

## Core-valence electron correlation effects in photodetachment of $\text{Ca}^-$ ions

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The  $R$ -matrix method has been used to perform a five-state ( $^1S$ - $^3P^o$ - $^3D$ - $^1D$ - $^1P^o$ ) close-coupling calculation on the photodetachment of  $\text{Ca}^-$  ions with photon energies from threshold to 4 eV. Calculations both with and without the core-valence electron correlation are carried out. The dominant core-valence electron correlation is included by exciting one  $3p$  electron to the valence orbitals. It has been found that the so-called core-valence correlation is quite crucial to the prediction of the position of the Cooper minimum and the distinct behavior of the photodetachment cross sections near  $^3P^o$  and  $^1P^o$  thresholds. The core-valence correlated calculation results in a Cooper minimum at 1.20 eV and a narrow shape resonance just above the  $4s4p$   $^1P^o$  threshold. These structures are in good agreement with experimental observations. The present result also supports the previous conclusion that core-valence electron correlation is responsible for reducing the electron affinity of valence-only results to much closer to the experiment.

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### I. INTRODUCTION

Negative alkaline-earth-metal ions have been extensively studied in the past decade. The growing interest in the study of alkaline-earth-metal negative ions has been stimulated by the discovery that one of these closed-shell atoms form stable negative ions [1,2]. In addition to the studies of the binding energies of the negative ions [3–14] and the studies of electron collisions with alkaline-earth-metal atoms [15–23], most recently photodetachment experiments were performed to probe the properties of the negative calcium ions. Measurement of the photodetachment cross section of the negative calcium ions can be traced back to an experiment by Heinicke *et al.* [24] more than 25 years ago. Though the total relative cross sections were obtained from 0.5 to 3.2 eV with a lesser energy resolution from a modern point of view, interesting structures, a Cooper minimum near 1.2 eV, a shoulder just above 2.0 eV, and a sharp peak around 3.0 eV were displayed clearly. More recently, relative cross sections from 1.1 to 3.1 eV were measured with a much higher energy resolution [25]. The position of the Cooper minimum was determined more precisely, and a much sharper shape resonance peak was also clarified just above the  $^1P^o$  threshold and used to determine the electron affinity of the negative ions. There have been three experiments to measure the absolute values of the cross sections. One is due to Kristensen *et al.* [26] and the other two are due to Lee *et al.* [27]. The absolute cross section at 1.39 eV was obtained by Kristensen *et al.* [26] using the state selective depletion technique, while a saturation method was used by Lee *et al.* [27] to get the absolute cross sections at 1.903 and 2.083 eV.

As for the theoretical study of the photodetachment of the negative calcium ions, only three calculations have so far been carried out. The first one is due to Gribakin *et al.* [28], the second one to Fischer and Hansen [29], and the last one to Yuan and Fritsche [30]. In the work of Gribakin *et al.* [28] the bound-state wave function of the negative ion was obtained by solving the Dyson equation to include the correlation effect. The reliability of the theory was, however, weakened by using a Hartree-Fock approximation to describe the

continuum wave function of the free electron. Fischer and Hansen dealt with a multiconfiguration Hartree-Fock scheme for both bound and free-electron states to ensure a relatively good accuracy. The calculation of Fischer and Hansen referred, however, to photodetachment cross sections below 0.12 Ry, and hence can only in part be compared to the earlier measurements of Heinicke *et al.* [24] and the later experiments of Walter and Peterson [25] and of Lee *et al.* [27]. The  $R$ -matrix method was used by Yuan and Fritsche to perform six-state close-coupling calculations on electron scattering by calcium atoms and on the photodetachment of negative calcium ions. Their results covered the energies from threshold to 4 eV and displayed the general features of the experimental result of Heinicke *et al.* [24]. Nevertheless, as energy levels of the atomic states included in the close-coupling expansion were not optimized very satisfactorily, the near-threshold behavior for  $^3P^o$  and  $^1P^o$  states showed a large distance from the most recent measurement of Walter and Peterson [25]. A mistake was also involved in the absolute value of the photodetachment cross section. The correct value should be the original one divided by 3, the orbital statistical weight of the negative ion ( $2L+1$ ), which was lost in the original program. The most significant incompleteness of the theory is that the so-called core-valence electron correlation was excluded completely. This problem exists in Fischer and Hansen's work too.

Many authors have investigated the binding energy of the negative calcium ion. In an extensive multiconfigurational Hartree-Fock (MCHF) calculation, Fischer [3] arrived at an electron affinity of 70 meV without the relativistic corrections. This value was believed to be the correct limit of a valence-only calculation. Nevertheless, the experiment of Walter and Peterson [25] gave a much smaller value of 18.4 meV compared with the earlier experiment [1] and the valence-only calculation [3]. More recently, accurate values of 24.55 and 19.73 meV were obtained in the experiment of Petrunin *et al.* [14], respectively, for the two fine-structure components  $4p_{1/2}$  and  $4p_{3/2}$  of the ionic ground state. Meanwhile, some calculations showed that the calculated electron affinity of  $\text{Ca}^-$  is reduced considerably when the core-

valence electron correlation is considered [10–12]. In our most recent calculation, it was shown that the core-valence electron correlation has considerable effects on the very-low-energy electron scattering from calcium atoms [31]. In that work, however, the energy levels of the atomic states were still far from satisfactory. In the present study, it will be shown that the core-valence electron correlation has more significant influence on the photodetachment cross sections of the  $\text{Ca}^-$  ion. In particular, the Cooper minimum and the shape resonance peak just above the  $^1P^o$  threshold can be predicted accurately when much better atomic levels are obtained by incorporating the core-valence electron correlation.

## II. METHOD OF CALCULATION

The  $R$ -matrix method for electron-atom and photon-atom interactions has been discussed in great detail by Burke *et al.* [32]. The present calculations have been carried out by using the latest Belfast atomic  $R$ -matrix codes [33]. In an  $R$ -matrix calculation, the wave function of the  $N+1$  electron system is given the form

$$\Psi_k(X_1 \dots X_{N+1}) = \hat{A} \sum_{ij} c_{ijk} \Phi_i(X_1 \dots X_N \hat{\mathbf{r}}_{N+1} \sigma_{N+1}) \times u_{ij}(r_{N+1}) + \sum_j d_{jk} \phi_j(X_1 \dots X_{N+1}), \quad (1)$$

where  $\hat{A}$  is the antisymmetrization operator to take the exchange effect between the target electrons and the free electron into account.  $X_i$  stands for the spatial ( $\mathbf{r}_i$ ) and the spin ( $\sigma_i$ ) coordinates of the  $i$ th electron. The functions  $u_{ij}(r)$  under the first sum construct the basis sets for the continuum wave functions of the free electron, and  $\Phi_i$  are the coupling between the target states and the angular and spin part of the free electron. The correlation functions  $\phi_j$  in the second sum are constructed by the square integrable orbitals to account for the correlation effects not adequately considered because of the cutoff in the first sum. The square integrable orbitals are cast as linear combinations of Slater-type orbitals

$$P_{nl} = \sum_j C_{jnl} r^{l+jn} \exp(-\xi_{jnl} r), \quad (2)$$

in which the number of Slater-type orbitals necessary to sufficiently approximate these orbitals  $P_{nl}$  increases as the number of spherical nodes of  $P_{nl}$  becomes larger. The pertinent parameters and coefficients  $C_{jnl}$  for  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ , and  $3p$  orbitals are nearly identical with those of the Hartree-Fock orbitals given by Clementi and Roetti [34] for the Ca ground state, but are readjusted after more electron configurations are included. In addition to these core orbitals, another set of seven valence orbitals ( $4s, 4p, 3d, \overline{5s}, \overline{5p}, \overline{4d}$ , and  $\overline{4f}$ ) is employed in constructing the wave function. The parameters in Eq. (2) are optimized independently by using the proven CIV3 computer code [35] to fit the energy levels of atomic Ca. To start the optimization procedure, the initial forms of

TABLE I. Calculated relative positions (in eV) of the first four excited states of Ca compared with experimental values.

| State | Theory           |                  | Experiment       |
|-------|------------------|------------------|------------------|
| $^1S$ | 0.0 <sup>a</sup> | 0.0 <sup>b</sup> | 0.0 <sup>c</sup> |
| $^3P$ | 1.8848           | 1.7319           | 1.8924           |
| $^3D$ | 2.5318           | 2.9479           | 2.5239           |
| $^1D$ | 2.7429           | 2.9528           | 2.7090           |
| $^1P$ | 2.8883           | 2.8905           | 2.9325           |

<sup>a</sup>The present core-valence correlated result.

<sup>b</sup>The present valence-only result.

<sup>c</sup>The experimental data from Ref. [37].

the above seven valence orbitals are chosen to be the one-configuration Hartree-Fock results. In the following multi-configurational calculations, the orbitals  $4s, 4p, 3d$ , and  $\overline{5s}$  are used to minimize the ground-state energy of the atom,  $\overline{5p}$  to minimize the energies of both the ground state and the first  $^1P^o$  excited state, and  $\overline{4d}$  and  $\overline{4f}$  to minimize the first  $^3D$  excited state. The procedure is repeated to arrive at a self-consistent result. The final forms of  $4s, 4p$ , and  $3d$  are not quite far from the initial ones, while  $\overline{5s}, \overline{5p}, \overline{4d}$ , and  $\overline{4f}$  are significantly different from the corresponding valence orbitals. The bar over the orbital symbols indicates their pseudo-orbital characteristics. Generally speaking, the first sum in Eq.(1) runs over an infinite number of excited bound states and continuum states of the atom [36]. In order to make the calculations manageable, some pseudostates are often included to account for the effects of the highly excited states and continuum states approximately [36]. Though in the present case the orbitals with a bar over them are included to improve the target states, they can take the effects of continuum states in part. The fact is that all the one-configuration states of the kind  $4s n\overline{l}$  except  $4s \overline{5p} ^3P^o$ , where  $n\overline{l}$  refers to the above pseudostate-type orbitals, lie above the Hartree-Fock ionization threshold of the atom. For the intermediate-energy processes, much more pseudo-orbitals must be included carefully in order to treat the excitation or ionization processes efficiently, but for the very-low-energy processes it is not necessary.

The calculated atomic energy levels are listed in Table I compared with the experimental data [37]. One can find that the core-valence electron correlation brings the atomic energy levels much closer to the experimental data. An  $R$ -matrix radius of 200 a.u. was chosen to ensure that the wave function of the very weakly bound electron is completely wrapped within the  $R$ -matrix sphere. In forming the  $(N+1)$ -electron configurations in Eq. (1), all possible excitations of the two  $4s$  valence electrons and a  $3p$  core electron, which takes the main part of the core-valence electron correlation into account, into any of the seven valence orbitals are allowed for only excluding the possibility of having more than two electrons in the  $\overline{4f}$  orbital. This rule is also applied to the calculation of the atomic eigenstates. As for the construction of the continuum states, each of the angular-momentum orbitals is expressed as a linear combination of 80 numerical basis functions.

### III. RESULTS AND DISCUSSION

To start our discussion, we give more details about the calculation of the atomic levels as well as the bound negative-ion states. We use a configuration-interaction (CI) wave function to describe the atomic ground and excited states appearing in the close-coupling expansion. The radial part of the wave function is constructed by using analytic Slater-type basis functions. As mentioned in Sec. II, the pertinent parameters have been optimized to fit the atomic levels. This is not a simple multiconfiguration Hartree-Fock self-consistent calculation, as we have to get all the five atomic states in the close-coupling expansion rather than only one of them, for example the ground state, fit the true position as close as possible. The practice showed that this is impossible unless the core-valence electron correlation is involved in the calculation. Even then these Slater-type bases are still less suited to describe the rather diffuse loosely bound negative-ion states. Fortunately, an algorithm for the bound state has been included in the *R*-matrix computer code employed in the present calculations. The CI expansion constructed by the analytic Slater-type basis functions for the negative-ion state is represented by the second term in the right-hand side of Eq. (1). It has been mentioned that this CI expansion for the negative-ion state is far from sufficient, in particular for the core-valence correlated calculation. This incompleteness can be improved effectively by the first term of the close-coupling wave function of Eq. (1). An electron affinity of 60 meV is obtained by our valence-only calculation, which is close to the valence-only calculation limit of 70 meV obtained by Fischer [3]. By including the core-valence correlation, our value is 29 meV, which is close to the most recent experiment of Petrunin *et al.* [14] who reported precise values with the fine structure being resolved. Without the first term, i.e., with a simple CI calculation by using the CIV3 computer code, we get the ground-state negative ion 93 meV above the ground state of the neutral atom for the valence-only treatment, and 121 meV for the core-valence correlated calculation. The new Belfast *R*-matrix code does not calculate the contributions to the matrix elements from the wave functions outside the *R*-matrix sphere, so that we have to choose a large enough *R*-matrix radius of 200 a.u. In order to make a convergent expansion, up to 80 numerical basis functions for each angular momentum are included in the first term of Eq. (1).

When the early experiment of Heinicke *et al.* [24] on the photodetachment of  $\text{Ca}^-$  ions was carried out, the existence of a stable negative  $\text{Ca}^-$  ion was not known yet and hence the interpretation of the experiment lacked conclusiveness. Nowadays, it is believed [38,25] that the  $\text{Ca}^-$  ion beam in the experiment of Heinicke *et al.* was predominantly in the  $^2P$  ground state. Therefore, comparisons will be given between our theory and the experiments of Heinicke *et al.* [24], of Walter and Peterson [25], of Kristensen *et al.* [26], and of Lee *et al.* [27].

The results of the present calculation on the total photodetachment cross section are shown in Fig. 1 along with the four sets of experimental data mentioned above. The first two sets of experimental data were originally given in arbitrary

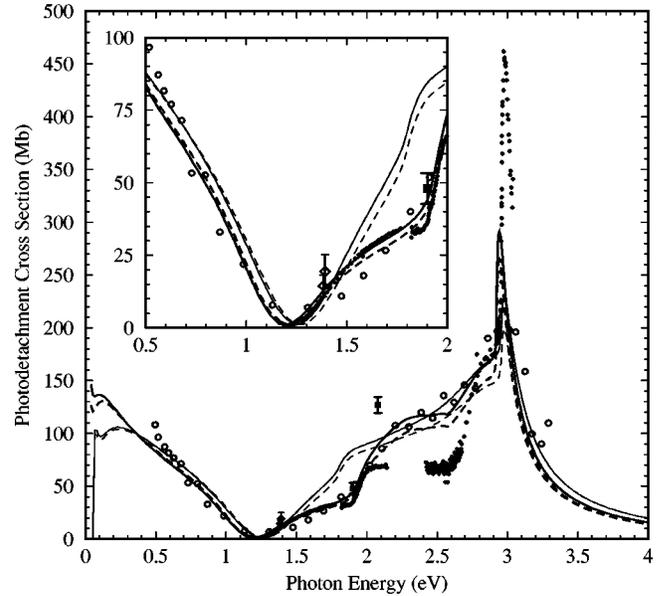


FIG. 1. Total photodetachment cross sections. The thick solid and dashed lines are, respectively, the length and velocity forms, respectively, of the present core-valence correlated results. The thin solid and dashed lines represent the length and velocity forms, respectively, of our valence-only calculation. Dots are the experimental data of Walter and Peterson [25]. Open circles represent the experimental points of Heinicke *et al.* [24]. The filled squares at 1.903 and 2.08 eV give the absolute values of Lee *et al.* [27] with error bars. Two open diamonds at 1.39 eV belong to the experiment of Kristensen *et al.* [26].

units. We have scaled them appropriately to alleviate a comparison with our results. The data of Heinicke *et al.* [24] are scaled to fit our results below the Cooper minimum point, because the theoretical results in this energy region are less sensitive to the threshold effect. The data of Walter and Peterson are scaled to our core-valence correlated result at 1.5 eV also below the first excitation threshold. Obviously the main features of the experiments are fairly well described by our calculation. In particular, for the photon energies below 2 eV, the core-valence correlated calculation gives good agreement with all the experiments. The position of the Cooper minimum is predicted accurately in coincidence with the higher-energy resolution measurement of Walter and Peterson. At 1.39 eV, our results go through within the error bar of the absolute measurement of Kristensen *et al.* The absolute cross section given by Lee *et al.* at 1.903 eV lies also very close to our core-valence calculation curves. The inset in Fig. 1 gives an expanded view of the comparison around the Cooper minimum. Above 2 eV, the opening of more than one photodetachment channels and the threshold effects complicate the problem. The experimental data are scattered among the plotted three sets. Apparently, the difference between Heinicke *et al.* and Walter and Peterson's experiments is hard to explain by the poor energy resolution used by the former authors. Our calculations reproduce the energy dependence of the photodetachment cross sections observed in the experiment of Heinicke *et al.* The shape resonance peak just above the  $^1P^o$  threshold explored by Walter and Peter-

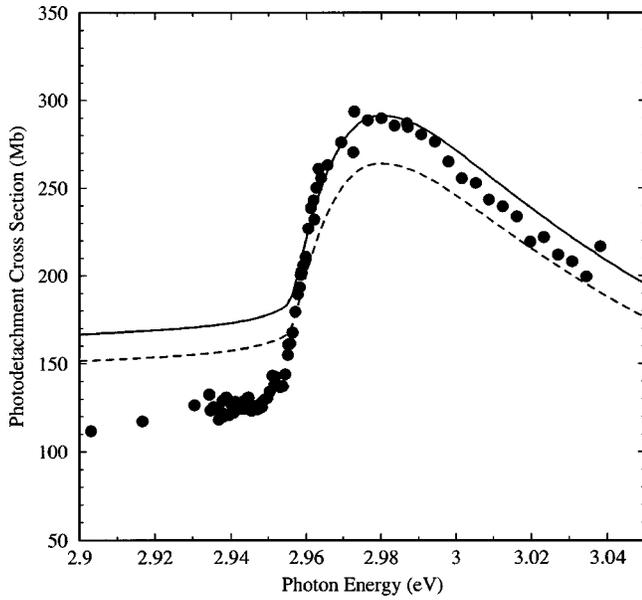


FIG. 2. A comparison in details between theory and experiment for the sharp peak at 3 eV. The measured top of the peak [25] is scaled to the length form of our core-valence correlated calculation, which has been shifted 0.04 eV to fit the observed  $^1P^o$  threshold energy.

son is predicted clearly by our calculation, though large discrepancies are found above 2 eV. Even the details in the shape and width of the structure are produced quite well. In Fig. 2, the top part of the measured shape resonance peak is scaled to our theory, but the theoretical curves are shifted 0.04 eV up to fit the measured threshold energy. One can see that both shape and width of the structure are fitted well in details.

A set of valence-only results is also presented in Fig. 1. This set of results is obtained by excluding any excitations of electrons from core to valence orbitals. In Table I, one has seen that the atomic levels are much worse for the valence-only calculation. Therefore, the shoulder observed in experiments around 2 eV is moved down to 1.8 eV in our valence-only results. The shape resonance just above the  $^1P^o$  threshold is produced with much lower magnitude. The Cooper minimum is also moved up about 0.05 eV from the correct position.

As for the comparison with other theories, we choose the MCHF calculations of Fischer and Hansen [29]. As the free electron is only described at a Hartree-Fock level, the calculation of Gribakin *et al.* [6] is not quite reliable and will not be discussed anymore. In comparing our results to those of Fischer and Hansen, we find reasonably good agreement with our valence-only results, except that their results showed slightly lower cross section near the photodetachment threshold and a slightly higher Cooper minimum position due to a more tightly bound electron in their calculations. The main difference between our calculation and theirs resides in the description of the atomic states. They used a numerical valence-only multiconfiguration Hartree-Fock scheme to minimize the ground-state energy of the atom and the ground-state energy of the negative ion [3,29]. With the

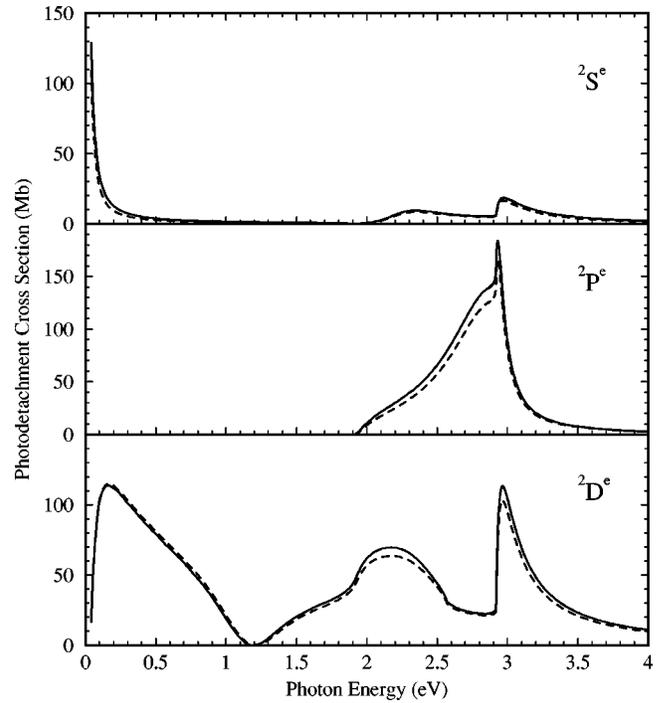


FIG. 3. Partial cross sections of the photodetachment process. The solid and dashed lines are, respectively, the length and velocity forms of the results.

same kind of basis functions (core plus  $4s, 4p, 3d, 5s, 5p, 4d, 4f$ ), our ground-state energy of the atom is  $-676.78631$  a.u. for the valence-only calculation, which is by only  $0.00074$  a.u. higher than their calculations. Our core-valence correlated ground-state energy of the atom is  $-676.80326$  a.u. As argued by Fischer and Hansen, a description of the neutral target within this range of accuracy should be sufficient because the photodetachment cross section is not sizably sensitive to the target state but rather to the continuum wave function and that of the extra electron bound to the neutral target. From our calculations, it has also been found that correct excitation energies of the atom are quite essential for an adequate description of the photodetachment process above the Cooper minimum. In the present calculations, not only the ground-state energy is minimized but also the first four excited states are calculated in good agreement with experiment. The largest error for the four excitation energies is less than  $0.045$  eV.

Partial cross sections are helpful to understand the origins of the structures presented in Figs. 1 and 2. One can see from Fig. 3, in which the partial cross sections are plotted, that the shoulder at 2 eV is a combined contribution of  $^2P$  and  $^2D$  symmetries. The increase of the  $^2P$  partial cross section is responsible for the increase of the cross section starting at 2.6 eV. The platform of the total cross section before this point is a result of the compensation between the increase of the  $^2P$  partial cross section and the decrease of the  $^2D$  partial cross section after passing a relatively broad maximum around 2.2 eV. Walter and Peterson [25] attributed the observed slower rise at 2.6 eV in their measurement to the opening of a photodetachment channel of a metastable state of the negative ions  $^4P \rightarrow ^3S + \epsilon p$ . The possible existence of

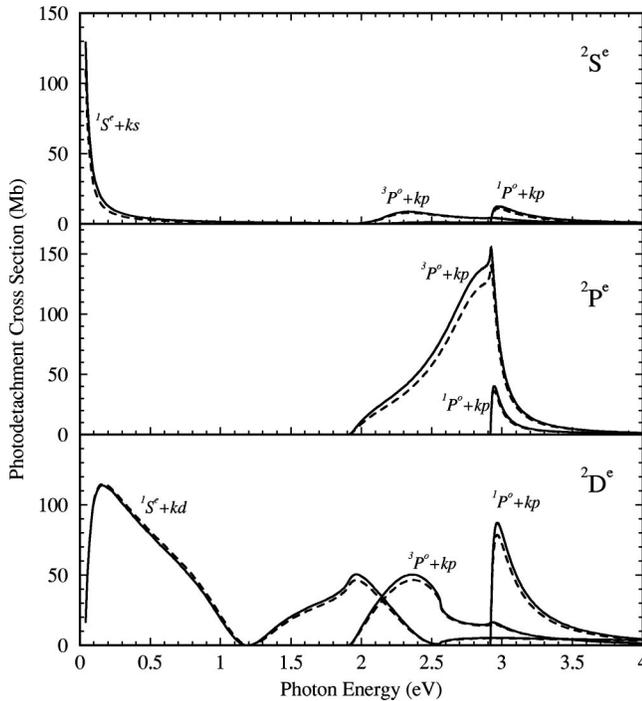


FIG. 4. The dominant contribution photodetachment channels for the three partial symmetries. The solid and dashed lines are, respectively, the length and velocity forms.

the photodetachment process of the metastable ions would make the story more complicated, because the result strongly depends on the population of the metastable ions in the ion beam and the decay rate. All the three symmetries contribute to the sharp peak just above the  $1P^o$  threshold, but the main rule is taken by the  $2D$  symmetry. Below the first excitation threshold, one is only dealing with the photodetachment channels  $(4s^21S + \epsilon s)^2S$  and  $(4s^21S + \epsilon d)^2D$ . The physics mirrored by these data is the same as that discussed by Fischer and Hansen in their  $s$ -wave and  $d$ -wave analysis.

We have also extracted from our calculation the contributions of the major ionization channels to the three partial cross sections. The result is shown in Fig. 4. As follows from the inspection of the top figure in Fig. 4, there are two weak

shape resonances related to the ionization channels  $(4s4p^3P + \epsilon p)^2S$  and  $(4s4p^1P + \epsilon p)^2S$ . From the middle of Fig. 4, it can clearly be seen that the increase of the total cross section at 2.6 eV originates mainly from the contribution of  $(4s4p^3P + \epsilon p)^2P$  ionization channel. This increase is most likely caused by the interaction between  $(4s4p^3P + \epsilon p)^2P$  and  $(4s4p^1P + \epsilon p)^2P$  channels. Channel contributions to the  $2D$  partial cross section are displayed in the bottom one of Fig. 4. The cusp around 2 eV in the detachment channel  $(4s^21S + \epsilon d)^2D$  and the broad maximum around 2.4 eV of the  $(4s4p^3P + \epsilon p)^2D$  channel reflect the channel interaction and are quite sensitive to the positions of the thresholds of  $3P^o$  and  $3D^e$ . From Fig. 4, it can be seen more clearly that the sharp peak near 3 eV is dominated by the shape resonance in  $(4s4p^1P^o + \epsilon p)$  detachment channel.

In summary, we have carried out calculations on photodetachment of  $\text{Ca}^-$  ions by using the  $R$ -matrix method. Core-valence electron correlation has been shown to be very important to reproduce the experimental observations. Accurate calculation for the Cooper minimum and the distinct threshold features depends upon adequate descriptions for both the negative-ion state and the atomic states included in the close-coupling expansion. This can only be achieved by a core-valence correlated calculation. The relative energy dependence of the photodetachment cross sections below 2 eV has been predicted in good agreement with the experiments. The absolute values of the calculated cross section at 1.39 and 1.903 eV lie also within the error bars of the experiments of Kristensen *et al.* [26] and of Lee *et al.* [27]. A shape resonance peak at 3 eV is also produced with the shape and width of the peak in good agreement with the experiment of Walter and Peterson [25]. Further independent experiments are required to clarify the scattered experimental data from 2 to 2.8 eV.

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- [1] D. J. Pegg, J. S. Thompson, R. N. Compton, and G. D. Alton, *Phys. Rev. Lett.* **59**, 2267 (1987).  
 [2] C. F. Fischer, J. B. Lagowski, and S. H. Vosko, *Phys. Rev. Lett.* **59**, 2263 (1987).  
 [3] C. F. Fischer, *Phys. Rev. A* **39**, 963 (1989).  
 [4] L. Kim and C. H. Greene, *J. Phys. B* **22**, L175 (1989).  
 [5] W. R. Johnson, J. Sapirstein, and S. A. Blundell, *J. Phys. B* **22**, 2341 (1989).  
 [6] G. F. Gribakin, B. V. Gul'tsev, V. K. Ivanov, and M. Yu. Kuchiev, *Pis'ma Zh. Tekh. Fiz.* **15**, 32 (1989) [*Sov. Tech. Phys. Lett.* **15**, 468 (1989)].  
 [7] P. Fuentealba, A. Savin, H. Stoll, and H. Preuss, *Phys. Rev. A* **41**, 1238 (1990).  
 [8] R. Cowan and M. Wilson, *Phys. Scr.* **43**, 244 (1991).  
 [9] V. Dzuba, F. Flambau, G. F. Gribakin, and D. Sushkov, *Phys. Rev. A* **44**, 2823 (1991).  
 [10] Hugo W. van der Hart, C. Laughlin, and J. E. Hansen, *Phys. Rev. Lett.* **71**, 1506 (1993).  
 [11] D. Sundholm and J. Olsen, *Chem. Phys. Lett.* **217**, 451 (1994).  
 [12] Sten Salomonson, H. Warston, and I. Lindgren, *Phys. Rev. Lett.* **76**, 3092 (1996).  
 [13] M.-J. Nadeau, X.-L. Zhao, M. Garwan, and A. Litherland, *Phys. Rev. A* **46**, R3588 (1992).  
 [14] V. V. Petrunin, H. H. Andersen, P. Balling, and T. Andersen, *Phys. Rev. Lett.* **76**, 744 (1996).  
 [15] I. I. Fabrikant, *Atomniye Protsessi* (Zinatne, Riga, 1975), p. 80 (in Russian).

- [16] N. I. Romanyuk, O. B. Shpenik, and I. P. Zapesochyi, *Pis'ma Zh. Éksp. Teor. Fiz.* **32**, 472 (1980) [*JETP Lett.* **32**, 452 (1980)]; N. I. Romanyuk, O. B. Shpenik, F. F. Papp, I. V. Chernysheva, I. A. Mandi, V. A. Kelemen, E. P. Sabad, and E. Yu. Remeta, *Ukr. Fiz. Zh. (Russ. Ed.)* **37**, 1639 (1992).
- [17] H. A. Kurtz and K. D. Jordan, *J. Phys. B* **14**, 4361 (1981).
- [18] M. Ya Amusia, V. A. Sosnivker, N. A. Cherepkov, and L. V. Chernysheva, *Zh. Tekh. Fiz.* **55**, 2304 (1985) [*Sov. Phys. Tech. Phys.* **30**, 1369 (1985)]; M. Ya Amusia and V. A. Sosnivker, *ibid.* **59**, 28 (1989); [**34**, 270 (1989)].
- [19] J. Yuan and Z. Zhang, *J. Phys. B* **22**, 2751 (1989); *Phys. Rev. A* **42**, 5363 (1990); J. Yuan, *ibid.* **52**, 4647 (1995).
- [20] A. R. Johnston, G. A. Gallup, and P. D. Burrow, *Phys. Rev. A* **40**, 4770 (1989).
- [21] G. F. Gribakin, B. B. Gul'tsev, V. K. Ivanov, M. Yu. Kuchiev, and A. R. Tančić, *Phys. Lett. A* **164**, 73 (1992).
- [22] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, *Phys. Rev. A* **44**, 4224 (1991).
- [23] R. Szmytkowski and J. E. Sienkiewicz, *Phys. Rev. A* **50**, 4007 (1994).
- [24] E. Heinicke, H. J. Kaiser, R. Rackwits, and D. Feldmann, *Phys. Lett.* **50A**, 265 (1974).
- [25] C. W. Walter and J. R. Peterson, *Phys. Rev. Lett.* **68**, 2281 (1992); J. R. Peterson, *Aust. J. Phys.* **40**, 293 (1992).
- [26] P. Kristensen, C. A. Brodie, U. V. Pedersen, V. V. Petrunin, and T. Andersen, *Phys. Rev. Lett.* **78**, 2329 (1997).
- [27] D. H. Lee, D. J. Pegg, and D. Hanstorp, *Phys. Rev. A* **58**, 2121 (1998); D. H. Lee, M. B. Poston, D. J. Pegg, D. Hanstorp, and U. Berzinsh, *ibid.* **60**, 715 (1999); D. H. Lee, M. B. Poston, D. Hanstorp, U. Berzinsh, and D. J. Pegg (unpublished).
- [28] G. F. Gribakin, B. V. Gul'tsev, V. K. Ivanov, and M. Yu. Kuchiev, *J. Phys. B* **23**, 4505 (1990).
- [29] C. F. Fischer and J. E. Hansen, *Phys. Rev. A* **44**, 1559 (1991).
- [30] Jianmin Yuan and L. Fritsche, *Phys. Rev. A* **55**, 1020 (1997).
- [31] Jianmin Yuan and C. D. Lin, *Phys. Rev. A* **58**, 2824 (1998).
- [32] P. G. Burke, A. Hibbert, and W. D. Robb, *J. Phys. B* **4**, 153 (1971).
- [33] K. A. Berrington, W. B. Eissner, and P. H. Norrington, *Comput. Phys. Commun.* **92**, 290 (1995).
- [34] E. Clementi and C. Roetti, *At. Data Nucl. Data Tables* **14**, 177 (1974).
- [35] A. Hibbert, *Comput. Phys. Commun.* **9**, 141 (1975).
- [36] M. P. Scott, P. G. Burke, and K. Bartschat, in *Photonic, Electronic and Atomic Collisions*, edited by F. Aumayr and H. Winter (World Scientific, Singapore, 1998), p. 229.
- [37] *Atomic Energy Levels*, edited by C. E. Moore, Natl. Bur. Stand. (U.S.) Title Series No. I (U.S. GPO, Washington, D.C., 1970), p. 242.
- [38] D. Hanstorp, P. Derynck, W. G. Graham, and J. R. Peterson, *Phys. Rev. Lett.* **63**, 368 (1989).