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Hari P. Saha  
*University of Central Florida*

C. Denise Caldwell  
*University of Central Florida*

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## ***K*-shell photoionization of beryllium**

Hari P. Saha and C. Denise Caldwell

*Department of Physics, University of Central Florida, Orlando, Florida 32816*

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The numerical multiconfiguration Hartree-Fock method is used to study in detail the photoionization of atomic beryllium near the  $1s$  threshold. Electron correlation effects, which are found to be very important in the  $K$ -shell partial photoionization cross section, have been taken into account very accurately through the configuration-interaction procedure. The present results are compared with experimental measurements of the relative contributions of the three major ionization channels and are found to be in excellent agreement. The existence of the principal resonances reported by the experiment has been confirmed and assignments made to these contributions based on accurate energy calculations.

### I. INTRODUCTION

Inner-shell photoionization cross sections of atoms are quantities of chemical and physical interest. Their accurate measurement and calculation, and their subsequent interpretation embody a broad spectrum of useful information about the dynamics of photoexcitation.<sup>1</sup> In general, multiple-excitation processes in atomic inner-shell photoionization occur with significant probability. The resulting final states are approximately described by configurations formed by removal of a core electron and excitation of additional electrons to higher bound states (shake up) or to the continuum (shake off).<sup>2-4</sup> These final states subsequently decay by electron or photon emission, giving rise to satellites in the Auger and x-ray spectra<sup>4</sup> and in the photoelectron spectra.<sup>2,5-7</sup> The study of these multiple-excitation processes is important because they provide important clues for the understanding of electron correlation and excitation dynamics. The energy dependence of the cross section for two-electron processes is particularly informative near threshold.

Recently, Krause and Caldwell<sup>8</sup> made an experimental study of the  $K$ -shell photoionization of atomic beryllium in the region of the threshold for production of the  $K$ -hole state of the  $\text{Be}^+$  ion,  $\text{Be}^+(1s2s^2S)$  at 123.56 eV. At energies just above this threshold, where other ionic channels open, they observed a strong correlation which led to production of  $\text{Be}^+(1s(2s2p)^3P)$  above 127.9 eV, and  $\text{Be}^+(1s(2s2p)^1P)$  above 130.2 eV. Their measurements of the partial cross sections show a number of autoionization resonances in each of these three ionic channels.

The only theoretical calculation of inner-shell photoionization of Be has been made by Bely-Dubau, and Petrini.<sup>9</sup> Their method is similar to that used by Dubau and Wells<sup>10</sup> for the outer-shell photoionization of Be. Until now, no theoretical work has been reported on the photoeffect in the  $1s$  shell of beryllium that can interpret the experimental results obtained by Krause and Caldwell.<sup>8</sup> Because of the relative simplicity of the Be atom, which facilitates theoretical calculations, and the importance of correlations among the different principal

shells, it is of great interest to have accurate calculations in order to identify the important interactions and to obtain accurate results for comparison with experiment.

It has already been established that the multiconfiguration Hartree-Fock (MCHF) approach<sup>11-13</sup> can achieve considerable success in the calculation of the photoionization cross section of atoms. This can be seen in the recent application of the method to the calculation of the photoionization of sodium and potassium atoms.<sup>11,12</sup> Very good agreement with experiment was obtained for both of these systems. This success has been possible via an extension of the traditional MCHF theory to allow the computation of continuum wave functions. In the present paper we report the application of this expanded MCHF technique to the calculation of the  $K$ -shell photoionization cross section of the beryllium atom for incident photon energies ranging from the  $(1s^{-1})2s^2$  threshold at 123.6 to 144 eV. We will see again that the calculation achieves quite good agreement with the experimental results. This is true not only for the continuum region, but the theory predicts autoionizing resonances exactly where they are found in experiment. This implies that these resonances can be readily identified with double electron excitations in the atom. Furthermore, due to the accuracy with which the MCHF scheme can determine energies, both thresholds and "bound" states can be specified quite accurately, thus highlighting another advantage of the use of the MCHF scheme in cross-section calculations.

### II. MCHF THEORY OF PHOTOIONIZATION

The photoionization cross section in the dipole approximation is given by the expression

$$\sigma(\omega) = 4\pi^2 \alpha a_0^2 \omega \sum_{f,m} |\langle \Psi_f | T | \Psi_i \rangle|^2,$$

where atomic units are employed. The symbol  $\alpha (= \frac{1}{137}$  a.u.) is the fine-structure constant,  $\omega$  is the energy of the incident photon, and  $a_0$  is the Bohr radius of the hydrogen atom.  $\Psi_i$  and  $\Psi_f$  are the initial- and the final-state eigenfunctions, respectively, and the sums run over all

final configurations and all magnetic quantum numbers.  $T$  is the dipole operator in either length

$$T = T_L = \sum_{j=1}^n z_j$$

or velocity

$$T = T_v = \sum_j \frac{\nabla_j^z}{i\omega}$$

forms. The length and the velocity forms of the cross sections will be identical when  $\Psi_i$  and  $\Psi_f$  are exact solutions of the same Hamiltonian.

The MCHF wave function for the final continuum state is expressed in terms of a continuum orbital  $\phi_{kl}$  coupled to the wave function for an  $N$ -electron ion, plus a sum of bound  $(N+1)$ -electron configurations to incorporate orthogonality and core polarization effects. The ionic-core wave function having energy  $E_c$  is written in the form

$$\Psi_c(L_c S_c; N) = \sum_{j=1}^{m_c} a_j \Phi(\gamma_j L_c S_c; N), \quad (1)$$

where  $\Phi(\gamma_j L_c S_c; N)$  is an  $N$ -electron bound configuration eigenstate of  $L_c$  and  $S_c$ , having configuration  $\gamma_j$  and mixing coefficient  $a_j$ . The MCHF wave function for a continuum final state with energy  $E$ , label  $\gamma$ , and term  $LS$  is written in the form

$$\Psi_f(\gamma LS; N+1) = \Psi_c(L_c S_c; N) \phi_{kl} + \sum_i^m c_i \Phi(\gamma_i LS; N+1), \quad (2)$$

where  $\phi_{kl}$  is the one-electron continuum orbital with orbital angular momentum  $l$ . The first term on the right-hand side represents the coupling of the  $N$ -electron ionic-core wave function with a single continuum electron to yield an antisymmetric configurational state for the  $(N+1)$ -electron system with the designated term value and configuration. The second term is the sum of  $(N+1)$ -electron bound-state configurations which are eigenstates with the same  $L$  and  $S$ , as indicated above, and are included to accommodate orthogonality and the effects of core polarization in the final-state wave functions.

The coefficients  $a_j$  and a set of radial functions  $P_j(r)$ ,  $j=1, 2, \dots, N_c$  describing the ionic-core wave function are determined from a separate MCHF calculation and are kept fixed for the purpose of the final-state continuum wave-function calculation. The coefficients  $c_i$  and a set of radial functions  $P_i(r)$ ,  $i=1, 2, \dots, N_f$ , which describe the bound and continuum orbitals, are determined variationally. All the radial functions  $P_i(r)$  are solutions of the coupled integro-differential equations of the form

$$\left[ \frac{d^2}{dr^2} + \frac{2Z}{r} - \frac{l(l+1)}{r^2} \right] P_i(r) = \frac{2}{r} [Y_i(r)P_i(r) + X_i(r) + I_i(r)] + \sum_{i'} \varepsilon_{ii'} P_{i'}(r), \quad (3)$$

where the off-diagonal energy parameters  $\varepsilon_{ii'}$  are related to Lagrange multipliers that ensure orthogonality assumptions. On the right-hand side  $(2/r)Y_i(r)$  is the screening potential,  $(2/r)X_i(r)$  is the exchange function, and  $(2/r)I_i(r)$  represents terms arising from interaction between the configuration states.

The boundary conditions satisfied by the bound radial functions are

$$P_i(r) \xrightarrow{r \rightarrow 0} r^{l+1}, \quad P_i(r) \xrightarrow{r \rightarrow \infty} 0. \quad (4)$$

In this case the diagonal energy parameters  $\varepsilon_{ii}$  are eigenvalues of the integro-differential equations and are to be determined. The radial functions for the continuum orbital satisfy the following boundary conditions:

$$P_i(r) \xrightarrow{r \rightarrow 0} r^{l+1},$$

$$P_i(r) \xrightarrow{r \rightarrow \infty} (2/\pi k)^{1/2} \sin[kr - l\pi/2 + (q/k)\ln(2kr) + \sigma_l + \delta_l], \quad (5)$$

where  $\sigma_l = \arg[\Gamma(l+1-iq/k)]$  is the Coulomb phase shift,  $q = Z - N$  is the net charge of the ion, and  $\varepsilon_{ii} = -k^2$ ,  $k^2$  being the kinetic energy of the photoelectron.

The coupled integro-differential equations are solved numerically by the iterative method. The multiconfiguration (MC) self-consistent field (SCF) procedure is applied to compute both the bound and the continuum wave functions, with the same numerical procedures being used for both. The bound radial functions are essentially localized and vary smoothly as  $r \rightarrow \infty$ . The continuum radial function is normalized by fitting the computed values at two adjacent points to the regular and irregular Coulomb functions as soon as the region is reached where the direct and exchange potentials are vanishingly small. This may be at a considerably smaller value of  $r$  than the asymptotic form represented by the boundary condition of Eq. (5).

The coefficients  $c_i$  are solutions of the system of equations

$$\sum_{i'=1}^m \langle \Phi_i | H - E | \Phi_{i'} \rangle c_{i'} + \sum_{j=1}^{m_c} \langle \Phi_i | H - E | \Phi_j \rangle a_j = 0, \quad i = 1, \dots, m \quad (6)$$

where

$$\Phi_j = \Phi(\gamma_j L_c S_c; N) \phi_{kl}, \quad j = 1, \dots, m_c$$

and

$$\Phi_i = \Phi(\gamma_i LS; N+1), \quad i = 1, \dots, m.$$

As indicated above, the  $a_j$  are regarded as constants for the calculation of the continuum function.

### III. COMPUTATIONAL PROCEDURE

Taking a clue from the experimental results, we considered the following processes:

$$\hbar\omega + \text{Be}(1s^2 2s^2 \ ^1S) \rightarrow \text{Be}^+(1s 2s^2 \ ^2S) + e^-(kp) \ ^1P^\circ, \quad (7a)$$

$$\hbar\omega + \text{Be}(1s^2 2s^2 \ ^1S) \rightarrow \text{Be}^+(1s 2s \ (^1S) 2p) + e^-(ks) \ ^1P^\circ, \quad (7b)$$

$$\hbar\omega + \text{Be}(1s^2 2s^2 \ ^1S) \rightarrow \text{Be}^+(1s 2s \ (^3S) 2p) + e^-(ks) \ ^1P^\circ. \quad (7c)$$

In order to study the effects of electron correlation in both the initial and the final states, we performed the calculations in the multiconfiguration Hartree-Fock approximation, as described in the previous papers.<sup>11–13</sup> Briefly, the set of bound radial functions was determined with the traditional MCHF method;<sup>14</sup> the modified MCHF method<sup>13</sup> was applied to determine a set of bound and continuum wave functions for a range of kinetic energies of the continuum electron.

Particular attention was paid to the inclusion of double electron excitations which give rise to the autoionization features that characterize the spectrum. In so doing we capitalize on the accuracy with which the MCHF theory can compute energy levels, thereby making possible identification of these resonances.

Let us first of all consider the ionization (7a). The initial state is the ground state of Be. The MCHF wave-function expansion for this state was over the set of two configurations  $\{1s^2 2s^2, 1s^2 2p^2\}$  coupled to form a  $^1S$  term. As they belong to the same complex, these two configurations mix very strongly. The  $1s$  radial function was kept fixed to the  $1s$  orbital of the initial ground state during the remainder of the calculation. Other orbitals and the mixing coefficients were obtained variationally.

The final-state continuum wave-function configuration adopted in the present study is comprised of the 16 terms arising from the configurations

$$\begin{aligned} &\{1s 2s^2 kp, 1s 2p^2 kp, 1s 2s \ (^1S) 2p 3s, 1s 2p^3, \\ &1s 2s \ (^3S) 2p 3s, 1s 2s \ (^1S, ^3S) 2p 3d, 2s^2 2p 3s, \\ &1s 2p 3s^2, 1s 2p \ (^1P, ^3P) 3s 3d, 1s 2s^2 2p, \\ &2s 2p^3, 1s 2p \ (^1P) 3d^2 \ (^1S, ^1D), 1s 2p \ (^3P) 3d^2 \ (^3P)\} \ ^1P^\circ. \end{aligned}$$

The  $1s$ ,  $2s$ , and  $2p$  orbitals are those obtained from the  $\text{Be}^+$  core state calculation, whereas the  $kp$  continuum function, the virtual  $3s, 3p$  orbitals, and the configuration-mixing coefficients  $c_i$  of Eq. (2) are optimized at each photon energy.

For the process (7b), we performed Hartree-Fock (HF) calculations for both the initial bound state and the final ionic-core state. In the HF calculation of the  $\text{Be}^+$  core state  $2s$  and  $2p$  orbitals are varied while keeping the  $1s$  orbital fixed to the HF  $1s$  orbital of the initial ground state. The final continuum state consists of two configurations  $\{1s 2s \ (^1S) 2p ks, 1s 2s \ (^3S) 3s 3p\}$  of the  $^1P^\circ$  state. Here the  $1s$ ,  $2s$ , and  $2p$  orbitals are kept fixed to the ionic-core state; the  $3s$  and  $3p$  orbitals are varied simultaneously along with the continuum  $ks$  orbital at each kinetic energy of the photoelectron.

Finally, in the process (7c), Hartree-Fock calculations were performed for the initial bound state and the final ionic-core state as in the previous case. In the HF calcu-

lation of the ionic state, the  $1s$  orbital is that obtained from the initial bound-state HF calculation, whereas the  $2s$  and  $2p$  orbitals are obtained variationally. Final continuum state wave functions are obtained from the MCHF calculation with two configurations  $\{1s 2s \ (^3S) 2p ks, 1s 2s \ (^1S) 3s 3p\}$  of the  $^1P^\circ$  state. In this case also, the virtual orbitals  $3s$  and  $3p$  and the continuum orbital  $ks$ , along with the virtual state mixing coefficients, are optimized at each kinetic energy of the photoelectron.

## IV. RESULTS

### A. Energy levels

As mentioned earlier, in process (7a) the initial bound-state wave functions were determined by the MCHF method.<sup>14</sup> The initial bound state of beryllium consists of two configurations  $\{1s^2 2s^2, 1s^2 2p^2\}$  which mix very strongly. The mixing coefficients for the set are  $\{0.9507313, 0.3100160\}$ , respectively. The binding energy obtained using this pair was  $-14.616063$  a.u. whereas the Hartree-Fock energy derived from use of a single configuration is  $-14.573023$  a.u. MCHF ionic-core wave functions are obtained from a similar set of two configurations which also mix strongly  $\{1s 2s^2, 2s 2p^2\} \ ^2S$ . The mixing coefficients for the set are  $\{0.932478, 0.361228\}$ , respectively.

In Table I, the HF energy levels of different states of the different configurations are presented relative to the ground state of the beryllium atom obtained in the HF approximation. In the HF calculation of  $1s 2s^2 \ ^2S$  and the  $1s 2s \ (^1S, ^3S) 2p \ ^2P$  states, the  $1s$  orbital was kept fixed to the HF  $1s$  orbital of the ground state. In the HF calculation of the remaining configurations all the orbitals were varied except  $1s$  and  $2s$ , which were kept frozen to the HF  $1s$  and  $2s$  orbitals of the ionic state.

TABLE I. Hartree-Fock (HF) energy levels relative to ground state of beryllium (HF energy =  $-14.573023$  a.u.).

Configuration state	Energy (eV)
$1s 2s^2 \ ^2S$	123.28
$1s 2s \ (^1S) 2p \ ^2P^\circ$	128.64
$1s 2s \ (^3S) 2p \ ^2P^\circ$	129.08
$1s 2s \ (^1S) 2p 3s \ ^1P^\circ$	126.28
$1s 2s \ (^3S) 2p 3s \ ^1P^\circ$	126.37
$1s 2p^3 \ ^1P^\circ$	126.31
$1s 2s \ (^3S) 2p 3d \ ^1P^\circ$	127.64
$1s 2s \ (^1S) 2p 3d \ ^1P^\circ$	127.63
$1s 2s \ (^3S) 2p 4s \ ^1P^\circ$	127.83
$1s 2s \ (^1S) 2p 4s \ ^1P^\circ$	127.78
$1s 2s \ (^3S) 3s 3p \ ^1P^\circ$	135.00
$1s 2s \ (^1S) 3s 3p \ ^1P^\circ$	138.40
$1s 2s \ (^3S) 3s 4p \ ^1P^\circ$	136.38
$1s 2s \ (^1S) 3s 4p \ ^1P^\circ$	139.22
$1s 2s \ (^1S) 3d 4p \ ^1P^\circ$	137.93
$1s 2s \ (^3S) 3d 4p \ ^1P^\circ$	141.18

In Table II, energy levels obtained from MCHF calculations are presented relative to the MCHF energy of the initial ground state. The energy of the  $^1P^\circ$  state of the configuration  $1s2s(^1S)2p3s$  was obtained using 14 bound state configurations

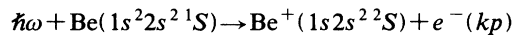
$$\{1s2s(^1S)2p3s, 1s2p^3, 1s2s(^3S)2p3s, \\ 1s2s(^1S, ^3S)2p3d, 2s^22p3s, 1s2p3s^2, \\ 1s2p(^1P, ^3P)3s3d, 1s2s^22p, 2s2p^3, \\ 1s2p(^1P)3d^2(^1S, ^1D), 1s2p(^3P)3d^2(^3P)\}^1P^\circ.$$

In this calculation,  $1s$ ,  $2s$ , and  $2p$  orbitals are taken from the MCHF calculation of the ionic-core state. The energies of the  $1s2p^3^1P^\circ$  and the  $1s2s(^3S)2p3s^1P^\circ$  states are obtained from a configuration-interaction (CI) calculation with the same 14 configurations.

### B. Cross sections

In Fig. 1 are shown the experimental results and the calculated results within the HF approximation for the three partial cross sections listed at the beginning of Sec. III. As the length and velocity forms of the calculation give results which are very close to each other, only the length forms are shown in the figure. The experimental results for all three final states, which were not absolute, have been normalized to the theoretical value for the  $^1S$  curve at an energy of 140 eV. This makes possible a comparison between the experimental partial cross sections and the theoretical partial cross sections for each channel. As this is a single-configuration calculation, no structure is seen in the theoretical curve. However, the agreement of the theoretical result with the experimental result for each channel is impressive. The only curve which stands out is the  $^1P$ , where the theoretical result is much smaller. However, the cross section itself is so small that the absolute value is more sensitive to the normalization. The agreement at threshold is quite good. The divergence at the higher energies could also be accounted for by contributions from resonances not included in the theory which are manifest in the experiment.

The calculated partial photoionization cross section using the full MCHF scheme over the region 123.6–130 eV for the process



is shown in Fig. 2. For comparison, the theoretical curve calculated in the HF approximation from Fig. 1 is shown.

TABLE II. Multiconfiguration Hartree-Fock (MCHF) energy levels relative to ground state of beryllium (MCHF energy =  $-14.616063$  a.u.).

Configuration state	Energy (eV) (theory)	Energy (eV) (experiment)
$1s2s^2^2S$	123.70	123.56
$1s2s(^1S)2p3s^1P^\circ$	125.15	125.10
$1s2p^3^1P^\circ$	126.80	126.90
$1s2s(^3S)2p3s^1P^\circ$	127.82	127.90

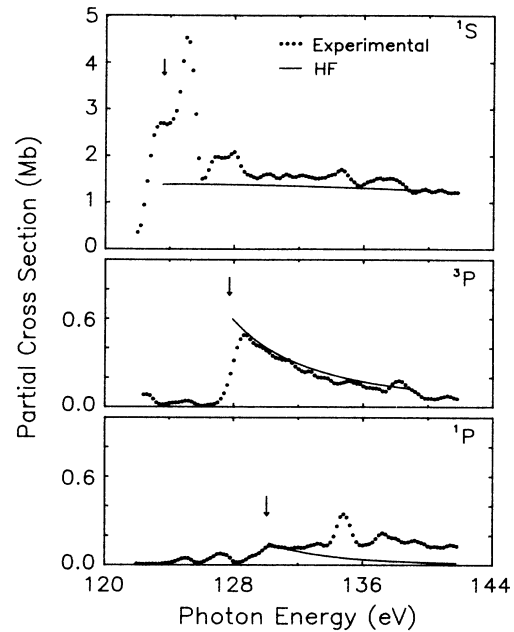


FIG. 1. Partial cross sections for the three major decay channels in  $K$ -shell photoionization of Be evaluated in the HF approximation. For comparison, shown are the experimental results (dotted lines) normalized to the theoretical value at 140 eV on the  $^1S$  curve. Arrows indicate the thresholds for production of the ionic states. In characterizing these states we have used the experimental  $^{1,3}P$  designations rather than the theoretical  $^{1,3}S$  designations given in Eq. (7).

Again, only the length cross section is plotted. Also shown are the experimental results of Krause and Caldwell,<sup>8</sup> normalized to the HF results at 140 eV as discussed above. From the figure, it is seen that the theoretical results are in excellent agreement with the experi-

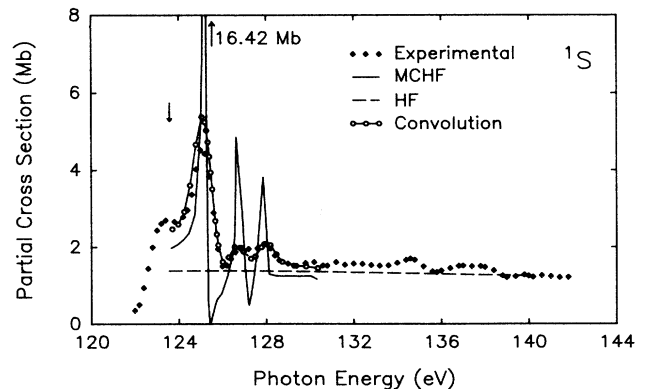
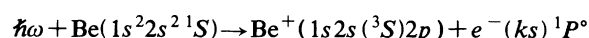


FIG. 2. Partial cross section for  $K$ -shell photoionization of Be resulting in the ground-state ion. The theoretical result (solid line) from threshold to 128 eV is a full MCHF calculation. For comparison, shown are the experimental results (dotted line) and a convolution of the theoretical result with a Gaussian slit function of width 272 meV (dot-dashed line). The HF results are given as the dashed line.

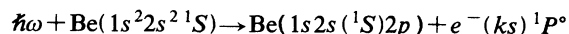
mental observations. The theoretical calculation shows three resonance structures in the  $^1S$  cross section. These resonances are due to the presence of the bound states  $1s2s(^1S)2p3s^1P^\circ$  at 125.15 eV,  $1s2p^3^1P^\circ$  at 126.80 eV, and  $1s2s(^3S)2p3s^1P^\circ$  at 127.82 eV. The positions of these resonances agree very well with the experimental identification. For better comparison, also shown is a convolution of the theoretical curve with a slit function characteristic of the monochromator. The resolution was good enough to separate the first state well, but the other two overlap in the experiments. At photon energies higher than 128 eV, the theoretical cross section decreases very slowly, which is in agreement with experiment.

The calculated partial photoionization cross section for the process



is presented in Fig. 3(a) as a function of photon energy. As before, experimental results are also plotted in the same figure with the same 140 eV normalization. It is seen from the theoretical curve that there is a sharp decrease in the cross section from threshold to 136 eV. This is in excellent agreement with the experimental results. Both theoretical and experimental results show a resonance at 138.40 eV. This autoionization resonance is due to the presence of the bound state  $1s2s(^1S)3s3p^1P^\circ$ .

In Fig. 3(b), the theoretical and experimental cross sections in the length form for the process



are plotted as a function of photon energy. The velocity cross sections agree very well so are not shown. The theoretical cross section shows a resonance at 135.00 eV due to the  $^1P^\circ$  state of the  $1s2s(^3S)3s3p$  configuration. The position of this resonance agrees remarkably well with that of the experimentally observed resonance. While it can be seen from the figure that the experimental cross section varies slowly with the increase in photon energy, this is not true of the theoretical result. The latter shows the same rather rapid decay characteristic of the  $^3P$  cross section for process (7b). For neither process (7b) nor (7c) were we able to perform a successful convolution analysis. This derives from the fact that the convolution analysis becomes very inaccurate when the resonance is extremely sharp compared to the slit width of the monochromator. While the results for process (7a) are reasonable, due to the fact that the resonance widths are large, the convolution for (7b) and (7c) would be meaningless.

It should be mentioned that the present MCHF method, at the moment, cannot handle the interchannel coupling between the open channels. However, the method very efficiently takes into account the coupling between a number of closed channels and a single open channel. The number of small features that are present in the experimental curves of Figs. 2 and 3 above 128 eV are not present in the theoretical results. This may be due to the neglect of the interchannel coupling between the open channels.

## V. CONCLUSIONS

While the application of the multiconfiguration Hartree-Fock method to calculations of photoionization cross sections for valence levels has already been shown to be quite effective,<sup>11,12</sup> the results obtained for the *K*-shell photoionization of Be show that it can also deliver quite good results for the calculation of inner-shell photoionization cross sections. Application of the technique to this process entails freezing the inner-shell orbitals to those appropriate to the atom or ion with the hole filled. However, given the quite good agreement that is obtained with the experiments of Krause and Caldwell,<sup>8</sup> doing this introduces negligible error in the calculation. The beauty of this MCHF technique is that the electron correlations can be introduced in an *ab initio* manner. These effects, which are found to be very important for the partial photoionization cross section leaving the ion in the  $^2S$  state, have been taken into account very accurately through the configuration-interaction procedure. Although not all autoionization resonances were included in the calculation, the positions of those which were included are in excellent agreement with the experimental values. Our success in this calculation convinces us once again that the modified MCHF technique should produce reliable quantitative results for a variety of photoionization phenomena.

## ACKNOWLEDGMENTS

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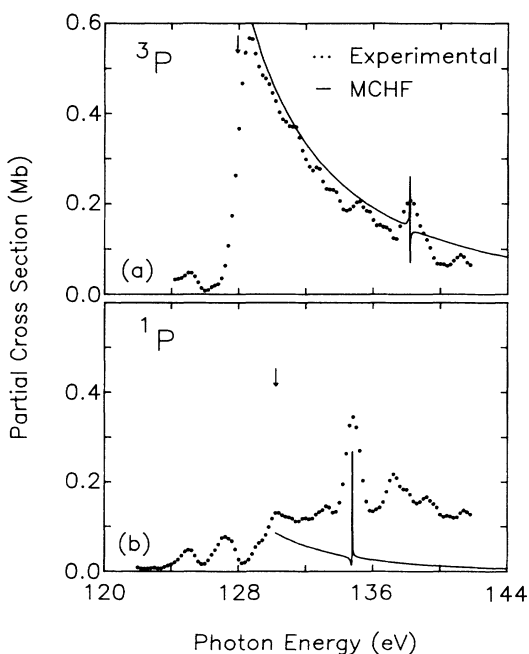


FIG. 3. Partial cross sections for production of excited-state  $\text{Be}^+$  ions following *K*-shell photoionization. (a)  $1s2s(^3S)2p$ ; (b)  $1s2s(^1S)2p$ . [Experimental *P* couplings are used rather than theoretical *S* couplings in Eq. (7)]. Dotted lines are experimental results. Note the excellent agreement between the location of the resonances in the theoretical and experimental curves.

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