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MANY-ELECTRON CORRELATION IN NEGATIVE-ION PHOTODETACHMENT

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Abstract: Photodetachment cross sections for Ba^- negative ions, calculated using the random phase approximation with exchange, are presented. The photodetachment cross sections are also calculated for the outer electron of this ion. When the polarization interaction is taken into account the minimum of the cross section is drastically moved towards to low energies. The results of r and ∇ forms in this case are closer (in the limits of the used approximation).

1. Introduction

Recently the field of the negative ion physics was clarified by some extremely interesting and exciting discoveries. It was shown experimentally [1] and theoretically [2,3,4,5,6] that the negative ions of alkaline earth atoms (Ca^- $4s^24p$, Sr^- $5s^25p$, Ba^-6s^26p and Ra^-7s^27p) are formed by binding an extra electron to an atom with closed subshells. The reason for this formation is the large value of the atom's dipole polarizability. The strong polarization potential which attract the electron to the atom plays an essential role during the photodetachment of the outer electron from the ion, too.

In order to solve the negative ion photodetachment problem it is convenient to use the Dyson equation method [6] which is very applicable to low-energy electron-atom scattering [7,8] and negative ion formation [3,9]

In the present paper, the Dyson equation method is used to calculate suitable data for the determination of the photodetachment cross section for Ba^-.

Throughout the paper the atomic units are used. The numerical values of the energy are given in Ry (or eV), and the cross section are given in Mb.

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2. Basic equations

The binding energy of an electron to an atom within the negative ion can be obtained from the Dyson equation method [6]. The wave function $\varphi_E(\vec{r})$ describing the motion of the electron with energy E in the atomic field, satisfies the equation

$$H^{HF}\varphi_E(\vec{r}) + \int \Sigma_E(\vec{r},\vec{r'})\varphi_E(\vec{r'})d\vec{r'} = E\varphi_E(\vec{r}) \tag{1}$$

where H^{HF} is the static Hartree-Fock (HF) Hamiltonian of the atom, $\Sigma_E(\vec{r},\vec{r'})$ is non local energy dependent potential and it is equal to self-energy part of the single particle Green's function. This potential includes completely the correlational interaction of the extra electron with the atom.

If an atom forms a stable negative ion with electron affinity $E_A > 0$, it has discrete and small negative energy $E = \varepsilon_0 \equiv -E_A$:

$$H^{HF}\varphi_0(\vec{r}) + \int \Sigma_{\varepsilon_0}(\vec{r},\vec{r'})\varphi_0(\vec{r'})d\vec{r'} = \varepsilon_0\varphi_0(\vec{r}) \tag{2}$$

where $\varphi_0(\vec{r})$ represents the weakly bound other electron in the negative ion. The spectrum of H^{HF} includes discrete states φ_ν^{HF}, $\nu = n\ell$ (corresponding to the filled subshells of the atomic ground state), and the continuum states φ_ν^{HF}, $\nu = \varepsilon\ell$. From equation (2), it is easy to obtain

$$\varepsilon_\nu C_\nu + \sum\!\!\!\!\!\!\int_{\nu'} \langle \nu | \Sigma_{\varepsilon_0} | \nu' \rangle C_{\nu'} = \varepsilon_0 C_\nu. \tag{3}$$

By using the orthogonal relations for $\varphi_0(\vec{r})$ the coefficients C_ν are

$$C_\nu = \int \varphi_\nu^{HF^*}(\vec{r})\varphi_0(\vec{r})d\vec{r}.$$

In the relation (3) $\sum\!\!\!\!\!\!\int_{\nu'}$ denotes the summation and integration over the whole spectrum of ν' states. Set of the states ν, ν'use HF states $n\ell, \varepsilon\ell$ with fixed momentum ℓ of the negative ion binding state. Equation (3) may be considered as the eigenequation for the matrix

$$\varepsilon_\nu \delta_{\nu\nu'} + \langle \nu | \Sigma_E | \nu' \rangle \qquad (E = \varepsilon_0) \tag{4}$$

when the self-energy matrix $\langle \nu | \Sigma_E | \nu' \rangle$ have to be calculated with energy E equal to the unknown ε_0 eigenvalue.

By solving the equation (3) we get a wave function for the negative ion's external electron [9]

$$\varphi_0(\vec{r}) = \sum\!\!\!\!\!\!\int_{\nu} C_\nu \varphi_\nu^{HF}(\vec{r}). \tag{5}$$

In this paper, we have considered the lowest approximation for the amplitude of the transition of the electron energy ε_0 and orbital momentum ℓ to the continuum state of energy ε and orbital momentum $\ell \pm 1$ after the absorption of a photon of the energy ω [3]

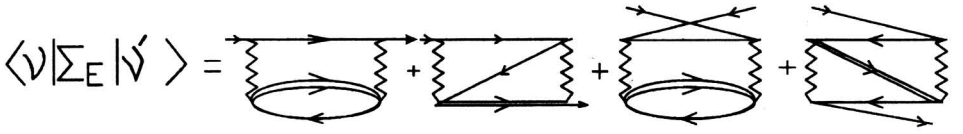
$$\mathcal{D}_{\ell\pm1}(\omega) = \int \varphi_{\varepsilon,\ell\pm1}^{HF^*} \hat{d}\varphi_0(\vec{r})\, d\vec{r}, \qquad (\varepsilon = \varepsilon_0 + \omega) \tag{6}$$

where $\hat{d}$ is the dipole operator for the interaction of the electron with the electromagnetic field. The photodetachment cross section for $\varepsilon\ell \to \varepsilon\ell \pm 1$ transition

$$\sigma_{\ell\pm1}(\omega) = \frac{4\pi^2\alpha}{\omega} |\mathcal{D}_{\ell\pm1}(\omega)|^2 \tag{7}$$

depends on the form (r or ∇) in which the $\hat{d}$ operator is used (α is the fine structure constant).

According to [8], the following basic approximation is used to calculate the self-energy matrix



where the wave function for the ν_2 excited states (double line) are calculated in the field of the atomic core with a hole ν_3 including the interaction of the ν_2 electron with the ν_3 vacancy within the second order diagrams [6].

3. Results and discussions

The wave function, presented in figure 1, was used to calculate the photodetachment cross section for Ba^- [3,9].

In the vicinity of the threshold the main contributions to the cross sections are given by the $6p \to \varepsilon s$ transitions. Wigner's law of the threshold $\sigma \sim \sqrt{\omega - |\varepsilon_0|}$ is valid in the very short interval. The photodetachment cross sections are presented in figure 2. The $6p \to \varepsilon d$ transitions dominate at larger energies and they give the main contributions to the dipole sum rule. The state of the other electrons in Ba^- is close to the single-particle state, and because of that, the dipole sum rule must be approximately valid for the photodetachment cross section

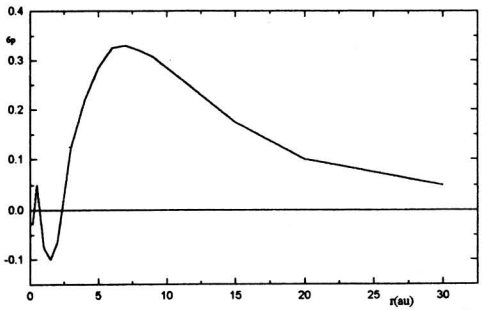


Fig 1. Radial wave function for 6p electron in Ba^-6s^26p ($\varepsilon_0 = -0.144\,eV$)[3]

$$\frac{1}{2\pi^2\alpha} \int_{|\varepsilon_0|}^{\infty} \sigma(\omega) d\omega \simeq 1. \tag{9}$$

For the $\sigma_{6p\to\varepsilon d}$ in Ba it yields 1.5 and 0.65 for the r and ∇ forms respectively. The published [11] show that electron d wave has a resonance in the field of Ba. In the HF approximation this resonance is located at larger energies. Because of that the action of polarization potential upon the d wave is essential and it needs to be taken into account.

The difference between the r and ∇ form of the cross section can be eliminated only by including the correlation corrections to the electromagnetic field operator exactly.

The minimum in the $\sigma_{6p\to\varepsilon d}$ appears because the $6p \to \varepsilon d$ transition amplitude passes though zero and changes its sign at this energy. The position of the minimum depends on what form of r or ∇ is used for the calculation of the cross section.

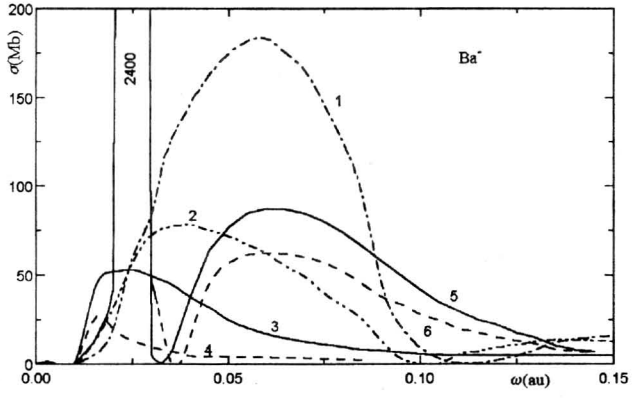


Fig 2. Cross section for 6p photodetachment in Ba^-: 1 and 2 -r and ∇ form, 6p – εd channel [3]; 3 and 4 -r and ∇ form, 6p – εs channel [3]; 5 and 6 -r and ∇ form, 6p – εd channel, with the polarization potential taken into account -present results.

When the polarization interaction is taken into account the minimum of the cross section is drastically moved towards low energies. The results of r and ∇ forms in this case are closer (in the limits of the used approximation)[8]

We think that the observed minimum in the Ba^- photodetachment cross section and expressive resonant behavior are very interesting for experimental investigations.

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MNOGOELEKTRONSKE KORELACIJE U FOTOOTKIDANJU ELEKTRONA OD NEGATIVNOG JONA

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U radu je računat efikasni presek fotootkidanja elektrona sa negativnog jona Ba^- primenom aproksimacije slučajnih faza sa izmenom. Pokazano je da se uzimanjem u obzir polarizacije minimum efikasnog preseka pomera ka nižim energijama, a rezultati korišćenja r i ∇ forme bliži su jedni drugima.