PHYSICAL REVIEW A VOLUME 36, NUMBER 11 DECEMBER 1, 1987

Double ionization of helium by multicharged ions with impact energy 1.4 MeV/amu

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(Received 1 June 1987)

We interpret recent experimental data on double ionization of helium by impact of ions with charges between 15 and 44. An independent-electron model is used. It is shown that quantitative agreement can be obtained when the "saturation" effect in the single-electron ionization probability is accounted for at small impact parameters.

Measurements on double ionization of He by fast multicharged ions have been performed by a number of authors.[1-3] The interest in these processes lies in two different aspects. The first one is to check whether double ionization can be interpreted in the framework of an independent electron model. As the ground state of helium is a singlet state, in the independent-electron model the single- and double-ionization cross sections may be written as

$$\sigma_s = 2\pi \int_0^\infty \rho d\rho 2P_I(\rho)[1-P_I(\rho)] \ , \qquad (1a)$$

$$\sigma_D = 2\pi \int_0^\infty \rho d\rho P_I^2(\rho) \ , \qquad (1b)$$

where $P_I(\rho)$ is the probability of ejecting a single electron in a collision with impact parameter ρ.

The second aspect lies in that double ionization can be expected to be much more sensitive to "saturation" effects[4] as the charge of the projectile increases. By saturation we mean that, for large projectile charges Z_P, the single-ionization (respectively double) cross section increases more slowly with Z_P than the Z_P^2 (respectively Z_P^4) behavior predicted by the Born approximation to $P_I(\rho)$. This can be generally correlated to situations where the Born values for $P_I(\rho)$ approach or exceed unity over some range of impact parameters. In this case, expression (1a) is meaningless. An example of such a situation is given here (see Fig. 1). For fast collisions, $P_I(\rho)$ decreases slowly with impact parameter due to the importance of the dipolar term in the ionization probability (i.e., the electron is ejected preferentially with angular momentum $l=1$). As a consequence, the single-ionization total cross section is determined by distant collisions where the capture probability is small and saturation effects are relatively weak. Conversely, as shown in Fig. 2, the important impact-parameter interval shrinks for double ionization which increases the weight of small impact parameters where saturation effects are much stronger, as demonstrated below (Figs. 1 and 2). Since the saturation effects are strongest for small impact parameters, which dominate the double-ionization cross section, it is clear that σ_D will show a larger deviation from Born approximation than σ_S.[3]

In the present work we evaluate by a nonperturbative method the double ionization and single ionization by ions with charge between 15 and 44 at an impact energy of 1.4 MeV/amu.

To be consistent with the independent-electron model, we describe the active electron target interaction through a potential $V_T(r)$. The initial and final electronic states are defined with the same potential. Instead of using the numerical Hartree-Fock potential, which leads to very good agreement with experiment,[5] we have used for convenience an analytical $V_T(r)$. Our results are not sensitive to the precise form of potential chosen. To calculate the Born values for $P_I(\rho)$, we have transformed the T matrix elements, calculated similarly as in Ref. 5, to impact-parameter-dependent probabilities through the usual Hankel transform.[6] Up to five partial waves have been introduced for the final continuum states, which was enough to reach convergence after integration over ejected electron energies.

Alternatively, we have carried out a nonperturbative calculation using a method first employed by Cheshire and Sullivan.[7] This method consists of solving the time-dependent Schrödinger equation for one electron in the projectile and target potentials through a multipole expansion defined on one center (MEDOC), in the target

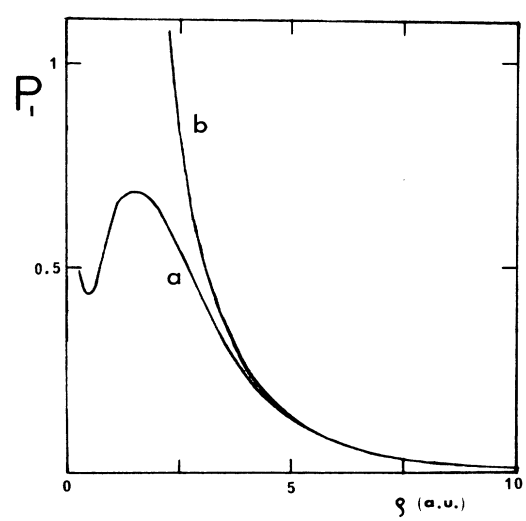

FIG. 1. Single-electron ionization probability $P_I(\rho)$ as a function of impact parameter for $Z_p=15$: (a) MEDOC, (b) Born. The Born values are larger than unity for $\rho < 2.5$ a.u. We have not plotted them since perturbation theory is then meaningless.

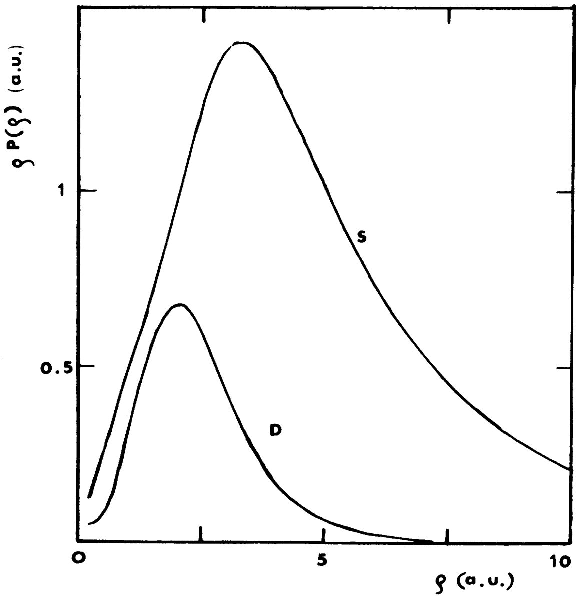

FIG. 2. Probability time impact parameter for single (S) and double (D) ionization of helium as a function of impact parameter for $Z_p=15$. $P_S=2P_I(\rho)[1-P_I(\rho)]$, $P_D=P_I^2(\rho)$. The quantities plotted (ρP_S and ρP_D) are the integrands in the definition of the total cross sections (1).

frame

$$\Psi(\mathbf{r},t)=\sum_{lm} Y_l^m(\theta,\phi)L_{lm}(r,t) \ , \qquad (2)$$

where $\mathbf{r}$ (r,θ,ϕ) is the electron vector with respect to the target. We then get coupled partial differential equations in r and t of the form

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+i\frac{d}{dt}+R_{lm}^{lm}(r,t)\right]L_{lm}(r,t) =\sum_{l'm'} L_{l'm'}(r,t)R_{l'm'}^{lm}(r,t) \ , \qquad (3)$$

which we solve by a finite-element method.

The most important feature of the MEDOC method is its nonperturbative nature in the sense that it involves no limitation on the strength of the electron-projectile interaction, but only on the angular momentum transfer to the electron. Furthermore, it enforces unitarity; hence, "saturation" effects can be accounted for.

The MEDOC method has two limitations: (i) It can be expected to be accurate only when the charge-exchange channels do not play an important role. For high enough energies, it has been shown[8] that saturation effects appear at small impact parameters even in the absence of appreciable capture. However, if the charge is large enough, capture is so important that no reasonable ionization probability can be determined without accounting for the competition with capture channels.[8] Therefore, we have evaluated the capture probabilities with the continuum-distorted-wave (CDW) approximation.[9] For $Z=20$, we get a total capture probability of 0.05 for $\rho=0.5$ with a rapid decrease for larger impact parameters. For $Z=36$, the capture probability is hard to calculate since it occurs mostly in highly excited states. For $\rho=0.5$ we get a probability of 0.13 to capture an electron into the $n=13$ state. Furthermore, the capture probability decreases more slowly as ρ increases. Therefore we think that capture is certainly very important for $Z=36$ and 44. We cannot expect a quantitative answer when neglecting the capture channels. (ii) We have limited the partial-wave expansion to $l=1$. This approximation is discussed further below.

Results are given in Table I together with the experimental values. For single charge exchange we also give the Born contribution for $l=2$–4. We see that it is much smaller than that for $l=0$–1 when $Z_p<20$. However, it is quite important for $Z_p=36$ and $Z_p=44$. Therefore, limiting our expansion to $l=1$ is certainly subject to criticism in these cases. Nevertheless, as we neglect capture as well, it was not worth the effort to introduce more terms in (2).

Results for double ionization are in very good agreement with experiment for $Z_p=15$ and 20 where our MEDOC calculations should be considered as accurate. The Born values are off by an order of magnitude in the case of $Z_p=15$ and by a factor of 20 for $Z_p=20$. This can be understood by looking to the ionization probabilities as given in Figs. 1 and 2. The double-ionization cross section is much more sensitive to the small impact parameter range where the saturation effects are maximum.

In conclusion, we think that our results show that the experimental data of Ref. 3 are compatible with an independent electron model if the single-electron ionization probability accounts for the saturation effects when the charge of the projectile increases. For the largest projectile charges ($Z_p=36$), the competition with capture channels needs to be evaluated to get a more quantitative agreement.

TABLE I. Ionization cross sections by impact of ions with charge Z_p at 1.4 MeV/amu (in cm^2).

	Single ionization					Double ionization		
Z_p	(a) Born	(b) MEDOC ($l=0,1$)	(c) Born ($l>1$)	(d) (b)+(c)	(e) Experiment	(a) Born	(b) MEDOC	(c) Experiment
1	1.6^{-17}		1.78^{-18}			5.7^{-20}		
15	3.6^{-15}	1.3^{-15}	3.96^{-16}	1.69^{-15}	1.79^{-15}	2.9^{-15}	3.0^{-16}	2.91^{-16}
20	6.4^{-15}	2.03^{-15}	6.96^{-16}	2.7^{-15}	2.60^{-15}	9.12^{-15}	4.8^{-16}	5.4^{-16}
36	2.07^{-14}	3.9^{-15}	2.26^{-15}	6.16^{-15}	5.72^{-15}	9.6^{-14}	1.4^{-15}	1.7^{-15}
44	3.1^{-14}	4.8^{-15}	3.37^{-15}	8.17^{-15}	7.21^{-15}	2.1^{-13}	2.0^{-15}	2.3^{-15}

The Laboratoire des Collisions Atomiques is "Equipe du Centre National de la Recherche Scientifique."

[1]M. B. Shah and H. B. Gilbody, J. Phys. B **18**, 899 (1985).

[2]H. Knudsen, L. H. Andersen, P. Hvelplund, G. Astner, H. Cederquist, H. Danared, L. Liljeby, and K. G. Reusfelt, J. Phys. B **17**, 3545 (1984).

[3]J. H. McGuire, A. Müller, B. Schuch, W. Groh, and E. Salzborn, Phys. Rev. A **35**, 2479 (1987).

[4]B. Brendlé, R. Gayet, J. P. Rozet, and K. Wohrer, Phys. Rev. Lett. **54**, 2007 (1985).

[5]S. T. Manson, L. H. Toburen, D. H. Madison, and N. Stolterfoht, Phys. Rev. A **12**, 60 (1975).

[6]R. McCarroll and A. Salin, J. Phys. B **1**, 163 (1968).

[7]I. M. Cheshire and E. C. Sullivan, Phys. Rev. **160**, 4 (1967).

[8]C. O. Reinhold, C. A. Falcón, and J. E. Miraglia, J. Phys. B **20**, 3737 (1987).

[9]Dž. Belkić, R. Gayet, and A. Salin, Comput. Phys. Commun. **32**, 385 (1984).