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Double Photoionization Cross Section of Ne ($1s^2\ 2s^2\ 2p^6$) $^1S_0^e$ Employing the Configuration Interaction (Ci) Wave Function For The Ground State

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ABSTRACT

In this paper, we have carried out the double photoionization cross section (DPICS) of Ne ($1s^2\ 2s^2\ 2p^6$) $^1S_0^e$ employing the configuration interaction (CI) wave function for the ground state and Brauner, Briggs and Klar (BBK) for the final state involved in the electric dipole transition matrix element exactly in the same as Tiwary and Kumar did in earlier work. Comparison is made with other available experimental and theoretical results. Our present calculated result is encouraging.

KEYWORDS: Atom, Photon, Double Photoionization Cross-section (DPICS).

I. INTRODUCTION

The subject of double photoionization of noble-gas atoms has been of growing interest to both experimentalists and theorists because double-electron photoionization in noble gases gives basic information on the electron correlation in atomic targets. A number of experiments and calculations have been carried out over the last several years for the inert-gas atoms. The integrated two-electron photoionization cross section as a function of the projectile (photon) energy for the helium atomic system ($1s^2$) $^1S^e$ has been measured by Carlson [1], Wight and van der Wiel [2], Schmidt et al [3] and Holland et al [4]. The double photoionization cross section (DPICS) for He has been calculated by Byron and Joachain [5], Brown [6], Amusia et al [7], Yurev [8], Varnavshikh and Labzovskii [9], Carter and Kelly [10] and Tiwary [22]. Furthermore, atomic photoionization has been reviewed by Schmidt [11, 12], Starace [13], Tiwary [23, 24, 25, 26], Becker and Shirley [14], Sonntag and Zimmermann [15] and Amusia [16], Tiwary and Kumar [31]. From a review of the literature, it is clear that there is a striking discrepancy between the recent experimental observations and theoretical predictions over not in the entire but near threshold impact-energy range of measurements, i.e., from threshold up to 240 eV. This long-standing unsatisfactory situation probably exists because of the absence of the electron-electron interaction, which plays a very important role in low-energy reactions, in the final-state wavefunction. Altick [17, 18] has examined this important problem and has obtained the correct asymptotic forms of the two-electron wavefunctions with

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a monopole interaction. For the first time Tiwary [22] has used the Altick wavefunction to calculate DPICS of He. Our investigation shows that the Altick wavefunction is not capable to yield encouraging results in the low-energy region. Brauner, Briggs and Klar (BBK) [19] have proposed a better double continuum wavefunction (DCWF). We [31] have employed BBK DCWF to calculate the DPICS of He. Result obtained is promising which reflects the adequacy of BBK DCWF.

Several experimental observations and theoretical predictions have been also made in heavier noble gas atoms [1-31]. Bizau and Wullemier [32] and Barlett et al [33] have measured the double photoionization cross sections of neon atomic system (Ne) from the threshold to 330 eV. Carter and Kelly [34], Chang and Poe [35], Carlson and Krause [36], Samson and Haddad [37] have performed theoretical calculation in the entire energy range of experimental data available. There is a discrepancy between experimental data and theoretical results. Earlier results of He [31] using BBK DCWF has encouraged to extend to calculate the double photoionization cross section of Ne. The primary purpose of the present work is to test the validity of the BBK DCWF in the case of double photoionization of Ne by single photon impact.

II. THEORY

The expression for the total double photoionization cross section can be written as

$$\sigma^{2+}\left(E_v\right) = \frac{4\pi^2 \alpha\, a_0^2}{E_v} \sum_l \int\int d\varepsilon\, d\varepsilon' \left| \left\langle \Psi_f \left| \sum_{j=1}^{2} \frac{\partial}{\partial z_j} \right| \Psi_i \right\rangle \right|^2 \delta\left(E_v - B_i - \varepsilon - \varepsilon'\right) \qquad (1)$$

where α is the fine-structure constant and a_0 is the first Bohr radius. E_v is the incident energy, and Ψ_i and Ψ_f are the wavefunctions of the initial and final states involved in the transition.

We have employed the configuration interaction (CI) wavefunction for the initial state as given below

$$\Psi_i = \sum_{k=1}^{M} a_k \Phi_k\left(\alpha_k LS\right), \qquad (2)$$

where $\{\alpha_k\}$ denote all the distinguishing features of Φ_k other than L and S [1-4].We now turn to the problem of representing the final continuum state Ψ_f of Ne with two free electrons and Ne^{++}. Byron and Joachain [5] and Brown [6] have represented two continuum electrons by a symmetrised product of uncorrelated Coulomb wavefunctions. We have employed the Brauner, Briggs and Klar double-continuum wavefunction (BBK DCWF) [19] as well as modified BBK DCWF which are given below:

$$\begin{aligned} \Psi_f^- = {} & (2\pi)^{-3/2} e^{i(\boldsymbol{k}_1.\boldsymbol{r}_1 + \boldsymbol{k}_2.\boldsymbol{r}_2)} \\ & \times {}_1F_1\left(-i\frac{Z}{k_1}, 1; -i\left(k_1 r_1 + \boldsymbol{k}_1.\boldsymbol{r}_1\right)\right) \\ & \times {}_1F_1\left(-i\frac{Z}{k_2}, 1; -i\left(k_2 r_2 + \boldsymbol{k}_2.\boldsymbol{r}_2\right)\right) \\ & \times {}_1F_1\left(i\frac{1}{2\kappa}, 1; -i\left(\kappa r_{12} + \boldsymbol{\kappa}.\boldsymbol{r}_{12}\right)\right) \end{aligned} \qquad (3)$$

with $\boldsymbol{\kappa} = \frac{1}{2}(\boldsymbol{k}_1 - \boldsymbol{k}_2)$ and $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. The essential property of this wave function is that it shows exact asymptotic behaviour in the Redmond [20] limit, i.e., for large particle separations.

An even better description of the double continuum state is achieved with the help of local space-dependent momenta [21]. Alt and Mukhamedzhanov [21] showed the necessity of modified momenta to correctly describe

the asymptotic form of the wavefunction in the limiting case of one particle far away from the remaining 2-body subsystem. We present here a slightly different viewpoint and proceed as follows. First, we separate off the plane wave factor for the electrons

$$\Psi_f^- = e^{i(\boldsymbol{k}_>.\boldsymbol{r}_> + \boldsymbol{k}_<.\boldsymbol{r}_<)}\,\overline{\Psi} \tag{4}$$

where $\overline{\Psi}$ describes the Coulomb modifications. $\boldsymbol{r}_{>,(<)}$ stands for the larger (smaller) electron-ion separation and $\boldsymbol{k}_{>,(<)}$ are the corresponding momenta. As in the BBK wavefunction, equation (4), we employ Coulomb waves for 2-body subsystems. The outer electron is located at $\boldsymbol{r}_>$ we use ordinary Coulomb waves for the 2-body subsystems as above,

$$\overline{\Psi} = A\,{}_1F_1\left(-i\frac{Z}{k_>},1;-i\left(k_>r_> + \boldsymbol{k}_>.\boldsymbol{r}_>\right)\right)\,{}_1F_1\left(i\frac{1}{2\kappa},1;-i\left(\kappa r + \boldsymbol{\kappa}.\boldsymbol{r}\right)\right) \propto Ae^{i\Phi} \tag{5}$$

where the phase Φ being chosen to produce correct asymptotic behaviour,

$$(\boldsymbol{k}_>.\nabla_> + \boldsymbol{k}_<.\nabla_<)\Phi = -\frac{Z}{r_>} + \frac{1}{r_{><}} \tag{6}$$

with the solution

$$\Phi = -\frac{Z}{k_>}ln\left(k_>r_> + \boldsymbol{k}_>.\boldsymbol{r}_>\right) + \frac{1}{2\kappa}ln\left(\kappa r_{><} + \boldsymbol{\kappa}\left(\boldsymbol{r}_> - \boldsymbol{r}_<\right)\right) \tag{7}$$

and $\boldsymbol{\kappa} = \frac{1}{2}\left(\boldsymbol{k}_> - \boldsymbol{k}_<\right)$. The amplitude in equation (5) describes the motion of the inner electron located at $\boldsymbol{r}_<$. For $r_> >> r_<$ the wave equation for $A = A(\boldsymbol{r}_<)$ reduces to

$$\left[\Delta_< + 2i\boldsymbol{\kappa}_{eff}.\nabla_< - \frac{2Z}{r_<}\right]A(\boldsymbol{r}_<) = 0 \tag{8}$$

with the solution

$$A = {}_1F_1\left(-i\frac{Z}{k_{<,eff}},1;-i\left(k_{<,eff}r_< + \boldsymbol{k}_{<,eff}.\boldsymbol{r}_<\right)\right) \tag{9}$$

where the effective momentum for the inner electron is given by

$$\boldsymbol{k}_{<,eff} = \boldsymbol{k}_< + \nabla_<\Phi \tag{10}$$

and Φ given by equation (7). This momentum modification (10) is identical to the result achieved by [19] to lowest order in $r_</r_>$. $\overline{\Psi}$ in equation (4) has correct asymptotic behaviour also if all three particle separations are large. This is easily seen because each of the confluent hypergeometric functions reduces then to a pure phase factor, and the effective momentum [20] approaches its static value in that limit. Equation (5) is still incorrect in the limit of two electrons close together but far away from the nucleus. We investigate therefore this limit now. To this end we introduce Jacobi coordinates $\boldsymbol{R} = \frac{1}{2}\left(\boldsymbol{r}_< + \boldsymbol{r}_>\right)$ and $\boldsymbol{r} = \boldsymbol{r}_> - \boldsymbol{r}_<$. For large values of **R** and finite values of r we expect a structure of the wavefunction like $\overline{\Psi} = B(\boldsymbol{r})e^{i\Lambda}$ where the phase Λ is now defined by the eikonal equation

$$\left(\boldsymbol{k}_>.\nabla + \boldsymbol{k}_<.\nabla\right) = -\frac{Z}{r_>} - \frac{Z}{r_<} \tag{11}$$

with the solution

$$\Lambda = -\frac{Z}{k_>} ln\left(k_> r_> + \boldsymbol{k}_> . \boldsymbol{r}_>\right) - \frac{Z}{k_<} ln\left(k_< r_< + \boldsymbol{k}_< . \boldsymbol{r}_<\right) \quad (12)$$

For the amplitude B we find then the wave equation (r << R)

$$\left[\Delta_r + 2i\boldsymbol{\kappa}_{eff} . \nabla_r - \frac{1}{r}\right] B(\boldsymbol{r}) = 0 \quad (13)$$

where $\boldsymbol{\kappa}_{eff}$ is given by

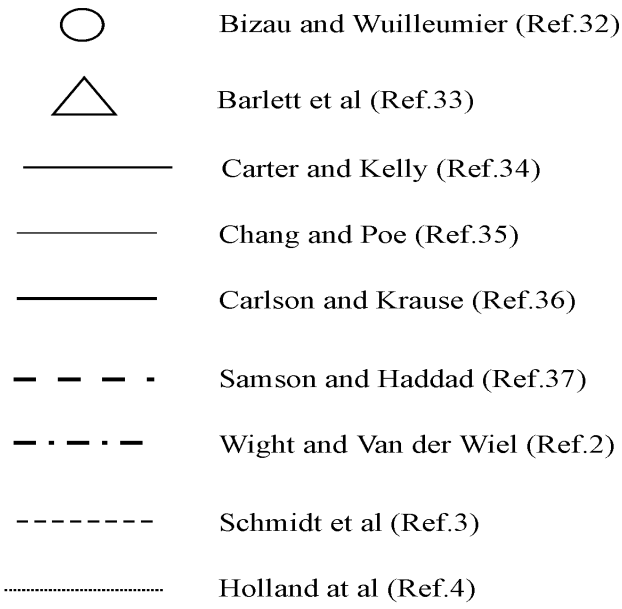
$$\boldsymbol{\kappa}_{eff} = \frac{1}{2}(\boldsymbol{k}_> - \boldsymbol{k}_<) + \frac{1}{2}(\nabla_> - \nabla_<)\Lambda \quad (14)$$

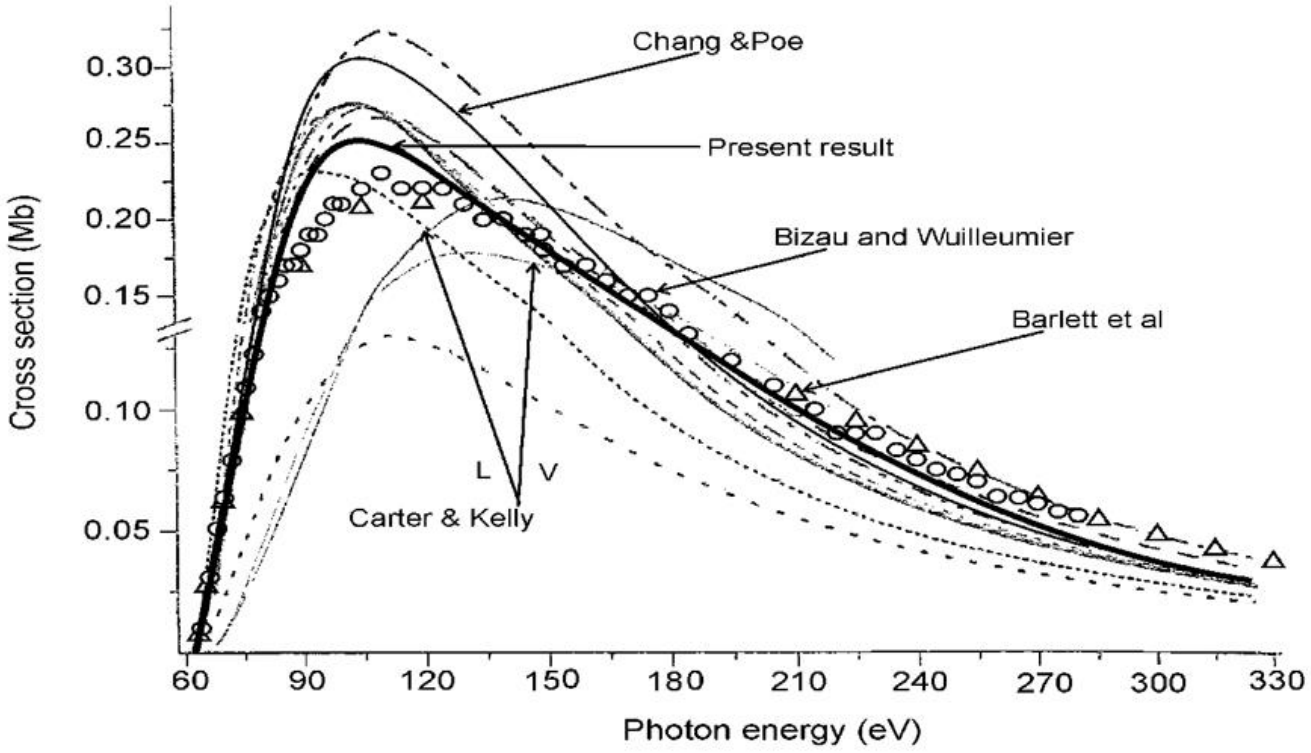
We conclude therefore that the wavefunction given by equation (5) should be an accurate solution of the Schrödinger equation provided the relative momentum $\boldsymbol{\kappa}$ is replaced by its effective value, see equation [14-23].

III.RESULTS AND DISCUSSION

In the present paper we have calculated DPICS of Ne using BBK DCWF for the final state and configuration interaction (CI) wavefunction for the initial state involved in the dipole matrix element [24-31]. It is clear from figure 1 that our present result is reasonably in good agreement with reliable experimental data of Bizau and Wuilleumier [32] almost in the entire energy range under present consideration which shows that BBK DCWF is better than other theoretical results. However, there is a discrepancy between the experiment and the present theoretical result in the close vicinity of the peak of the cross section which reflects that BBK DCWF does not include full correlation. A wavefunction with modified momentum is also employed in the present work. BBK DCWF with effective momentum yields encouraging results but disagreement remains in the close vicinity of the peak of the cross section which suggests to development of further accurate DCWF to obtain high-precision results.

Figure 1: Double photoionization cross section (Mb) for Neon (Ne).





Graph: 1

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