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Near-threshold photodetachment cross section of negative atomic boron ions

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By using the close-coupling R-matrix method, photodetachment cross sections of negative boron ion are studied. We calculate the electron affinity for the $B^-(2s^22p^2)$ and find that results agree better with experimental results, after taking into account excitations from $1s$ shell. We clarify both total photodetachment and partial cross section and discuss its threshold structure. Reasonable agreement of cross section between calculations and experimental data has been achieved.

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I. INTRODUCTION

Negative atomic ions play an important role in various branches of physics, ranging from astrophysics, atmospheric, and plasma physics to surface physics and accelerator physics. Now it is widely used for dating samples of archaeological or geophysical interest, oceanography, hydrology, and biomedicine [1,2]. Negative boron ions are also a good example to illustrate electron correlation effects and special attention has been paid to the photodetachment process for decades [2–5]. The major reason is that the B^- ground-state binding energy studies showed very clearly the importance of properly calculated core-core and core-valence correlation in order to obtain an accurate treatment of this six-electron system [2]. Experimental measurements for the photodetachment cross section of boron ion were performed and given at the photon energies 1.871 and 2.077 eV by Lee *et al.* [3] and with photon energies ranging from 3.37 to 4.83 eV by Kristensen *et al.* The behavior of the cross section above the threshold indicates the presence of the theoretically predicted quasibound $B(2s2p^3\ {}^3P,{}^3D)$ states [4]. In parallel to those experimental developments, there were several theoretical simulations of the photodetachment cross section. One calculation [5] was based on the many-body method in the framework of the spin-polarized random-phase approximation with exchange (SPRPAE) and thereby analogous to the calculations for the negative ions of C, Si, and Ge [6–8], which predicted a window resonance just below the excited $B(^4P)$state. However, limitations of the method of calculations were pointed out, which was developed for half-filled shells and not for open shells such as the B^- ion. The experimental results also did not reveal the window resonance structure. Ramsbottom *et al.* [9] achieved better agreement between calculations and experiment using the R-matrix method with a slight curve shift in energy owning to an improper wave function and neglect of the core-valence correlation.

Kashenock *et al.* [10] reinvestigated the collective effects in B^- photodetachment using many-body theory taking interchannel interactions, dynamic-core polarization, and screening effects into consideration. However, as the first step forward in this direction, their results for the length and velocity forms were poor because they were not self-consistent, resulting in a nonequivalence of cross sections calculated with the dipole operator in length and velocity forms. To the best of our knowledge, no better calculations results were achieved. In the present study, by using the nonrelativistic close-coupling R-matrix approach with consideration of core-valence interaction, the photodetachment cross section from threshold to 5 eV of B^- is calculated and compared with the experimental results.

II. THEORETICAL METHODS

The R-matrix method for electron-atom and photon-atom interactions has been discussed in great detail by Burke *et al.* [11]. The present calculations have been carried out by using the Belfast atomic R-matrix code [12]. The method was improved to be efficient and useful in studying photodetachment process of negative ions by our group [13,14], We will just give an outline as follow. In an R-matrix calculation, the wave function of the $N+1$ electron system is given by the form

$$\begin{aligned}\Psi_k(X_1\cdots X_{N+1}) &= \hat{A}\sum_{ij} c_{ijk}\Phi_i(X_1\cdots X_N\hat{r}_{N+1}\sigma_{N+1})\,u_{ij}(r_{N+1}) \\ &\quad + \sum_j d_{jk}\Phi_j(X_1\cdots X_{N+1}),\end{aligned} \tag{1}$$

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 (r_i) and the spin (σ_i) for coordinates of the i electron. The functions $u_{ij}(r)$ in the first sum construct the basis sets for the continuum wave functions of the free electron, and Φ_i is the coupling between the targets and the angular and spin part of the free electron. The correlation functions Φ_j in the second sum are formed from the same set of bound orbitals and must be included to compensate for the incompleteness of the continuum orbitals. They can also be used to compensate 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

$$P_{nl} = \sum_j C_{jnl} r^{I_{jnl}} \exp(-\xi_{jnl} r), \tag{2}$$

where the number of Slater-type orbitals necessary to sufficiently approximate these orbitals P_{nl} increase as the number of spherical nodes of P_{nl} becomes larger.

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TABLE I. Calculated relativistic energy levels (in eV) of the first four low-lying excited states of boron atom and electron affinity (EA) (in eV) for boron negative ion compared with experimental results.

State	A	B	C	Expt.
$2s^22p\ ^2P^o$	0.0	0.0	0.0	0.0000[a]
$2s2p^2\ ^4P$	3.5713	3.5958	3.5563	3.5518[a]
$2s^23s\ ^2S$	8.0133	7.9548	4.8869	4.9643[a]
$2s2p^2\ ^2D$	5.9848	5.9930	5.9631	5.9335[a]
EA for B^-	0.2464	0.2584	0.2584	0.2797[b]

[a] Experimental results from Ref. [15].
[b] experimental result from Ref. [16].

In the present calculations, eleven orbitals ($1s,2s,2p,3s,3p,3d,4s,4p,4d,4f,5g$) were included. Ten targets in total were taken into account, i.e., the dominant electron configurations are $1s^22s^22p(^2P^o)$, $1s^22s2p^2(^4P)$, $1s^22s^23s(^2S)$, $1s^22s2p^2(^2D)$, $1s^22s^23p(^2P^o)$, $1s^22s^23d(^2D)$, $1s^22s^24s(^2S)$, $1s^22s^24p(^2P^o)$, $1s^22s^24d(^2D)$, $1s^22s^24f(^2F^o)$. The pertinent parameters and coefficients for the first three orbitals are chosen from the Hartree-Fock orbitals given by Clementi *et al.* [17]. The rest are optimized independently using the CIV3 code [18] to make the first four energy levels of the boron atom as low as possible for the importance of these four energy levels for the position of the threshold. Meanwhile, electron affinity (EA) makes effects on the photodetachment cross section, especially on the threshold position and structure, so we take it into consideration. Table I shows the lowest four energy levels of atomic boron and the EA value of B^- ion in three cases we studied, together with the experimental energy levels of the boron atom and EA value of the negative boron ion. Case A stands for the situation where all the electrons on the $1s$ shell are kept frozen when the electrons on the $2s$ and $2p$ shells can be excited; case B where only one electron on the $1s$ shell can be excited; case C where two electrons on the $1s$ shell can be excited. In all the cases, only two electrons can be excited at the same time. We can see from Table I that better agreement is achieved between the boron atom energy levels as well as the electron affinity of the negative boron ion with the experimental result after considering the excitation of two electrons on the $1s$ shell. Especially for the B ($2s^23s\ ^2S$) state, the energy level fits the experimental one very well after considering the core-valence electron correlation effects, suggesting that the B ($2s^23s\ ^2S$) state has a strong configuration interaction with the B ($2s^24s\ ^2S$) state. In contrast to the cases of alkaline-earth-metal atoms [19,20] whose core-valence correlations reduce the EA considerably, the effects of the core electron excitations are to increase the EA of the negative boron ions.

III. RESULTS AND DISCUSSION

Some of the total photodetachment cross sections for B^- are given in Fig. 1. The solid line and dot-dashed line in Fig. 1 are the length form and velocity form of the photodetachment cross sections from our calculation, respectively. The empty circles and filled circles are the experimental results of Lee *et al.* [3] and Kristensen *et al.* [4], respectively. As shown in the figure, our length and velocity form agrees well with each other, which should be owing to the proper wave function and reasonable optimization. From the length form and velocity form formulas for photodetachment cross sections, one conclusion can be attached that the value of the R-matrix radius makes obvious effects on the length form. With larger radius, the length form result has a better precision, and the wave function approximation will be more accurate in average [11]. In the present calculation, we set the radius to 80 a.u., enough to ensure the accuracy. In Fig. 1, we also provide the theoretical result of Ramsbottom *et al.* [9] by the violet dotted line as well as length form and velocity form results of Kashenock *et al.* [10] by the green dot-dashed line and blue dashed line, respectively. Two results in the R-matrix method, by Ramsbottom *et al.* [9] and us, respectively, have similar structure, while differing much from results in SPRPAE by Kashenock *et al.* [10] with photo energy ranging from 1.5–2.5 eV. Although the present results agree well with the experimental results, there is still some discrepancy between the photon energy from 3.5–4 eV. The experimental results show a small peak, which does not appear in all the theoretical studies. We will discuss it thoroughly by analyzing the partial wave cross section and individual ionization channels cross section.

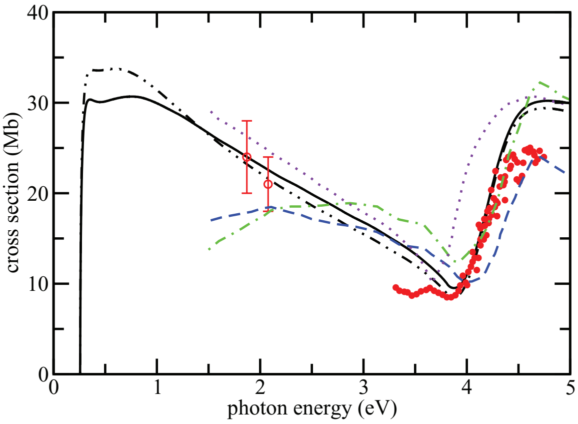

FIG. 1. (Color online) Total photodetachment cross sections of B^- for the length form (black solid line) and the velocity form (black dot-dashed line). Different colored markers correspond to different results: Experimental data: red empty circle, Lee *et al.* [3]; green filled circle, Kristensen *et al.* [4]. Other calculations: violet dot line, Ramsbottom *et al.* [9]; green dot-dashed line and blue dashed line, length form and velocity form results of Kashenock *et al.* [10].

In Fig. 2, we give three partial wave cross sections included in our calculation, where (a), (b), and (c) are partial wave cross sections from boron negative ion ^3P to $^3S^o$, $^3P^o$ and $^3D^o$ symmetry respectively, in which black solid lines stand for the length form of cross section while red dashed lines stand for the velocity form of cross section. As shown in Fig. 2, compared with $^3D^o$ and $^3P^o$ symmetry, the contribution by the $^3S^o$ symmetry is rather small. Our two forms of results agree with each other rather well, which are almost the same near the threshold position, where new channels open.

In Fig. 3, we show the main contribution of individual ionization channels to each symmetry, where solid lines stand

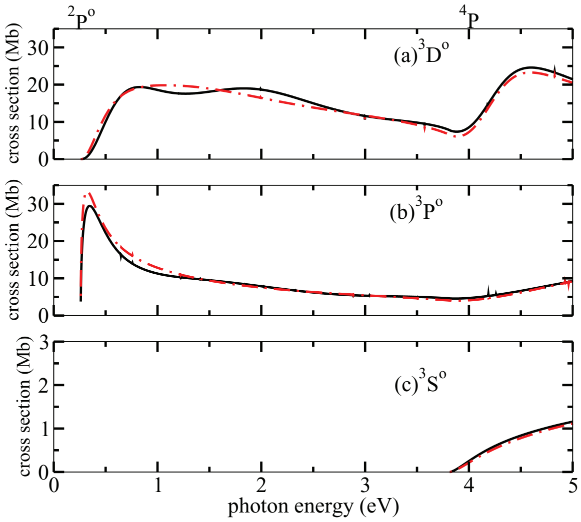

FIG. 2. (Color online) Partial cross sections in the present calculations: (a)–(c) transition from B$^-$ bound state to ^2D symmetry, from B$^-$ bound state to ^2P symmetry, and from B$^-$ bound state to ^2S symmetry, respectively. The black solid and red dashed lines denote the length and the velocity form of the cross sections, respectively.

for the length form of the cross section and dashed lines stand for the velocity form. Two forms of cross sections agree well with each other. Figures 3(a)–3(c) show partial cross sections for transition from negative boron ion bound state ^3P to boron atom $^3D^o$, $^3P^o$, and $^3S^o$ symmetry respectively. In Fig. 3(a), we plot the contribution from channels $(^2P^o + kd)\,^3D^o$, $(^4P + kp)\,^3D^o$ to the $^3D^o$ partial cross section, where $(^2P^o + kd)\,^3D^o$ is the notation of the system of a $^2P^o$ boron atom and a continuum d electron. In the present result, there is also contribution from channel $(^4P + kf)\,^3D^o$, which is small enough to be neglected. In Fig. 3(b), one can see that at lower photon energy, the cross section of the $(^2P^o + ks)\,^3P^o$ ionization channel shows typical s-wave structure [21], which is much larger than that of the $(^2P^o + kd)\,^3P^o$ ionization channel. The two cross sections come closer with increasing photon energy. When the photon energy reaches the electron affinity plus the energy of transition from atomic boron ground state to the first ionized state $2s2p^2\ ^4P$, the $(^4P + kp)\,^3P^o$ channel opens, whose contribution is relatively small. Figure 3(c) shows that the transition from ^3P to $^3S^o$ symmetry is mainly caused by the $(^4P + kp)\,^3S^o$ channel. As shown in Figs. 2 and 3, there are not any signatures identifying the existence of resonance structure between 3.5 eV and 4 eV in the experimental results we have mentioned before, so experimental results in that range could be checked out if possible.

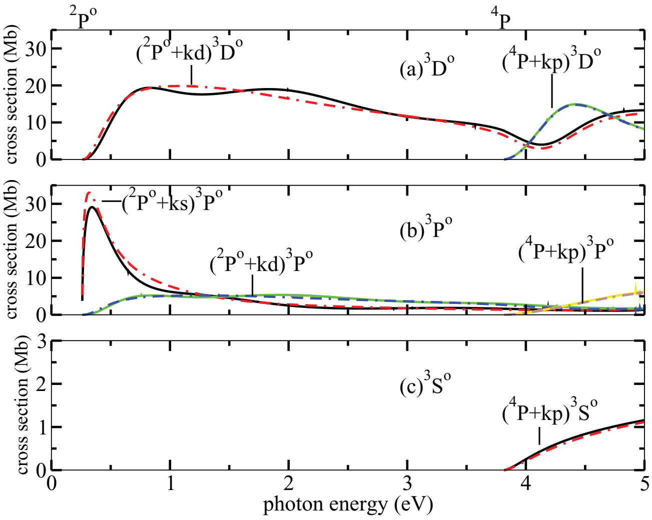

FIG. 3. (Color online) Main contribution of the individual ionization channels to the partial cross sections of B$^-$ state: (a) $(^2P^o + kd)\,^3D^o$ and $(^4P + kp)\,^3D^o$; (b) $(^2P^o + ks)\,^3P^o$, $(^2P^o + kd)\,^3P^o$ and $(^4P + kp)\,^3P^o$; (c) $(^4P + kp)\,^3S^o$. The solid and dashed lines donate the length and the velocity form of cross sections, respectively.

IV. CONCLUSION

In summary, the photodetachment cross section of B$^-$ we have obtained by the R-matrix method proves that the core-valence correlation plays an important role in the photodetachment process of B$^-$. Our results our in good agreement with the experimental data. To clarify the threshold structure of the B$^-$ photodetachment, both the partial cross section and the main contributions of the individual ionization channels to the partial cross sections were given. Further analyzing of the partial wave cross section shows that there should not be any resonance structure from 3–4 eV.

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