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Interference between direct and rearrangement mechanisms for double ionization

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In double ionization at very high collision velocities Becker has pointed out that so-called direct mechanism obeys the dipole selection rule while the rearrangement mechanism is a monopole transition, and since s and p waves cannot interfere in total cross sections, interference between these mechanisms is forbidden. It is shown here that interference is possible due to dipole-forbidden contributions to the direct mechanism or rearrangement process.

At high collision velocities it is well established that the cross section for single ionization of helium by electrons and protons of the same velocity is the same. This result is in agreement with the first Born approximation[1] which varies as Z^2, where Z is the charge of projectile, and it has recently been shown[2,3] that antiprotons give the same cross section as protons (or electrons) at $v \geq 5$ atomic units (a.u.) on helium. However, the double ionization cross sections at about $v = 10$ a.u. differ by a factor of 2 between protons and antiprotons[2] or protons and electrons.[3]

The difference in double, but not single, ionization cross sections has been explained[4] in terms of an interference between two mechanisms for double ionization, namely direct and rearrangement mechanisms. In the direct mechanism, the projectile interacts directly with each electron. Using the Born approximation for each interaction the probability amplitude for this process is given[4] by

$$a_D = a_1 \cdot a_2 = \langle \phi_1^f \mid V_1 \mid \phi_1^i \rangle \langle \phi_2^f \mid V_2 \mid \phi_2^i \rangle = CZ^2/v^2 , \quad (1)$$

where C is a complex number independent of z and v. In the rearrangement mechanism, double ionization occurs because of final-state rearrangement of the target following direct ionization of the first electron by the projectile. In the Born approximation, ignoring the Pauli principle, this amplitude is simply estimated by

$$a_R = a_1 \langle \phi_2^f \mid \phi_2^i \rangle = C'Z/v . \quad (2)$$

When a_R and a_D are comparable in magnitude interference can cause an observable difference opposite signs of Z since $\mid a_R + a_D \mid^2$ contains a term cubic in Z, i.e., a term which changes sign as $Z \rightarrow -Z$.

Becker, however, has[5,6] found an argument against this interference interpretation. In total cross sections s and p waves cannot produce interference effects since the sp coherence goes to zero by orthogonality. In the high velocity limit, the Born approximation obeys a dipole selection rule. Hence electron 2 initially in an s state must go to a p state, due to the dipole selection in $\langle \phi_2^f \mid V_2 \mid \phi_2^i \rangle$ of Eq. (1) in the direct mechanism. And again since s and p waves are orthogonal, the amplitude $\langle \phi_2^f \mid \phi_2^i \rangle$ of the rearrangement mechanism is purely s wave when ϕ_i is an s wave. In other words the direct mechanism produces p-wave continuum electrons and the rearrangement mechanism produces s-wave continuum electrons. And since

$$\int Y_0(\hat{k}_2) Y_1(\hat{k}_2) d\hat{k}_2 = 0$$

interference between such a_D and a_R amplitudes cannot be present in total cross sections.

This insightful argument was not considered in the original work.[4] We begin to address this useful objection by noting that the Born amplitude contains significant contributions from dipole-forbidden transitions for p (or $\bar{p}, e$ or $\bar{e}$) on helium at $v \cong 10$ a.u. For $p \rightarrow \text{He}$ we have evaluated the contributions from various partial waves (Fig. 1). The dipole-allowed transition with a p wave as a final state is only about 75% of the total contribution. Each of the dipole-forbidden monopole (s wave) and quadrupole (d wave) transitions account for approximately 5% and 10%, respectively. These parts of the amplitude, however, can interfere with the direct amplitude and can produce a dependence of the double ionization cross section on the sign of the charge of the ionizing particle as observed in the experiment. We consider in the following only the effect of dipole-forbidden contributions in the rearrangement channel. We point out that a similar interference effect can rise from the direct process. We now give a crude estimate for the size of the effect. We note first that in the transition region between the shake off dominated and double scattering dominated double ionization

$$\mid a_D \mid \cong \mid a_R \mid . \quad (3)$$

Now consider the rearrangement amplitude a_R corresponding simply to single ionization followed by ejection of a second electron due to correlation. This final rearrangement contribution is often simply expressed in terms of an overlap of nonorthogonal initial- and final-state wave functions. We assume that the initial ionization part of a_R may be represented by the first Born approximation for single ionization. Decomposing the rearrangement amplitude into an interfering part I and a noninterfering part N

$$a_R = a_R^N + a_R^I \ , \tag{4}$$

the double ionization cross section is given as a collisional average

$$\langle \, | a_D \pm a_R \, |^2 \rangle = \langle \, | a_D \, |^2 + | a_R^N \, |^2 + | a_R^I \, |^2 \rangle \pm 2 (\langle \, | a_R^I \, |^2 \rangle \langle \, | a_D \, |^2 \rangle)^{1/2} \langle \cos\phi \rangle \tag{5}$$

when the $\pm$ sign refers to negatively and/or positively charged projectiles. An accurate estimate of interference effect requires the determination of the average interference phase angle $\langle \cos\phi \rangle$. Instead of attempting this we leave $\langle \cos\phi \rangle$ as free parameter and show that the experimentally observed cross-section portion can be explained by a collisional average with $| \langle \cos\phi \rangle | \leqq 1$. From the partial-wave decomposition (Fig. 1) we get as a conservative estimate

$$\frac{\langle \, | a_R^I \, |^2 \rangle}{\langle \, | a_R^I \, |^2 + | a_R^N \, |^2 \rangle} \gtrsim 0.1 \tag{6}$$

if we take into account only the d-wave contribution.

Using Eqs. (3)–(6) leads to a ratio

$$R = \frac{\langle \, | a_D + a_R \, |^2 \rangle}{\langle \, | a_D - a_R \, |^2 \rangle} \cong \frac{(1 + 0.316 \langle \cos\phi \rangle)}{(1 - 0.316 \langle \cos\phi \rangle)} \ . \tag{7}$$

The experimentally observed ratio $R \cong 2$ can therefore be reproduced with a full phase coherence of $\langle \cos\phi \rangle \cong 1$.

In our simple estimate we have used only d waves, and ignored various other effects including s waves, nonhydrogenic effects in the ground state, helium wave functions, and final-state correlation. The result of this simple estimate is marginal, i.e., a factor of two effect is possible only with full coherence, i.e., $\langle \cos\phi \rangle = 1$. Using the s-wave contributions from Fig. 1 alone in our estimate, an interference effect of a factor of two is not possible. We note that our conclusions are consistent with recent calculations and analysis[7] by Reading and Ford.

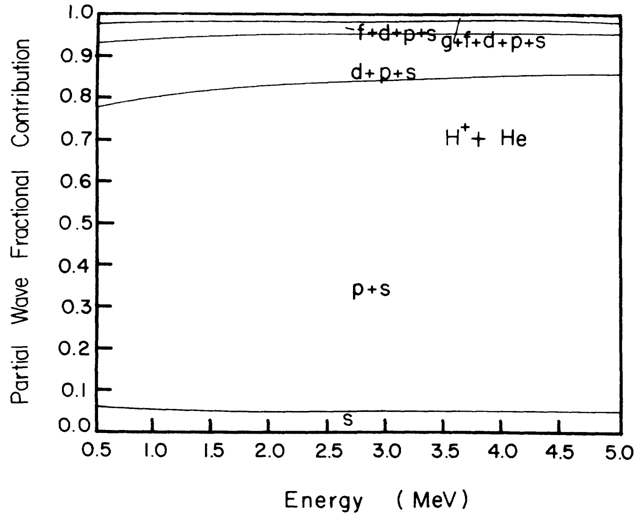

FIG. 1. Partial-wave contribution to the total cross section for ionization of a single electron at various incident proton energies. About 75% of the cross section is due to the dipole-allowed p-wave contribution in the energy range shown here for $p + \mathrm{He}$.

In summary, the sign dependence in the double ionization cross section on the charge of the projectile can be explained as an interference effect between the direct and a dipole-forbidden part of the rearrangement amplitude using s,p- and d-wave contributions.

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