Indian J. Phys. **71B** (3), 415–420 (1997)

IJP B
— an international journal

A simple procedure for the calculation of the shake-off ratio of double-to-single ionization of a helium–like ion by photoabsorption of a high-energy photon

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Abstract: A simplified, but accurate procedure is proposed for the calculation of the shake-off ratio of double-to-single ionization of a helium–like ion by photoabsorption of a high-energy photon. The procedure is based on the observations that: i) the high-energy shake-off ratio of double-to-single ionization for photoeffect is determined by the behavior of a two–electron wave function in the region where one electron is near the nucleus, and ii) the two–electron wave function, in this region can be determined employing only the monopole term of the electron–electron interaction (i.e replacing $1/|\mathbf{r}_1-\mathbf{r}_2|$ of the exact Hamiltonian of a He–like system by $1/r_>$ where $r_>$ is a larger of r_1 and r_2). The proposed procedure might be helpful in evaluating double-to-single photoabsorption ratios for more complex systems.

Keywords: double photonization, photoeffect, Helium

PACS numbers: 32.80.Fb, 32.30.Rj

In recent years the double ionization of two–electron atoms by one photon has attracted significant attention both experimentally and theoretically [1]. The study has particularly focused on the ratio $R = \sigma^{++}/\sigma^{+}$ of double-to-single ionization. Measurement and prediction of this observable for the simplest many-body system is considered to provide a good test of our understanding of electron–electron correlation in complex systems. Generally, both Compton scattering and photoeffect contribute to ionization at high photon energies [2,3], with Compton scattering becoming dominant over the photoeffect for energies above 6 keV for Helium. It is now becoming possible to measure these contributions separately [4,5]. Here we are concerned with the photoeffect contribution.

The first experimental studies of R using He atoms as a target [6] were performed with relatively low energy photons (ω). At such energies, for which the incoming photon momentum ($k = \omega/c$) is several times smaller than the average momentum of the bound electrons (p_{av}), the dipole approximation for photoeffect was assumed to be sufficient for the theoretical calculations. With the advent of modern synchrotron light sources, experiments measuring the ratio R have become available [7] which extend into a higher energy region.

The calculation of the asymptotic high-energy limit of the ratio R stems from works beginning in the 1960's [8-10], using what is generally called the sudden approximation [11], leading to the shake–off mechanism. In these pioneering works it was shown that, in the dipole approximation using velocity or acceleration gauge, the limit as $\omega \to \infty$ is

$$R = 1 - \frac{\sum_{\mathrm{B}} \left| \int \Phi_{\mathrm{B}}^*(\boldsymbol{r}_1) \Psi_i(\boldsymbol{r}_1, 0) d\boldsymbol{r}_1 \right|^2}{\int |\Psi_i(\boldsymbol{r}_1, 0)|^2 d\boldsymbol{r}_1} . \tag{1}$$

Here $\Psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2)$ represents the initial state wave function, $\Phi_{\mathrm{B}}(\boldsymbol{r}_1)$ is a bound state hydrogen–like electron wave function (in the potential of charge Z), and the summation is over all bound states. Using the best available correlated two electron wave functions this formula gives for He $R = 0.0166$ (1.66%) [10]. Experimental observations in accord with this prediction were reported for photon energies above 2.5 keV [4,5]. Note that the evaluation of the shake–off ratio from the Eq. (1) is separate from the issue of calculation of the photoionization cross sections themselves.

The shake–off approach assumes that in most cases one electron takes almost all the photon energy with the other electron of low energy. In such a situation, the recoiled nucleus takes the rest of the momentum, which is approximately equal and opposite to the momentum of the fast electron. Recently, Drukarev [12] has called attention to an additional mechanism of double photoeffect which would first manifest itself as a linear rise of the ratio with energy, causing roughly a 10% correction to the shake-off limit at about 12 keV. However, even though the shake-off ratio may not be the high-energy limit of the photoeffect ratio, it is a physically well defined quantity which we may measure [4].

The usual procedure in evaluating Eq. (1) is straightforward, although somewhat cumbersome. It requires evaluation, usually using variational method, of the ground-state He–like wave function in, generally, six dimensional configuration space. After obtaining this function we put $r_2 = 0$ and substitute it in the Eq. (1). Here we propose a different approach based on the results of Altick [13] and recent results of Surić et al. [14], and demonstrate that Altick's one parameter ground-state wave function can be used for accurate evaluation of the photoionization shake-off ratio.

In his work Altick simplified the exact Hamiltonian for two electron atom by just keeping the first term (monopole) in the multipole expansion of the electron–electron interaction, that is

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \rightarrow \frac{1}{r_>}, \tag{2}$$

where $r_>$ is a larger of $\mathbf{r}_1$ and $\mathbf{r}_2$. Altick has chosen, as an approximation to the ground state of the Hamiltonian with monopole electron–electron interaction, the wave function of the form

$$\Psi_i(\mathbf{r}_1, \mathbf{r}_2) = \exp\left(-Zr_< + \alpha\frac{r_<^2}{r_>} - \beta r_>\right), \tag{3}$$

where the variables $r_<$ and $r_>$ are the lesser and greater of $\mathbf{r}_1$ and $\mathbf{r}_2$; Z is the atomic number, β is an unspecified parameter and α is fixed by the requirement that Ψ have continuous first derivatives at $r_1 = r_2$. Using variational method, treating β as variational parameter and fixing its value by minimizing the energy Altick has obtained the following values for β: $\beta = 0.42$ for $Z = 1$, $\beta = 1.47$ for $Z = 2$, and $\beta = 2.48$ for $Z = 3$. For our discussion here the parameter β is of primary interest and we shall discuss this parameter from the point of view of the recent results of Surić, Pisk and Pratt [14].

In their recent paper Surić, Pisk and Pratt [14] consider charge dependence of the ratio of double-to-single ionization of a helium–like ion by Compton scattering of a high-energy photon. They introduce the concept of the effective shake–off charges which, according to their discussion, determine ratios of double-to-single photoionization (photoabsorption or Compton scattering). Their discussion on effective shake–off charge for photoabsorption, made in Coulomb gauge and in velocity form, is relevant for our discussion here.

The shake–off mechanism for ionization of two–electron system assumes that one of the two electrons is suddenly removed. The other electron feels a sudden change of potential, from the potential of two electrons in a field of charge Z to the potential of one electron in a field of charge Z. According to Surić, Pisk and Pratt, the state in which this remaining electron is found can roughly be described by some effective charge which they call the effective shake–off charge $Z^{2eP}{}_{\text{eff}}$ for photoeffect. They evaluate $Z^{2eP}{}_{\text{eff}}$ through the procedure beginning with highly correlated He-like wave functions $\Psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2)$. In the high-energy limit the fast electron is removed from the origin and the other electron is left in the state described by the function $\Psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2)$. They normalize this function and obtain $\phi(\boldsymbol{r}_1)$, the wave function of the remaining electron. They try, as a simplest approach, to find the Coulombic ground-state wave function in a field of an effective charge which has the largest overlap with $\phi(\boldsymbol{r}_1)$. The effective charge found in such way is $Z^{2eP}{}_{\text{eff}}$. They find that for all Z the double photoeffect effective shake–off charge can, within few percent accuracy, be written as

$$Z^{2eP}{}_{\text{eff}} \cong Z - 0.53 . \tag{4}$$

Surić, Pisk and Pratt interpret the number 0.53 as the screening which the slow electron sees when the fast electron has left the system from the origin. They have used $Z^{2eP}{}_{\text{eff}}$ to predict the double ionization ratio [14].

Repeating the procedure of Surić, Pisk and Pratt we obtain $Z^{2eP}{}_{\text{eff}} = 0.43$ for $Z = 1$, $Z^{2eP}{}_{\text{eff}} = 1.47$ for $Z = 2$, and $Z^{2eP}{}_{\text{eff}} = 2.48$ for $Z = 3$.

Comparing these values for $Z^{2eP}{}_{\text{eff}}$ with the Altick parameter β we may conclude that they are the same (within the numerical accuracy).

Following the procedure of Ref. [14], we project hydrogenic ground-state wave functions of the charges given above (0.43, 1.47 and 2.48), on the hydrogenic $Z = 1$, $Z = 2$, and $Z = 3$ scattering states, and obtain results for R which agree exactly (within the numerical accuracy) with those obtained with Hylleraas wave functions and Eq. (1) [14].

Therefore, we may conclude that: i) the concept of the effective shake–off charge allows us to calculate the high-energy shake-off photoabsorption ratio exactly without need to know any other information about the ground state of a helium–like ion, and ii) the effective shake–off charge can be obtained through the variational method using only the monopole term of the electron–electron interaction.

In this paper we presented a simplified procedure for the calculation of the high-energy shake-off photoabsorption ratio for helium-like ions. It is demonstrated that this ratio is completely determined by the effective photoeffect shake–off charge, as defined by Surić, Pisk and Pratt [14]. To obtain this effective charge a simple variational procedure of Altick [13], using a one parameter wave function, is sufficient and, therefore it is not necessary to employ highly-correlated, many-parameter, ground-state wave functions. High-energy shake-off photoabsorption ratio (for helium-like systems), therefore, contains the information on monopole, ground-state electron–electron interaction only.

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