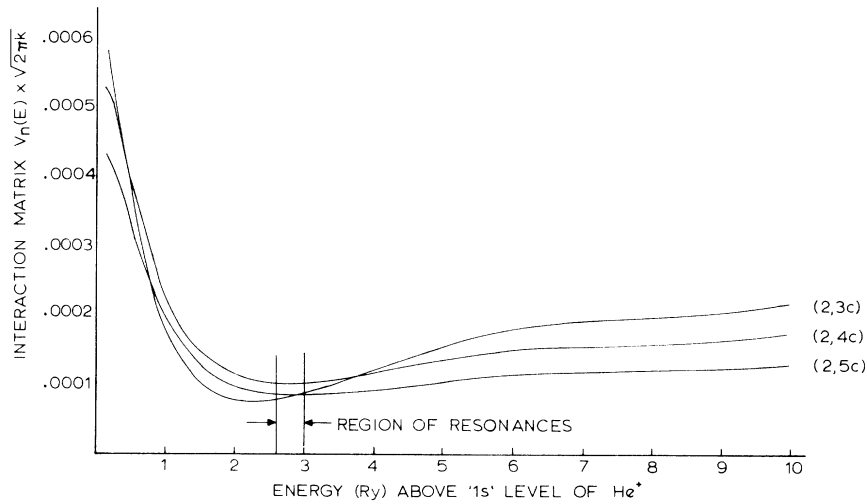


FIG. 4. Dependence of the interaction matrices  $V_n(E)(2\pi k)^{1/2}$  as a function of energy (Ry), for the three lowest  $c$ -series doubly excited states in  $^1P^0$  helium. The  $V_n$ 's are defined by Eq. (7a).

state is determined by the value of  $\Gamma$  for that particular state at the energy of the resonance.

#### V. HYDROGEN NEGATIVE ION

The method described in this paper is equally applicable to all two-electron systems. The only

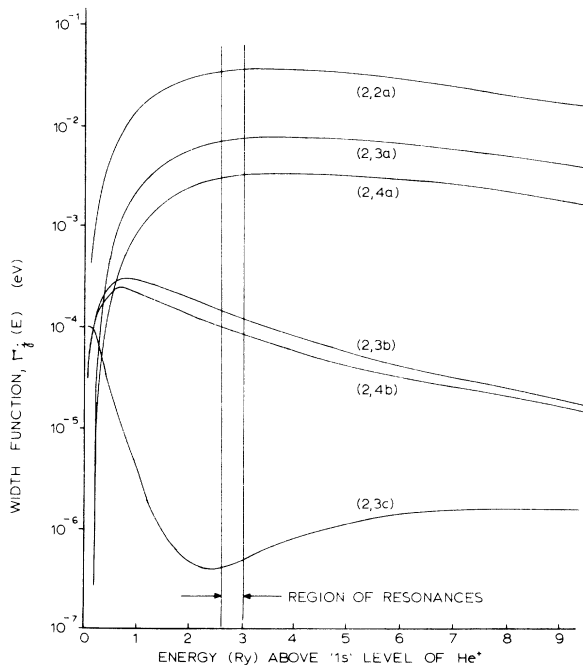


FIG. 5. Dependence of the width functions,  $\Gamma_n$  on energy for the six lowest doubly excited states in  $^1P^0$  helium. The width of each state is the value of its  $\Gamma$  function in the resonance region. Note that the  $\Gamma$  scale is logarithmic, so the  $a$ ,  $b$ , and  $c$  series differ by orders of magnitude above 1 Ry. The  $\Gamma$ 's are defined by Eq. (8).

question is whether TDM calculations can give good results for hydrogen, since the outer electron sees a polarized, neutral atom, whereas the TDM functions are all hydrogenic. In any case, these calculations for  $^1P^0$  yield only one level below the  $N=2$  threshold. Its energy, wave function and width are given in Table IV. The energy of  $-0.12602689$  a.u., is lower than the variational calculation of O'Malley and Geltman<sup>7</sup> who found two levels, the lower one of which was at  $(-0.125965)$  a.u.

An examination of the hydrogenic components in Table IV shows that the configuration mixing of this state is very similar to the  $(2,3b)$  state in helium, implying therefore that there is no  $2s2p$  state in  $H^-$ . This is in agreement with the work of Macek and Burke.<sup>21</sup> The width calculated here is  $0.311 \times 10^{-4}$  eV, and matches the  $b$ -series widths in He. Lin,<sup>20</sup> following Macek, has calculated an energy value for the  $(2,3b)$  state of  $-0.125955$  a.u., and has calculated potential curves which show why the  $a$  series does not produce Feshbach resonances.

#### VI. COMPARISON WITH OTHER CALCULATIONS

##### A. Close coupling

Burke and McVicar<sup>5</sup> performed a three-state CC calculation of  $^1P^0$  and  $^3P^0$  helium, results of which are in Table V and compared with the results of this paper. Several points of comparison between CC and this work are enumerated here. (1) All series  $a$  states agree to within 0.01 eV, and have comparable widths (although our results are consistently 20% narrower). (2) The calculations of the  $(2,3b)$  state agree very closely as to

TABLE IV. Energy, width, and configuration mixings of the lowest  $1P^o$  doubly excited states below the  $N=2$  threshold in  $H^-$  [classified as (2,3*b*)].

Energy (a.u.)	-0.126 027
Energy (eV)	10.165 809
Width (eV)	$0.311 \times 10^{-4}$
$n_1$ $l_1$ $n_2$ $l_2$	
2 0 2 1	-0.024 522
2 0 3 1	-0.316 661
2 0 4 1	0.477 804
2 0 5 1	-0.330 664
2 0 6 1	0.167 707
2 0 7 1	-0.055 900
2 0 8 1	0.019 355
2 0 9 1	-0.000 683
2 0 10 1	0.005 663
$\sum (2snp)^2$	0.470 168
3 0 2 1	0.336 638
4 0 2 1	-0.451 759
5 0 2 1	0.307 690
6 0 2 1	-0.152 874
7 0 2 1	0.051 965
8 0 2 1	-0.016 803
9 0 2 1	0.001 408
10 0 2 1	-0.003 647
$\sum (ns2p)^2$	0.438 453
2 1 3 2	-0.098 639
2 1 4 2	0.215 255
2 1 5 2	-0.160 464
2 1 6 2	0.085 136
2 1 7 2	-0.028 299
2 1 8 2	0.010 474
2 1 9 2	0.000 037
2 1 10 2	0.003 733
$\sum (2pnd)^2$	0.089 986
$\sum (\text{other})^2$	0.001 392
Classification	(2,3 <i>b</i> )

both width and position. (3) Except for the (2,3*b*) state, both the *b* and *c* series differ by more than the expected 0.01 eV. (4) In both calculations, the *b* series is the broader and *c* is the narrower of the two series. However, in CC *b* is not as broad and *c* is not as narrow as our calculation. (5) The states classified as (2, (*n*+1)*b*) are very close in energy to the corresponding states labeled (2,*nc*); however, in CC the *b*'s are slightly lower, while in TDM they are slightly higher.

The differences between the two calculations, especially item (5) above, deserve further investigation. It was mentioned in Sec. III that TDM and CC could be expected to be in close agreement as to the positions of the various resonances if the same channels are represented. But the three-state CC calculation only includes the *2skp*, *ks2p*, and *2pkd* channels, whereas the TDM calculation also includes among other things, the *3dkf* channel. We therefore ran a restricted 67 configuration calculation which excluded all configurations which had orbitals with an  $l > 2$ . Those results are also included in Table V. The energy comparison between the 67- and 83-state TDM calculations is also made in Fig. 6, where the quantum defects are plotted against the energy of the states.

We see immediately that the 67 configuration calculation is again in very close agreement with the three-state CC calculations as to energies, thereby indicating that the Burke-McVicar work does not correctly predict the properties of the *b* and *c* series, because it does not include all contributing channels. A similar situation occurred in the study of  $^1S$  helium. There, CC and TDM differed in the calculation of the (2,2*b*) state by 0.5 eV. The TDM calculation showed that the (2,2*b*) state had 3.5% of  $d^2$  configurations, and a recalculation by Macek,<sup>22</sup> using a six-state code yielded an energy value which agreed with TDM to less than 0.01 eV. In the  $1P^o$  case, the contribution to *b* and *c* series from "other" channels is less than 0.2%. Even so, their effects cannot be neglected. Part of this sensitivity is certainly due to the closeness in energy of the two series, where even a small perturbation can have a large influence.

Thomas, Ormonde, and Lipsky<sup>23</sup> have made calculations for  $1P^o$  helium, using a six-state close-coupling code which included the 3*s*, 3*p*, and 3*d* target states. Their values for the energies of the (2,3*c*) and (2,4*b*) states agree very closely with our 83-state calculations. They are 64.1255 and 64.1405 eV, respectively, within 5 meV of the values quoted in Table I. They have had great difficulty in calculating the widths however, since these have proven to be highly dependent on the step size in the radial coordinate chosen to numerically solve the differential equations. This is not entirely unexpected. O'Shea<sup>24</sup> has shown in other cases, that the energy position of a resonance will stabilize even while the line profile is still uncertain. The line profile (and the apparent width) will eventually stabilize also if the step size of integration is made small enough. In general, the smaller the width, the smaller the step size must be.

TABLE V. Comparison of 83-state TDM calculation with that of the close-coupling calculation (Ref. a), several variational calculations (Refs. b and c) and a restricted 67-state TDM calculation, for  $^1P^o$  and  $^3P^o$  helium below the  $N=2$  threshold. The 67-state calculation does not include any configurations which have orbital angular momentum greater than 2. The CC calculation is a three-target-state calculation, including  $1s$ ,  $2s$ , and  $2p$  targets. All energy levels in eV were obtained using the second formula of Table III.

Classification	Energies (eV)					Widths (eV)			
	TDM 83 state	TDM 67 state	Burke and McVicar <sup>a</sup>	Bhatia and Temkin <sup>b</sup>	Chung and Chen <sup>c</sup>	TDM 83 state	TDM 67 state	Burke and McVicar <sup>a</sup>	Bhatia and Temkin <sup>b</sup>
Singlet $P$ odd, below the $N=2$ threshold in helium									
(2, 2a)	60.2771	60.2791	60.2687	60.1537	60.1602	$0.3405^{-1}$	$0.341^{-1}$	$0.4375^{-1}$	$0.363^{-1}$
(2, 3a)	63.6905	63.6918	63.6905	63.6828	63.6649	$0.7266^{-2}$	$0.730^{-2}$	$0.8718^{-2}$	$0.10^{-1}$
(2, 4a)	64.4811	64.4814	64.4811	-	64.4738	$0.3104^{-2}$	$0.311^{-2}$	$0.3690^{-2}$	-
(2, 5a)	64.8244	64.8245	64.8244	-	64.8249	$0.1600^{-2}$	$0.161^{-2}$	$0.1891^{-2}$	-
(2, 6a)	65.0051	65.0057	-	-	65.0120	$0.9282^{-3}$	$0.932^{-3}$	-	-
(2, 3b)	62.7750	62.7754	62.7726	62.7607	62.7606	$0.1312^{-3}$	$0.133^{-3}$	$0.1394^{-3}$	$0.1165^{-3}$
(2, 4b)	64.1453	64.1381	64.1342	-	64.1396	$0.8680^{-4}$	$0.341^{-4}$	$0.5032^{-4}$	-
(2, 5b)	64.6643	64.6604	64.6579	-	64.6618	$0.4325^{-4}$	$0.144^{-4}$	$0.2300^{-4}$	-
(2, 6b)	64.9171	64.9149	-	-	65.0120	$0.2383^{-4}$	$0.750^{-5}$	-	-
(2, 7b)	65.0592	65.0578	-	-	65.0621	$0.1443^{-4}$	$0.441^{-5}$	-	-
(2, 3c)	64.1288	64.1625	64.1716	-	64.1232	$0.461^{-6}$	$0.379^{-4}$	$0.1539^{-5}$	-
(2, 4c)	64.6555	64.6717	64.6756	-	64.6545	$0.679^{-6}$	$0.220^{-4}$	$0.7759^{-6}$	-
(2, 5c)	64.9122	64.9210	-	-	64.9135	$0.465^{-6}$	$0.128^{-4}$	-	-
(2, 6c)	65.0562	65.0615	-	-	65.0584	$0.289^{-6}$	$0.795^{-5}$	-	-
Triplet $P$ odd, below the $N=2$ threshold in helium									
(2, 2a)	58.3745	-	58.3599	58.2872	58.2880	$0.1392^{-1}$	-	$0.1064^{-1}$	$0.890^{-2}$
(2, 3a)	63.1345	-	63.1412	63.0969	63.0926	$0.4113^{-2}$	-	$0.3101^{-2}$	$0.261^{-2}$
(2, 4a)	64.2543	-	64.2551	-	64.2368	$0.1615^{-2}$	-	$0.1231^{-2}$	-
(2, 5a)	64.7119	-	64.7119	-	64.7041	$0.7682^{-3}$	-	$0.5928^{-3}$	-
(2, 6a)	64.9421	-	-	-	64.9405	$0.4211^{-3}$	-	-	-
(2, 7a)	65.0739	-	-	-	65.0764	$0.2548^{-3}$	-	-	-
(2, 3b)	63.2657	-	63.2757	63.2533	63.2527	$0.4560^{-4}$	-	$0.7764^{-4}$	$0.488^{-4}$
(2, 4b)	64.3328	-	64.3336	-	64.3281	$0.1570^{-4}$	-	$0.3157^{-4}$	-
(2, 5b)	64.7545	-	64.7543	-	64.7532	$0.7823^{-5}$	-	$0.1592^{-4}$	-
(2, 6b)	64.9671	-	-	-	64.9668	$0.4469^{-5}$	-	-	-
(2, 7b)	65.0897	-	-	-	65.0896	$0.2829^{-5}$	-	-	-
(2, 3c)	64.0820	-	64.1211	-	64.0756	$0.3301^{-5}$	-	$0.4528^{-5}$	-
(2, 4c)	64.6281	-	64.6453	-	64.6275	$0.1833^{-5}$	-	$0.2725^{-5}$	-
(2, 5c)	64.8963	-	-	-	64.9024	$0.1041^{-5}$	-	-	-
(2, 6c)	65.0463	-	-	-	65.0521	$0.6387^{-6}$	-	-	-

<sup>a</sup> Reference 4.

<sup>b</sup> Reference 8 (1975).

<sup>c</sup> Reference 11 (1972 for  $^1P^o$  and 1974 for  $^3P^o$ ).

### B. Variational calculations

There have been numerous variational calculations of the lowest  $^1P^o$  and  $^3P^o$  states in helium. Table V contains two of the more recent sets of results, those of Bhatia and Temkin (1975),<sup>8</sup> and Chung and Chen.<sup>11</sup> All energy levels were obtained using the second conversion formula of Table III. Almost invariably, variational calculations provide lower energy eigenvalues for the first few members of each series [a notable exception is the (2, 3b)  $^1P^o$  state for  $H^-$ ], but for in-

creasing  $n$ , the TDM values get better, and in all but one case, provide lower eigenvalues for the higher members of each series.

There are very few width calculations available. Bhatia and Temkin (1975),<sup>8</sup> using their variational wave functions together with the same continuum functions as used here evaluated the widths of the three lowest states in both  $^1P^o$  and  $^3P^o$  helium. We see from Table V, that where comparison can be made, agreement is reasonable. Note, however, that for the  $a$  series in  $^3P^o$  helium, our disagreement with Bhatia and Temkin is as much

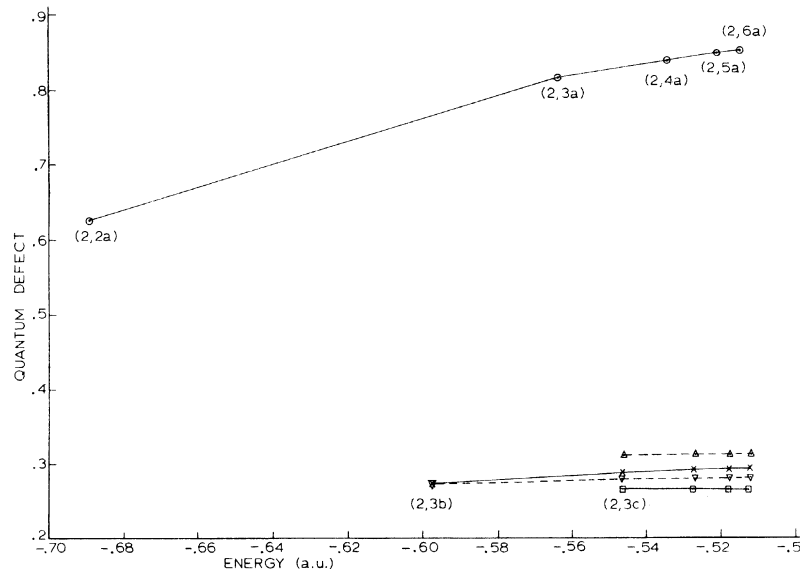


FIG. 6. Quantum defects ( $n^* - n$ ) of the various doubly excited states in  $1P^o$  helium below the  $N=2$  threshold, plotted against their energies. The defects are plotted modulo 1, making  $-0.2$  the same as  $0.8$ . Thus, the  $(n+1)$   $b$  level, with quantum defect near  $-0.7$  interacts closely with the  $n$ th  $c$  series level with quantum defect near  $0.3$ . "○" are both 83 and 67-state TDM calculations for  $a$  series. × and □ are 83-state TDM calculations, although  $(2,3b)$  has the same value for the 67-state calculation. "△" and "▽" represent  $c$  and  $b$  series respectively for the 67-state calculation. Note that although each solid line is below a dotted line (in accordance with the Hylleraas-Undheim theorem), the  $b$  series have actually moved up in going from 67 to 83 states.

as 50%, whereas Burke and McVicar are halfway in between. On the other hand, for the  $b$  series in  $3P^o$ , this paper and Bhatia and Temkin are very close, and Burke and McVicar differ by 70%.

Since Bhatia and Temkin do not quote any width values for the narrowest ( $c$ ) series for either  $1P^o$  or  $3P^o$ , we can make no comparisons here. It has been recognized, however, that calculation of such narrow widths is difficult indeed.

## VII. SUMMARY

The method described in this paper has shown itself to be a practical and efficient way to systematically calculate autoionization widths for all doubly excited states in two-electron systems.

It can be applied in an automatic, straightforward manner. No heuristic effects (such as deciding when a root has stabilized or hunting for rapid changes in phase shifts) are necessary.

## ACKNOWLEDGMENTS

The authors would like to thank Professor Kenneth Smith, under whose auspices this research was begun. They would also like to thank J. Macek, C. D. Lin, R. Anania, M. Ahmed, J. N. Bardsley, and R. Shakeshaft for helpful comments. The computational aspects of this work were carried out on the University of Nebraska's Lincoln Computing Facility.

<sup>1</sup>(a) L. Lipsky and A. Russek, *Phys. Rev.* **142**, 59 (1966);  
(b) P. L. Altick and E. N. Moore, *Phys. Rev. Lett.* **15**, 100 (1965).

<sup>2</sup>See P. G. Burke and K. Smith [Rev. Mod. Phys. **34**, 458 (1962)] for a review of both the static-exchange and close-coupling approximations.

<sup>3</sup>L. Lipsky, M. J. Connelly, and S. Ormonde, in *Proceedings of the Sixth International Conference on the Physics of Electronic and Atomic Collisions, Cambridge, Mass., 1969*, edited by I. Amdur (MIT Press, Cambridge, 1969).

bridge, 1969).

<sup>4</sup>R. A. Anania, L. Lipsky and M. J. Conneely (unpublished).

<sup>5</sup>P. G. Burke and D. D. McVicar, *Proc. Phys. Soc.* **86**, 989 (1965).

<sup>6</sup>Y. Hahn, T. F. O'Malley, and L. Spruch, *Phys. Rev.* **128**, 932 (1962).

<sup>7</sup>T. F. O'Malley and S. Geltman, *Phys. Rev.* **137**, A1344 (1965).

<sup>8</sup>A. K. Bhatia, A. Temkin, and J. F. Perkins, *Phys. Rev.*

- 153, 177 (1967); A. K. Bhatia and A. Temkin, *Phys. Rev. A* **11**, 2018 (1975).
- <sup>9</sup>P. L. Altick and E. N. Moore, *Phys. Rev.* **147**, 59 (1966); D. R. Herrick and O. Sinanoğlu, *Phys. Rev. A* **11**, 97 (1975).
- <sup>10</sup>H. Feshbach, *Ann. Phys. (N. Y.)* **19**, 287 (1962).
- <sup>11</sup>K. T. Chung and I-hsiun Chen, *Phys. Rev. Lett.* **28**, 783 (1972); *Phys. Rev. A* **10**, 997 (1974).
- <sup>12</sup>M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957).
- <sup>13</sup>U. Fano, *Phys. Rev.* **124**, 1866 (1961).
- <sup>14</sup>R. Bruch, G. Paul, J. Andra, and L. Lipsky, *Phys. Rev. A* **12**, 1808 (1975).
- <sup>15</sup>W. C. Martin, *J. Phys. Chem. Ref. Data* **2**, 257 (1973).
- <sup>16</sup>R. A. Bain, J. N. Bardsley, B. R. Junker, and C. V. Sukumar, *J. Phys. B* **7**, 2189 (1974); see also D. J. Drachman's appendix in Ref. 8 (1975).
- <sup>17</sup>J. W. Cooper, U. Fano, and F. Prats, *Phys. Rev. Lett.* **10**, 518 (1963).
- <sup>18</sup>U. Fano and J. Macek, NBS Report 8993, Project No. 100.0120 (1965).
- <sup>19</sup>J. Macek, *J. Phys. B* **1**, 831 (1968).
- <sup>20</sup>C. D. Lin, *Phys. Rev. Lett.* **35**, 1150 (1975); *Phys. Rev.* **12**, 493 (1975).
- <sup>21</sup>J. Macek and P. G. Burke, *Proc. Phys. Soc.* **92**, 351 (1967).
- <sup>22</sup>J. Macek [private communication in Ref. 1(a)].
- <sup>23</sup>K. Thomas, S. Ormonde, and L. Lipsky (unpublished).
- <sup>24</sup>B. O'Shea, Ph.D. thesis (University of London, 1970) (unpublished).