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# ANGULAR DISTRIBUTION OF PHOTOELECTRONS FROM $Ba^-$

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**Abstract:** In this paper we have determined the angular anisotropy parameters in $r$ and $\nabla$ form. In exact treatment, $r$ and $\nabla$ form give the some results. We used HF approximation in the work to determine the transition amplitude $d_{n\ell} \to \varepsilon(\ell \pm 1)$ and elastic scattering phases $\delta_\ell$. On the basis of these values we determined the angular anisotropy parameter and showed that the results $r$ and $\nabla$ agree qualitatively in applied approximation.

## 1. Introduction

Methods of photoelectronic spectroscopy in atomic physics offer a possibility to make very precise measurements of total and partial cross section of photoionization $\sigma_{n\ell}$ and angular distributions $\beta_{n\ell}(\omega)$, i.e. the parameter of angular anisotropy of ejected electrons. The comparison of experimental terms with theoretical calculations gives a detail information about the transition matrix elements and phases of elastic scattering. The calculations done by different approximations show that ionization cross section and angular photoelectron distribution are very sensitive to wave function choosing [1,2,3]. Characteristic oscillations $\beta(\omega)$ which are verified experimentally can be reproduced theoretically only by taking into account sufficient number of correct wave functions of Hermann-Skilman, Hartree-Fock (HF) functions as well as those got by the theory of many particle systems [3].

The theoretical calculations of total photoionization cross section showed that its size is mainly determined by main transition $n\ell \to \varepsilon, \ell+1$ ($\ell$ is an orbital momentum of ionized electron). In Ref [4] are investigated strong interaction correlations within that transition. Furthermore, by investigating only this type of section, we practically have no chance to get an information of the influence of weak transition $n\ell \to \varepsilon, \ell-1$ (the contribution is ten time smaller). Suth information can be obtained by investigation of angular distribution of photoelectron.

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## 2. Basic formulas

The angular distribution of photoelectrons which are ejected from subshell with quantum numbers $n$, $\ell$ when nonpolarized atom is illuminated by nonpolarized light is given by the expression [5]

$$\frac{d\sigma_{n\ell}(\omega)}{d\omega} = \frac{\sigma_{n\ell}(\omega)}{4\pi}\left[1 - \frac{1}{2}\beta_{n\ell}(\omega)P_2(\cos\theta)\right], \tag{1}$$

where $P_2(x)$ is Legendre's polinomial; $\omega = \varepsilon + \varepsilon_{n\ell}$ is the injected photon energy; $\varepsilon_{n\ell}$ –ionization energy of the given subshell; $\sigma_{n\ell}$ total cross section of $n\ell$ -subshell photoionization; $\theta$ –angle between photon and electron momentum; $\beta_{n\ell}$ –angular anisotropy parameter.

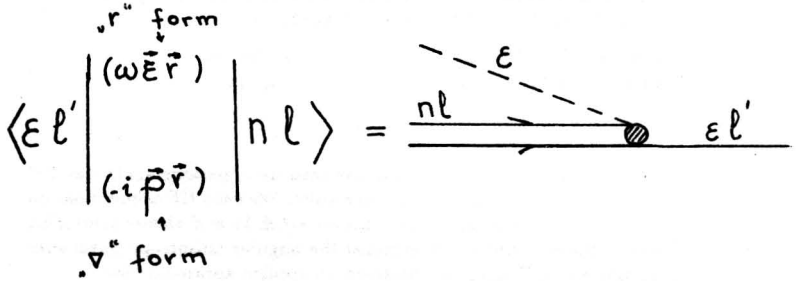


FIGURE 1 .

The matrix element which determines the amplitude of photoejection of external electron is given in fig. 1: $|n\ell>$ is a wave function of external electron of a given negative ion ($6p$ for $Ba^-$); $|\varepsilon\ell'>$ -wave function of electron in the atom field with orbital momentum $\ell = \ell \pm 1$. State $|\varepsilon\ell'>$ is formed from continuum spectrum of $s$ or $d$ electrons. In the given single-particle approximation we consider that the electrons at the final and of the initial states in the process of photoejection move independently. By considering that angular and spin dependencies of HF state $|n\ell>$ and $|n\ell'>$ are known [3], in the matrix element (Fig. 1) integration over angular variable and summarizing over projection of angular and spin momentum (independently of radial variables) can be done. Under this conditions cross section for partial photoejection transition $n\ell \to \varepsilon\ell'$ is

$$\sigma^r_{n\ell\to\varepsilon\ell'}(\omega) = \frac{4}{3\omega}\pi^2\alpha\frac{N_{n\ell}}{2\ell+1}\left|\langle\varepsilon\ell'\|d^r\|n\ell\rangle\right|^2 \tag{2}$$

$$\sigma^\nabla_{n\ell\to\varepsilon\ell'}(\omega) = \frac{16}{3\omega}\pi^2\alpha\frac{N_{n\ell}}{2\ell+1}\left|\langle\varepsilon\ell'\|d^\nabla\|n\ell\rangle\right|^2 \tag{3}$$

where $\alpha$ is fine structure constant, $N_{n\ell}$ number of electrons in the subshell $n\ell$, $\omega = \varepsilon - \varepsilon_{n\ell}$ photon energy. In this paper we use atomic system of units. The reduced matrix elements $\langle\varepsilon\ell'\|d^r\|n\ell\rangle$ of $r$ form and $\langle\varepsilon\ell'\|d^\nabla\|n\ell\rangle$ of $\nabla$ form are given by

$$d^r_{n\ell\to\varepsilon\ell'} \equiv \langle\varepsilon\ell'\|d^r\|n\ell\rangle = \omega\sqrt{[\ell'][\ell]}\begin{pmatrix}\ell' & 1 & \ell\\ 0 & 0 & 0\end{pmatrix}\int_0^\infty P_{\varepsilon\ell'}(r)\,r\,P_{n\ell}(r)dr \tag{4a}$$

and

$$d^{\nabla}_{n\ell\to\varepsilon\ell'} \equiv \langle \varepsilon\ell' \| d^{\nabla} \| n\ell \rangle = [\ell'][\ell] \begin{pmatrix} \ell' & 1 & \ell \\ 0 & 0 & 0 \end{pmatrix} \int_0^{\infty} P_{\varepsilon\ell'}(r) \left( \frac{d}{dr} \pm \frac{\ell+\ell'+1}{2r} \right) P_{n\ell}(r) dr \tag{4b}$$

where $[\ell] \equiv (2\ell+1)$ and $P_{n\ell}$ and $P_{\varepsilon\ell}$ are radial wave functions. When the wave functions for the states $|\varepsilon\ell'>$ and $|n\ell>$ are exact then the forms (4a) and (4b) must be equivalent. The differences in calculations of $\sigma^r$ and $\sigma^{\nabla}$ show the accuracy of applied method.

The total cross section is given by

$$\sigma_{n\ell}(\omega) = \sigma_{n\ell\to\varepsilon(\ell-1)}(\omega) + \sigma_{n\ell\to\varepsilon(\ell+1)}(\omega). \tag{5}$$

The equality of the $r$ and $\nabla$ forms demand satisfying of sum rule, i.e.

$$\sum_{n\ell,n'\ell'} f_{n\ell,n'\ell'} + \frac{1}{2\pi^2\alpha} \sum_{n\ell} \int_{|\varepsilon_{n\ell}|} \sigma_{n\ell}(\omega) d\omega = N \tag{6}$$

where $f_{n\ell,n'\ell'}$ are oscillator strengths for transition from $n\ell$ shell to discrete excitation state $n'\ell'$, $\sigma_{n\ell}$ is cross section for photoejection electron from $n\ell$ shell. Summing up in (5) is over all filled atom shells. Sum rule is satisfied approximately for partial subshells

$$\sum_{n'\ell'} f_{n\ell,n'\ell'} + \frac{1}{2\pi^2\alpha} \int_{|\varepsilon_{n\ell}|}^{\infty} \sigma_{n\ell}(\omega) d\omega \simeq N. \tag{7}$$

Since in our case there is no discrete photoexcitations the first parts of the left sides of equations (5) and (6) are equal to zero. For negative ion $Ba^-$ $N_{n\ell} = 1$. The wave function $\varphi_E(\vec{r})$ which describes moving of the electron with energy $E$ in the atomic field satisfies the equation

$$H^{HF}\varphi_E(\vec{r}) + \int \Sigma_E(\vec{r},\vec{r}')\varphi_E(\vec{r}')dr' = E\varphi_E(\vec{r}). \tag{8}$$

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

Let's consider the problem of determining the wave functions and bind energy of negative ion. If there is a stable negative ion with the ground state energy $E_0^{N+1}$, then

$$E = \varepsilon_0^+ = E_0^{N+1} - E_0^N = -E_A \le 0$$

where $E_A$ $(> 0)$ is the affinity energy. For determination of the Green's function for the negative ion the external electron can be used [3]

$$G_E(\vec{r}_1,\vec{r}_2) = G_E^{(0)}(\vec{r}_1,\vec{r})\Sigma_E(\vec{r},\vec{r}')G_E(\vec{r}',\vec{r}_2)d\vec{r}d\vec{r}' \tag{9}$$

where $G_E^{(0)}$ is Green's function for the zero approximation. In our case, the zero approximation is HF approximation so that

$$\left(E - H^{(0)}\right) G_E^{(0)}(\vec{r}_1,\vec{r}_2) = \delta(\vec{r}_1 - \vec{r}_2). \tag{10}$$

By using the relation (9) and formula for $G_E^{(0)}$ and by changing the limits $E \to \varepsilon_0$ we find a linear homogeneous equation for the determination of the negative ion wave function

$$\varphi_0(\vec{r}) = \int G_{\varepsilon_0}^{(0)}(\vec{r},\vec{r}_1)\Sigma_{\varepsilon_0}(\vec{r}_1,\vec{r}_2)\varphi_0(\vec{r}_2)d\vec{r}_1\,d\vec{r}_2. \tag{11}$$

Acting on the left side (11) by operator $(E_H^{(0)})$ we find

$$\varepsilon_0\varphi_0(\vec{r}) = H^{(0)}\varphi_0(\vec{r}) + \int \Sigma_{\varepsilon_0}(\vec{r},\vec{r}_1)\varphi_0(\vec{r}_1)d\vec{r}_1. \tag{12}$$

In the representation of the HF self functions $\varphi_\nu^{(0)}(\vec{r})$ the following equation gives solution of (12) [6]

$$H^{(0)}\varphi_\nu^{(0)}(\vec{r}) = \varepsilon_\nu\varphi_\nu^{(0)}(\vec{r}) \tag{13}$$

where full set $\left\{\varphi_\nu^{(0)}(\vec{r})\right\}$ contains HF functions for discrete spectra states $|n\ell>$ and continuum spectra states $|\varepsilon\ell>$. The expanding of $\varphi_0(\vec{r})$ over $\varphi_\nu^{(0)}(\vec{r})$ gives

$$\varepsilon_0 c_\nu = \varepsilon c_\nu + \sum\!\!\!\!\!\!\int_{\nu'} \langle\nu\,|\Sigma_{\varepsilon_0}|\,\nu'\rangle\, C_{\nu'}, \tag{14}$$

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

The symbol $\sum\!\!\!\!\!\!\int_{\nu'}$ assign a summing up and an integration over all spectrum of the $\nu'$ states. Set of the states $\nu$, $\nu'$ use HF states $n\ell$, $\varepsilon\ell$ with fixed momentum $\ell$ of the negative ion binding state. By solving the equation (12) we get a wave function for the negative ion's external electron

$$\varphi_0(\vec{r}) = \sum\!\!\!\!\!\!\int_{\nu} C_\nu\varphi_\nu^{HF}(\vec{r}). \tag{15}$$

This function is used in the calculation of the cross section for photoejection the of the corresponding electron [3,7]. In this paper, we used the lowest approximation order to calculate the electron transition amplitude from the state with the energy $\varepsilon_0$ $(\varepsilon_{n\ell})$ and the orbital momentum $\ell$ into the continuum state with the energy $\varepsilon$ and the orbital momentum $\ell+1$. This transitions is conditioned by the absorption of the photon with the energy $\omega$. The results of the calculation of the wave functions and cross section for photoejection are given in [3,7].

Near the threshold, the $np \to \varepsilon s$ transitions give the main contribution to the cross section . Wigner's law of the threshold $\sigma \sim \sqrt{\omega - |\varepsilon_0|}$ is valid in the very short interval. The transitions $np \to \varepsilon d$ are dominant at the higher energies and they give the main contribution to the dipole sum rule.

The parameter of the angular anisotropic $\beta_{n\ell}(\omega)$ (1) have been calculated over photoejection amplitude and scattering phases $\delta_{\ell\pm1}$ of photoelectrons on the neutral atomic core

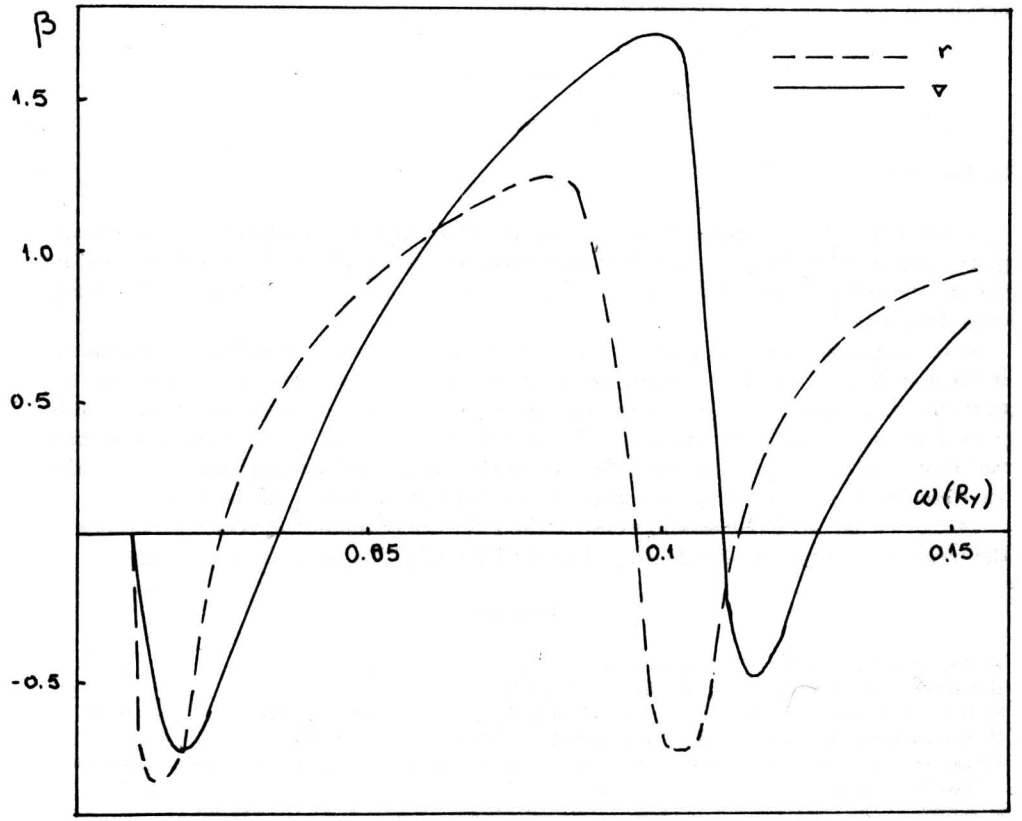


FIGURE 2 .

(atomic core is negative ion with the vacansy in the shell $n\ell$) [3].

$$\beta_{n\ell}(\omega) = \frac{(\ell+2)d^2_{n\ell\to\varepsilon(\ell+1)} + (\ell-1)d^2_{n\ell\to\varepsilon(\ell-1)}}{(2\ell+1)\left(d^2_{n\ell\to\varepsilon(\ell+1)} + d^2_{n\ell\to\varepsilon(\ell-1)}\right)} + \\ + \frac{\sqrt{6(\ell+1)}d_{n\ell\to\varepsilon(\ell+1)}d_{n\ell\to\varepsilon(\ell-1)}\cos(\delta_{\ell+1}-\delta_{\ell-1})}{(2\ell+1)\left(d^2_{n\ell\to\varepsilon(\ell+1)} + d^2_{n\ell\to\varepsilon(\ell-1)}\right)}. \tag{16}$$

Phase shifts $\delta_\ell$ are determined over asymptotic radial part of the wave functions [6]

$$P_{\varepsilon\ell} \sim \frac{1}{\sqrt{\pi k}} \sin\left(kr - \frac{1}{R}\ln 2kr - \frac{\pi\ell}{2} + \delta_\ell\right), \tag{17}$$

where $k = \sqrt{\varepsilon}$ is electron's momentum, and $\delta_\ell$ are HF scattering phases. On the low energy dipole matrix elements have the following form

$$d_{n\ell\to\varepsilon\ell'} \sim \varepsilon^{(2\ell'+1)/4} \quad \text{for} \quad \varepsilon \to 0,$$

and for limits $\varepsilon \to 0$ parameter $\beta$ have the form

$$\beta_{n\ell} \sim \frac{\ell - 1}{2\ell + 1}; \qquad (\ell \geq 1)$$

## 3. Results

In the figure 2, the results of the calculating of the angular anisotropy parameters are given. The amplitudes $d_{n\ell} \to \varepsilon(\ell \pm 1)$ and elastic scattering phases $\delta_\ell$ were calculated in the HF approximation. According to amplitudes $d^r$ and $d^\nabla$ ($r$ and $\nabla$ form) $\beta^r_{n\ell}$ and $\beta^\nabla_{n\ell}$ were determined.

In the range of low energies, the two mimimums and two maximums clearly determined. In the points of amplitude sign changing, the parameter $\beta$ changes rapidly from its maximal to its minimal value. Zero value (roots) of the $\beta_{n\ell}$ correspond the zero value of amplitude $p \to d$ transition and they are $\omega = 0.11$ for $r$ form, $\omega = 0.99$ for $\nabla$ form. the second two roots are determined by the difference in the elastic scattering phases, i.e. by the interference of the $s$ and $d$ waves which become from photoejecting of the $p$ electron.

In the further work one should examine the influence of manyelectronic correlations in the framework of the already developed method RPAE [7] by using Dyson's method.

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## UGAONA RASPODELA FOTOELEKTRONA IZBAČENIH IZ $Ba^-$

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U radu smo odredivali parametar ugaone anizotropije u koordinatnoj i impulsnoj formi.U tačnom tretiranju koordinatna i impulsna forma daju isti rezultat. U radu smo koristili Hartrre-Fockovu aproksimaciju da bi odredili amplitudu prelaza $d_{n\ell} \to \varepsilon(\ell \pm 1)$, i faze elastičnog rasejanja $\delta_\ell$. Na osnovu ovih vrednosti odredili smo parametar ugaone anizotropije i pokazali da se rezultati u koordinatnoj i impulsnoj formi kvalitativno poklapaju u ovoj aproksimaciji.