PHYSICAL REVIEW A VOLUME 44, NUMBER 1 1 JULY 1991

Photoionization of two-electron atoms using a nonvariational configuration-interaction approach with discretized finite basis

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(Received 30 January 1991)

We present an extension of a simple configuration-interaction procedure to the photoionization of two-electron atoms. By using a finite basis set constructed from B splines, this nonvariational approach does not rely on any optimum procedure, which is often required in other more elaborate configuration-interaction calculations. The quantitative accuracy of this procedure is tested by examining the photoionization cross sections at photon energies immediately above the first ionization threshold, as well as near the doubly excited $2s2p\ ^1P$ resonance structure. The S- and P-wave phase shifts for the electron-hydrogen scattering calculated with this procedure are also presented. The excellent agreement between the present calculation and other existing theoretical and experimental results, in addition to the extensive recent applications of this procedure to the bound excited states of divalent atoms, has further demonstrated the effectiveness of this simple configuration-interaction procedure.

I. INTRODUCTION

A complete and detailed characterization of the asymptotically oscillating continuum wave functions is not necessarily required in the determination of transition amplitudes for transitions from a bound state confined in a finite volume to a continuum extending to infinity. The transition matrix can often be evaluated accurately if the short-range interaction can be represented adequately by an *effective* continuum wave function, which is a linear combination of a discretized finite basis confined in a finite volume and normalized with proper boundary condition consistent with its asymptotic behavior at a large distance. An earlier attempt by Heller, Reinhardt, and Yamani [1] has shown that the matrix constructed in an L^2 integrable basis can represent effectively an operator with a continuous spectrum. Subsequent applications of the J-matrix method [2,3] have also led to successful theoretical results for the electron-hydrogen scattering and photoejection of one and two electrons from H^-. The positions and widths of the open-channel doubly excited autoionization states embedded in the continuum (i.e., Feshbach resonances) can also be estimated by a rotated complex-coordinate method using a straightforward configuration-interaction (CI) procedure with a simple L^2 finite basis [4]. The theoretical positions and widths of the Feshbach resonances of two-electron atoms evaluated with a more elaborate Hylleraas functions in a complex-coordinate calculation [5,6] are often considered as reliable as any of the most accurate theoretical calculation [7–9] involving direct determination of the scattering phase shifts.

More recently, Moccia and Spizzo [10,11] have also successfully developed an L^2 calculational procedure to represent the continuum spectrum by employing a set of elaborate one-electron orbitals including a modified Slater-type orbital (STO) with an explicit $\cos(kr)$ dependence. By extending the calculation to a fairly large sphere of radius R, Moccia and Spizzo are able to link directly the calculated wave function at a distance r smaller than R to the true continuum wave function. The resonance structure in the continuum is then determined by the energy variation of the calculated scattering phase shifts and the normalization constants moving across a doubly excited resonant state. An attempt has also been made by Martin and co-workers [12,13] to determine the phase shifts of continuum functions by using the usual STO basis in a smaller sphere with the help of an elaborate fitting procedure. By modifying an earlier multiconfiguration Hartree-Fock (MCHF) approach for the continuum [14] with an L^2 spline-based procedure, Froese Fischer and Idrees [15] have extended successfully the MCHF approach to the study of resonance structure for the photoionization of He.

The purpose of this paper is to demonstrate that a simple nonvariational CI procedure, which has been applied extensively with success to the bound excited states of divalent atoms in a frozen-core Hartree-Fock (FCHF) approximation [16–18], can also be extended to the continuum above the ionization threshold. The effectiveness of this approach to represent the two-electron Coulomb interaction between positive-energy orbitals is shown in our recent application to the H^- atom [19]. Briefly, in this CI approach, a nearly complete set of discretized one-electron radial hydrogenic functions $\chi_{\nu l}$ corresponding to orbital angular momentum l and nuclear charge Z, defined by

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\frac{Z}{r}+\frac{1}{2}\frac{l(l+1)}{r^2}\right]\chi_{\nu l}=\epsilon_{\nu l}\chi_{\nu l}\ , \tag{1}$$

is employed in the construction of the L^2 basis in calculating the Hamiltonian matrix for the two-electron atom. The solutions $\chi_{\nu l}$ of Eq. (1) are expanded in terms of a set of B splines defined between $r=0$ and $r=R$ [16,20,21]. By diagonalizing the Hamiltonian matrix corresponding to a total spin S and a total orbital angular momentum L in the LS coupling, an energy eigenstate of total energy E, identified by a set of quantum numbers $\Lambda \equiv \{S, L, M_S, M_L\}$, is represented by a state wave function Φ_E^Λ, which is a linear combination of orthogonal two-electron configuration functions constructed from both negative- and positive-energy χ_{vl}.

In Sec. II, we first introduce the use of a sinelike knot sequence for the B-spline set, which helps to extend the applicability of this simple CI procedure to the continuum spectrum. The scattering phase shifts for the outgoing electron will be determined directly from the calculated wave functions confined in a finite volume. The position and width of the resonance structure in the continuum can then be determined by the energy variation of the phase shifts. A simple procedure will be introduced to calculate the photoionization cross section from a bound state. In Sec. III, we present the numerical results of this theoretical procedure including scattering phase shifts, the positions and widths of the resonance structures, and the photoionization cross sections for H^- and He atoms.

II. THEORETICAL PROCEDURE

In a bound-state calculation, the set of B splines of order K and total number n is often defined with an exponentially increasing knot sequence [16,21]. The choice of such a knot sequence satisfies the need for a more *densely* populated set of B splines near the nucleus in order to accommodate the fast raising inner s orbitals at small r. On the other hand, a more *evenly* populated set of B splines at larger r is required if the oscillating behavior of the positive-energy orbitals at large distance can also be properly represented. As a result, for transitions involving both a bound state and a continuum, we have chosen a sinelike knot sequence d_v defined by

$$d_v = R \sin\left[\frac{\pi}{2}\left[\frac{(v-1)\Delta h}{R}\right]^y\right], \quad v = 1, 2, \ldots, n-K+2, \qquad (2)$$

where $\Delta h = R/(n-K+1)$. The distribution of knot points can be adjusted by changing the position of the first nonzero knot d_2, which in turn determines the value of y according to Eq. (2). By employing such a knot sequence, we are able to limit the size of the B-spline set to a modest n (e.g., $n = 70-90$, $K = 7-9$ for $R = 120a_0$ in our H^- calculation), which is sufficiently large to take into account adequately both the small- and large-r behavior of the orbital functions.

Similar to our earlier bound state calculation [16,18,19], the one-electron radial hydrogenic functions χ_{vl} are subject to the boundary conditions

$$\chi_{vl}(r=0) = \chi_{vl}(r=R) = 0\ . \qquad (3)$$

In the present calculation, by applying the same numerical procedure presented earlier [16,18,19] with the knot sequence defined by Eq. (2), all positive-energy radial functions, with energy eigenvalues up to few Ry, exhibit an oscillating behavior identical to the analytical Coulomb function at the same energy. The phase shifts determined from our numerical one-electron radial functions χ_{vl} confined in a sphere of radius R, agree with the analytical Coulomb phase shift δ_C to at least seven figures. For the positive-energy orbitals, with energy ϵ_{vl} up to few Ry, only those with momentum $k_{vl} = (2\epsilon_{vl})^{1/2}$ that satisfy the boundary condition given by Eq. (3), i.e.,

$$k_{vl}R + \frac{Z}{k_{vl}}\ln(2k_{vl}R) - \frac{l\pi}{2} + \delta_C = m\pi\ , \qquad (4)$$

appear in the nearly complete set of discretized radial hydrogenic functions χ_{vl}.

The Hamiltonian matrix is constructed from a basis set consisting of a number of two-electron configuration series $\mu l l'$ [17–19]. Each $\mu l l'$ series includes a set of LS-coupled two-electron Slater determinant wave functions $\psi_{\mu l v l'}^\Lambda$ with one of the electrons (e.g., the inner electron) occupying a fixed hydrogenic orbital μl and the other l' electron extended from negative to positive energy $\epsilon_{vl'}$ over an entire set of eigenfunctions $\chi_{vl'}$ of Eq. (1). After diagonalizing the Hamiltonian, the state wave function for a state $|E>$ corresponding to a total energy E is given by

$$\Phi_E^\Lambda = \sum_{\mu l l'} \Xi_{E,\mu l l'}^\Lambda\ , \qquad (5)$$

where the configuration series function

$$\Xi_{E,\mu l l'}^\Lambda = \sum_v C_E^\Lambda(\mu l, v l')\psi_{\mu l v l'}^\Lambda \qquad (6)$$

represents the contribution to the state wave function from the $\mu l l'$ configuration series. A complete set of coefficients $C_E^\Lambda(\mu l, v l')$ forms the eigenvector of the state $|E>$.

At energy above the first ionization threshold of a two-electron atom, the spectrum is dominated by a series of doubly excited autoionization states embedded in a single continuum open-channel $1sl$. The state wave function Φ_E^Λ can be separated into two parts, i.e.,

$$\Phi_E^\Lambda = \Xi_{E,1sl}^\Lambda + \sum_{\mu_0 l_0 l'} \Xi_{E,\mu_0 l_0 l'}^\Lambda\ , \qquad (7)$$

where the first term represents the ionization channel and the second term denotes the combined contribution from doubly excited configurations from all closed channels. The kinetic energy ϵ and the momentum k of the ionized electron are given by

$$\epsilon = \tfrac{1}{2}k^2 = E + E_I\ , \qquad (8)$$

where E_I is the ionization energy of the remaining $1s$ electron.

Asymptotically, the correct wave function of an outgoing l electron with momentum k, evaluated in a direct scattering calculation, is given by the expression

$$\left[\frac{2}{\pi k}\right]^{1/2} \sin\left[kr + \frac{q}{k}\ln(2kr) - \frac{l\pi}{2} + \delta_C + \delta_l\right] \quad \text{as } r \to \infty\ , \qquad (9)$$

where q is the effective nuclear charge experienced by the outgoing electron and δ_l is the scattering phase shift due to the short-range interaction. The scattering phase shift can be extracted from the present calculation by comparing the configuration series function $\Xi^{\Lambda}_{E,1sl}$ for the $1sl$ open channel with the asymptotic expression given by Eq. (9). First, the configuration series function $\Xi^{\Lambda}_{E,1sl}$ can be expressed in a form identical to the Slater determinant function $\psi^{\Lambda}_{1s\xi_{\epsilon l}}$, where one of the radial hydrogenic functions is replaced by a one-particle radial function

$$\xi_{\epsilon l}(r)=\sum_{\nu} C^{\Lambda}_{E}(1s,\nu l)\chi_{\nu l}(r) \ . \tag{10}$$

Second, the numerical function $\xi_{\epsilon l}(r)$ is matched at a finite r against an asymptotic expression employed by Burgess, i.e., [22],

$$\xi_{\epsilon l}(r)\rightarrow A\left[\frac{k}{\zeta(r)}\right]^{1/2}\sin[\phi(r)+\delta_l] \quad \text{as } r\rightarrow R \ , \tag{11}$$

where ζ and ϕ are functions of r. As $r\rightarrow\infty$, $\zeta\rightarrow k$ and

$$\phi\rightarrow\left[kr+\frac{q}{k}\ln(2kr)-\frac{l\pi}{2}+\delta_C\right] \ . \tag{12}$$

An accurate representation of the continuum by a discretized finite basis set, of course, depends critically on its ability to match the calculated radial function against the correct asymptotic expression over a large portion of r with a constant amplitude A. In Fig. 1, we present the calculated radial functions $\xi_{\epsilon l}(r)$ at two different momenta in the $1ss$ open channel for the electron-hydrogen scattering below the $n=2$ threshold. The matching between our calculated $\xi_{\epsilon l}(r)$ and Eq. (11) is nearly perfect. The scattering phase shift δ_l can be determined easily without the help from any elaborate fitting procedure such as the one proposed by Martin and Salin [12]. As expected, the numerically determined amplitude A (or the "normalization constant" [10–13]) equals approximately $(2\rho_{1sl}/R)^{1/2}$, where

$$\rho_{1sl}=\sum_{\nu}|C^{\Lambda}_{E}(1s,\nu l)|^2=\langle\psi^{\Lambda}_{1s\xi_{\epsilon l}}|\psi^{\Lambda}_{1s\xi_{\epsilon l}}\rangle$$
$$=\langle\xi_{\epsilon l}(r)|\xi_{\epsilon l}(r)\rangle \tag{13}$$

is the probability density due to the $1sl$ configuration series. We note that for a two-electron atom, the effective nuclear charge q equals $Z-1$ even when $\xi_{\epsilon l}(r)$ is, in fact, a sum of one-particle hydrogenic functions which are subject to a nuclear charge of Z asymptotically. At energy near the Feshbach resonances below the $n=2$ threshold, the phase shift increases rapidly by a total of π. Consequently, a set of closely populated energy eigenvalues is required to describe the detail energy variation of the scattering phase shift across the resonance. This is carried out by repeating our calculations at slightly varied values of R. The energy E_r and the width Γ of the resonance are determined by a least-squares fit of the phase shifts to the usual expression [23, 24]

$$\delta_l(E)=\sum_{i=0}^{2}a_iE^i+\tan^{-1}\frac{\Gamma/2}{E_r-E} \ . \tag{14}$$

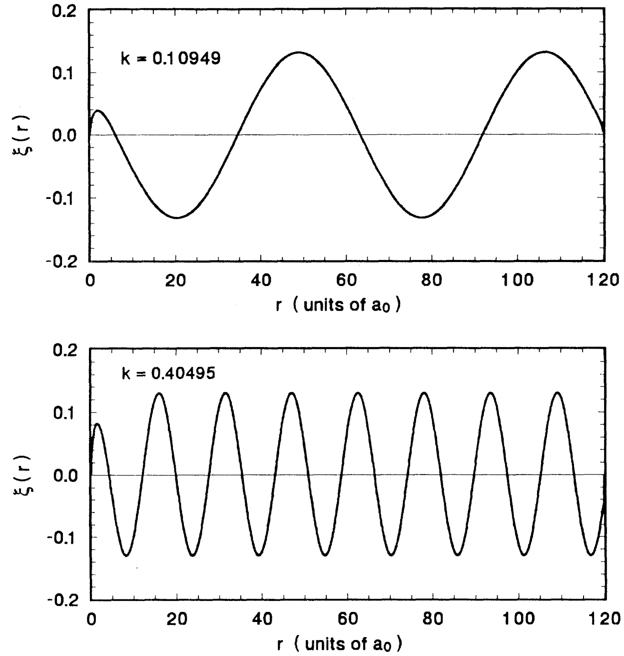

FIG. 1. The calculated one-particle functions $\xi(r)$ representing the H^- $1ss$ configuration series at momenta $k=0.10949$ and 0.40495.

The cross sections (in unit of a_0^2) for the photoionization from an initial state $|I>$ are given by

$$\sigma=\tfrac{8}{3}\pi^2\alpha g(E_\gamma)|D_{EI}|^2 \ , \tag{15}$$

where α is the fine-structure constant and $g(E)=E$ and E^{-1} for the dipole length and velocity approximations, respectively. The photon energy E_γ is given in atomic units. The dipole matrix between the initial state $|I>$ and the final state $|E>$ is given by

$$D_{EI}=\langle\Phi^{\Lambda}_{E}|\hat{D}(1,2)|\Phi^{\Lambda}_{I}\rangle \ , \tag{16}$$

where

$$\hat{D}(1,2)=D(\mathbf{r}_1)+D(\mathbf{r}_2) \ , \tag{17}$$

and D represent the position and gradient operators for the length and velocity approximations, respectively.

When the final-state wave function Φ^{Λ}_{E} is calculated by using the discretized finite basis set, the usual normalization constant $(2/\pi k)^{1/2}$ is replaced by the amplitude A given in Eq. (11). As a result, a constant

$$N_k=\frac{2/(\pi k)}{A^2} \tag{18}$$

should be added to Eq. (15) when we replace the dipole matrix D_{EI} by D^{d}_{EI}, i.e.,

$$\sigma=\tfrac{8}{3}\pi^2\alpha g(E_\gamma)N_k|D^{d}_{EI}|^2 \ . \tag{19}$$

The new dipole matrix D^{d}_{EI}, also defined by Eq. (16), is evaluated using the state wave functions Φ^{Λ}_{E} and Φ^{Λ}_{I} calculated with the discretized finite basis set. Alternatively, the photoionization cross section can be expressed in terms of the oscillator strength f_{EI} for absorption by the simple relation

$$\sigma=\frac{4\pi\alpha}{kA^2}f_{EI}\ , \tag{20}$$

where f_{EI} can be calculated numerically following the same procedure for the bound-bound transitions given in detail earlier [25].

III. RESULTS AND DISCUSSION

The accuracy of the present simple CI procedure is first illustrated in Fig. 2 by the excellent agreement between our calculated S- and P-wave phase shifts for the electron-hydrogen scattering and few selected earlier and recent theoretical calculations [9,26–28]. The energy variations of the calculated phase shift near the lowest ^1S Feshbach resonances below the $n=2$ threshold of H^- and He are presented in Fig. 3. Our calculated energy and width for the lowest H^- ^1S resonance at $-0.297\,563$ and 3.49×10^{-3} Ry, respectively, are in very good agreement with some of the most accurate theoretical results, including the recent R-matrix calculation by Scholz, Scott, and Burke [9], the earlier complex-coordinate calculation by Ho [5], and the electron-hydrogen scattering calculation using Hylleraas correlation function by Ho, Bhatia, and Temkin [7]. A complete summary of other earlier theoretical [29,30] and experimental [31,32] results is given recently by Pathak, Kingston, and Berrington [33]. A second ^1S resonance for H^- is found to locate at $-0.252\,035$ Ry with a width of 1.87×10^{-4} Ry (or, about 2.54 meV). This is about 0.87 meV *above* the ^1P resonance according to our calculation, which is also consistent with the experimental observation by Bryant *et al.* [34]. The overlapping ^1S and ^1P states are easily coupled by the electric field, as the width of the ^1S resonance is greater than the separation between these two states. An earlier scattering calculation by Callaway [35] has suggested initially that the ^1S state lies about 0.6 meV *below* the ^1P state with a width of about 5.6 meV, but a subsequent calculation by Callaway and Rau [36] has found that the ^1S state lies about 2.3 meV *above* the ^1P state. Our calculated width of 2.54 meV for this ^1S state agrees well with the value of 2.6 meV from recent R-matrix calculations by Pathak, Kingston, and Berrington [33]. We again refer to Ref. [33] for a review of other earlier theoretical results for this ^1S state. Our calculated excitation energy and width of 57.8562 and 0.142 eV, respectively, for the He $2s^2\,^1S$ state also agree very well with the available theoretical [5,23,37–39] and experimental [40,41] results reviewed recently by Froese Fischer and Idrees [15].

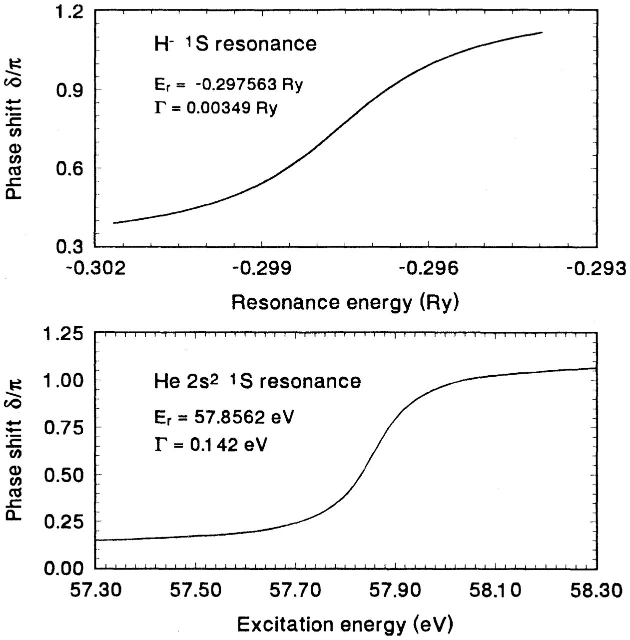

FIG. 3. The energy variation of the phase shifts for the lowest ^1S Feshbach resonance below the $n=2$ threshold for H^- and He.

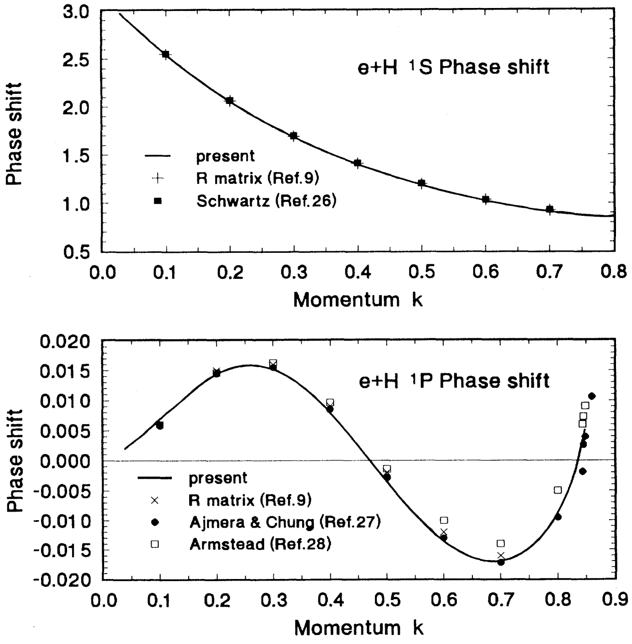

FIG. 2. The calculated S- and P-wave phase shifts for the electron-hydrogen scattering. The R-matrix results are taken from Ref. [9]. Other data shown are taken from Refs. [26], [27], and [28].

The calculated photoionization cross sections below the resonance structure for H^- and He, using the procedure outlined in Sec. II, are presented in Fig. 4. The present photodetachment cross sections from the ground state of H^- agree very well with some of the most accurate earlier theoretical calculations [2,42–44]. A collection of the earlier theoretical results has been given by

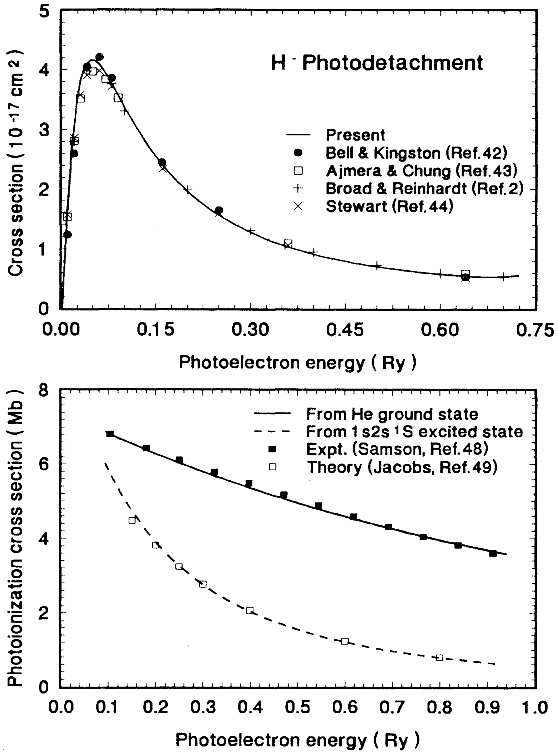

FIG. 4. The photoionization cross sections below the resonance structure for H^- and He. Comparisons are made with data taken from Refs. [42], [43], [2], [44], [49], and [48].

Daskhan and Ghosh [45]. A simple model calculation by Crance and Aymar [46] has led to cross sections that are significantly smaller at the low-energy side but larger on higher energies than most of the more elaborate theories. In contrast, a more recent calculation, using the hyperspherical coordinates [47], yields cross sections in the length form that are slightly higher near the peak region and slightly lower at higher energy than other theoretical results. Only the dipole-length results from the present calculation are plotted in Fig. 4. The agreement between our dipole-velocity and dipole-length results is about 1–2 % or better for the entire energy range. Our calculated photoionization cross sections from the ground state of He agree very well with the experimental data compiled recently by Samson [48], which are accurate to 1–2 %. The present photoionization cross sections from the excited $1s2s\ ^1S$ state of He are also in close agreement with the earlier calculation by Jacobs [49]. Similar to the photoionization from the ground state, our length and velocity results agree to about 1–2 % or better, and only the length results are plotted.

Photoionization of He at energy near the lowest $2n+$ doubly excited resonance (i.e., the $2s2p\ ^1P$ state observed first in detail by Madden and Codling [50] and classified later by Cooper, Fano, and Prats [51]) provides perhaps the best quantitative benchmark test for any theoretical and experimental approach intended for the study of multielectron interactions. The results of the present calculation are shown in Fig. 5. The position and width of the He $2s2p\ ^1P$ resonance, derived from the energy variation of the calculated phase shifts, at 60.1825 and 0.0397 eV, respectively, compare very well with most of the existing theoretical and experimental results. Detailed summaries, including many earlier and recent theoretical [5,38,39,52,53] and experimental [50,54,55] studies, are given recently by Sánchez and Martin [13], Wu and Xi [56], Froese Fischer and Idrees [15], Gersbacher and Broad [57], and Hamacher and Hinze [58]. The resonance profile parameters $q=2.68\pm0.06$ and $\sigma_0=1.40$ Mb are in very good agreement with other existing data. A maximum cross section close to 12 Mb is also in good agreement with the recent theoretical results by Sánchez and Martin [13], Gersbacher and Broad [57], Hamacher and Hinze [58], and Salomonson, Carter, and Kelly [53]. A more symmetric resonance profile representing the photoionization from the He $1s2s\ ^1S$ excited state is also shown in Fig. 5. A maximum cross section near 500 Mb at energy close to the resonance energy agree well with the maximum cross section of 541 Mb calculated by Doyle, Oppenheimer, and Dalgarno [59]. Our result is about 25% higher than the maximum value of 383 Mb calculated by Jacobs [49]. This disagreement may be partially attributed to the approximately 10% overestima-

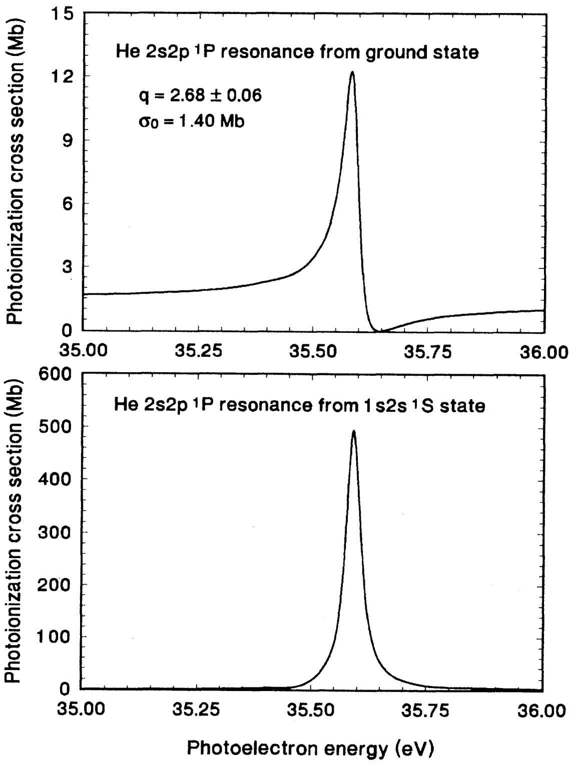

FIG. 5. The photoionization cross sections in the vicinity of $2s2p\ ^1P$ resonance from both the ground state and the $1s2s\ ^1S$ excited state of He.

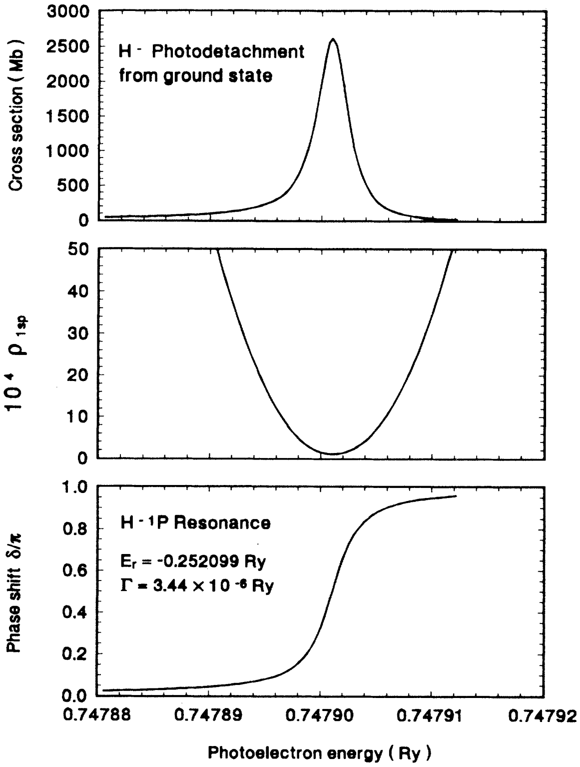

FIG. 6. The H^- photodetachment cross sections near the ^1P Feshbach resonance below the $n=2$ threshold from the ground state. The calculated probability densities ρ_{1sp} due to the $1sp$ configuration series and the corresponding phase shifts are also plotted as functions of photoelectron energy for comparison.

tion in width from Jacobs's calculation when compared with most of the existing theoretical values. Again, the overall agreement between our length and velocity results is about 1–2 % or better.

In Fig. 6, we present our calculated H^- photodetachment cross sections from the ground state at energies in the vicinity of the lowest ^1P Feshbach resonance. The phase shifts and the probability densities ρ_{1sp} for the $1sp$ ionization channel are also plotted on the same energy scale for comparison. As the energy approaches the resonance position, the value of ρ_{1sp} is seen to reach a minimum. This confirms the expectation that at the resonance, the combined probability density of all closed channels dominated by the doubly excited configurations is at its maximum. The position of the resonance at $-0.252\,099$ Ry from the present calculation is in close agreement with the earlier close-coupling calculation by Callaway [35], the complex coordinates calculation by Wendoloski and Reinhardt [4] and the recent R-matrix calculation by Pathak, Kingston, and Berrington [33]. The width of this narrow resonance is about 10^{-6} Ry, which is not resolved experimentally. Some of the calculated widths are listed in Table I. Clearly, additional theoretical calculation is required if the width of this resonance is to be determined more precisely. The width from the present calculation is about 40% smaller than the J-matrix result [2] compiled by Bryant *et al.* [34]. On the other hand, a peak cross section at about 2600 Mb from the present calculation is about 80% higher than the J-matrix result. In addition, as we pointed out recently [19], the numerical convergence of the transition matrix from the ground state depends critically on the accurate account of the continuum-continuum interaction between positive-energy orbitals included in the ground-state wave functions. The use of an enlarged basis set for a more accurate representation of the continuum spectrum in the present calculation has limited our ability to exhaust the continuum-continuum interaction included in the ground state on a relatively modest work station. In fact, the present calculation yields an oscillator strength of approximately 0.001 45, which is about 30% larger than the value of 0.001 08 from a more complete recent calculation [19]. As a result, a converged calculation should yield a maximum cross section perhaps slightly less than 2000 Mb.

TABLE I. Comparison of the theoretical width Γ in 10^{-6} Ry for the H^- ^1P Feshbach resonance blow the $n=2$ threshold.

Theory	Γ (10^{-6} Ry)
Present	3.44
Taylor and Burke (Ref. [29])	3.31
Seiler, Oberoi, and Callaway (Ref. [30])	1.78
Ajemera and Chung (Ref. [27])	2.10
Broad and Reinhardt compiled by Bryant *et al.* (Refs. [2] and [34])	5.43
Callaway (Ref. [35])	2.73
Wendoloski and Reinhardt (Ref. [4])	76.00

In conclusion, the numerical results from the present calculation clearly establish the quantitative reliability of the nonvariational finite basis CI procedure presented in this paper. The extension to divalent atoms, following its extensive recent applications to the bound-bound transitions [16,18], should be straightforward. In fact, our preliminary calculation for the Be $2p^2\,{}^1S$ resonance yields a width of 76.0 cm^{-1} which is in close agreement with the experimental value of 74.9 cm^{-1} by Clark *et al.* [6] as well as the theoretical value of 72.4 cm^{-1} by Moccia and Spizzo [11]. The accuracy of the present calculation can be improved easily if the numerical works are carried out on a more powerful computer when required.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation (NSF) under Grant Nos. PHY89-03384 and PHY89-13521 and the Department of Energy (DOE) under Grant No. DE-FG03-87ER60504. One of us (T.N.C.) would like to thank J. A. R. Samson for the use of his recent compilation of He photoionization data prior to its publication.

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