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LETTER TO THE EDITOR

Double-electron excitation of beryllium by proton and antiproton impact

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Abstract. The double-electron excitation cross section of the $1s^22p^2\ ^1D$ stationary discrete state of the beryllium atom by proton and antiproton impact is calculated within the expansion of scattering amplitude up to second order. We discuss the role of electron correlations in the two-electron excitation of the beryllium atom.

Two-electron transitions, such as double excitation, double ionization, ionization–excitation etc, have been the subject of intensive investigations during recent years. Study of these transitions in collisions with protons and antiprotons has provided a deeper insight into the dynamics of atomic collisions and the nature of electron correlations (Pedersen 1990).

The two-electron excitation process is a rather simpler process than the other two-electron ones. So far efforts both experimental (Pedersen and Hvelplund 1989, Giese *et al* 1990) and theoretical (Fritsch and Lin 1990, McGuire and Straton 1991, Moribayashi *et al* 1991, Winter 1991) have been confined to the double excitation of helium by charged particles. Attention has been particularly directed to the effects of the sign of the projectile charge. However, the states of helium atom with two excited electrons are autoionizing states. Recently, Godunov *et al* (1992) have demonstrated that inteference with single ionization processes together with Coulomb interaction in the final state play a significant role in the excitation of autoionizing states of helium. It was shown also that the charge sign effects in excitation of autoionizing states have a very intricate nature (Godunov *et al* 1990a, b). Therefore, atomic systems with the states of two-electron excitation lying under the first ionization limit are a more proper object to study the nature of the double-excitation process itself.

A four-electron system is the smallest for which a stationary discrete state with two excited electrons is possible. The beryllium atom has only one such state, $1s^22p^2\ ^1D$ (Osanai *et al* 1989). It is the purpose of the present work to study the process of two-electron excitation of the beryllium atom ($1s^22s^2\ ^1S$–$1s^22p^2\ ^1D$) by proton and antiproton impact along with the role of electron correlations.

Correlative and two-step excitation mechanisms are the leading ones at intermediate and high impact energies. In the first case only one atomic electron interacts with the projectile, but because of correlation caused by the electron–electron interaction the second is also excited. This is the first-order mechanism and the resulting cross secton scales as Z_p^2. If the two-electron transition is determined by projectile interaction with each of the target electrons then such a mechanism is called a two-step mechanism and the cross section scales as Z_p^4. The expansion of scattering amplitude in powers of the projectile–target interaction (in a Born series) up to second order is a suitable approach to study the double-electron

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excitation of an atomic system along with the role of electron correlations. The interference of the first- and second-order mechanisms results in a Z_p^3 dependence term and hence in the effects of the sign of the projectile (McGuire 1987).

The first-order excitation amplitude after integration over the coordinate of a projectile is given by

$$f_1 = -\frac{2m_p Z_p}{Q^2}\langle f|V(Q)|i\rangle \tag{1}$$

where

$$V(Q) = Z_t - \sum_{j=1}^{N}\exp(iQr_j)$$

is the projectile–target interaction potential, $|i\rangle$ and $|f|\rangle$ are respectively the antisymmetrized wavefunctions of coupled momenta for initial and final states, $Q = k_i - k_f$ is the momentum transfer, k_i and k_f are the momenta of incident and scattered particles, Z_p and Z_t are the projectile and target nucler charges, m_p is the mass of the projectile. Note that the projectile–atom interaction $V(Q)$ is a sum of one-electron operators and only allowing for the electron correlations results in a non-zero first-order amplitude for the two-electron excitation process.

Performing the integration over the coordinate of projectile, the second-order term takes the form (Godunov *et al* 1991)

$$f_2 = \frac{2m_p^2 Z_p^2}{\pi^2}\lim_{\varepsilon\to 0}\sum_{\alpha}\int d^3k \frac{\langle f|V(k-k_f)|\alpha\rangle\langle\alpha|V(k_i-k)|i\rangle}{(k-k_f)^2[k_i^2 - 2m_p E_\alpha - k^2 + i\varepsilon](k_i-k)^2} \tag{2}$$

where E_α is the energy of an intermediate state. In accordance with the relation

$$\frac{1}{k_n^2 - k^2 + i\varepsilon} = \frac{P}{k_n^2 - k^2} - i\pi\delta(k_n^2 - k^2) \tag{3}$$

the second-order amplitude can be represented as

$$f_2 = f_2^{vp} - i\pi f_2^{pol}. \tag{4}$$

The first term corresponds to the off-shell scattering amplitude (principal value part), the second term is the on-shell part of the scattering amplitude (pole part). The analysis of matrix elements in equations (1) and (2) has shown that the quantities f_1, f_2^{vp} and f_2^{pol} are purely real to within common phase factor. For fast ion–atom collisions the main contribution to the total cross section is determined by small momentum transfer or small scattering angles where the principal value part f_2^{vp} is a small portion of pole part f_2^{pol}. Potvliege *et al* (1987) have reported that in this kinematic regime the term $(f_2^{vp})^2$ proportional to Z_p^4 has the same order as term $f_1\,\mathrm{Re}(f_3)$ which is also proportional to Z_p^4. Therefore, we omit the term $(f_2^{vp})^2$ from further consideration. With the above comments in mind, the total cross section can be written as

$$\sigma = \frac{k_f}{k_i}\int[f_1^2 + 2f_1 f_2^{vp} + \pi^2(f_2^{pol})^2]\,d\Omega_{k_f}. \tag{5}$$

The exact calculation of the first-order amplitude does not present difficulty but the second order does. One of the problems that arises in the evaluation of the second-order amplitude is the infinite sum and integral over a complete set of intermediate states. The closure approximation (Holt and Moiseiwitsch 1968) is widely used to avoid such problems. In our opinion this method should be used with care in the studies of charge sign differences in two-electron excitation process. Usually, the choice of closure energy E_α in this approximation has little effect on the total cross section for excitation (Madison and Winters 1987). As mentioned above, the contribution to the total cross section from the second-order amplitude is determined by the f_2^{pol} part. But it is interference of the principal value term f_2^{vp} with the first-order amplitude that gives the term proportional to Z_p^3 with more intricate dependence on closure energy E_α. Using the substitution $p = k - Q/2$ in equation (2) along with cylindrical coordinates, it is easily shown that in the case of fast collisions at $E_\alpha = \Delta E/2$, where ΔE is the energy of the two-electron excitation, the value of f_2^{vp} is near zero as far as we have integration of asymmetric functions in symmetric limits. Therefore a little variation of closure energy E_α changes considerably the difference between the proton and antiproton double-excitation cross section. In the present work the second-order amplitude was calculated with direct summation over the intermediate states which bring a basic contribution to the cross section. The Cauchy principal value integral in the principal value part was integrated numerically.

In the following we discuss the total cross section for two-electron excitation of the stationary discrete state $1s^2 2p^2\ ^1D$ of beryllium by proton and antiproton impact with energy 0.1–1.5 MeV. The calculation has been carried out with expansion of the scattering amplitude up to second order (equation (5)).

Electron correlation has been recognized as very important in the formation of the structure and spectra of the beryllium atom. The correlated wavefunctions describing the ground, single-excited and double-excited states of beryllium have been obtained using the configuration interaction method (Hibbert 1975, Cowan 1981). The configuration set includes all configurations of $|1s^2 nln'l'\rangle$ type with $n, n' \leqslant 3$. For the lowest states of ^1D symmetry the 2s4d and 2s5d configurations are also included. The radial part of each orbital was expanded in terms of Slater-type orbitals.

Firstly, we consider the role of electron correlation in the first- and second-order amplitudes separately. The result of calculation for the first-order amplitude shows that the first-order cross section for the double-electron excitation allowing for correlation in the final state only is about three and a half times larger than the cross section calculated allowing for correlations in the initial state only. This relation is relatively independent of impact energy in the considered energy range. Such a result can be explained by strong interaction of the $1s^2 2p^2\ ^1D$ state with the $1s^2 2snd\ ^1D$ series and as a result one-electron quadrupole transition 2s–*n*d is possible. The mixture of leading configurations $1s^2 2s^2$ and $1s^2 2p^2$ in the initial ^1S state is not so significant. Unlike the first-order amplitude the second-order amplitude is out of zero with uncorrelated functions. However, allowing for electron correlations gives rise to a probability of the two-step excitation mechanism. The greater the impact energy the stronger this influence. At 100 keV impact energy such an effect is near 20% but at 1.5 MeV the correlations increase the cross section of double excitation by more than half.

We next consider the role of intermediate states for the calculation of the second-order amplitude in more detail. We found that the following five intermediate states $[1s^2]2s^2\ ^1S$, $2s2p\ ^1P$, $2s3p\ ^1P$, $2s3s\ ^1S$, $2p^2\ ^1D$, provide more than 90% of the contribution to the total cross section from the two-step mechanism of excitation. This result is in accordance with the analysis of the structure of the configuration interacting wavefunctions of the beryllium

atom. These intermediate correlated states allow the two-electron transition to proceed as a sequence of two dipole one-electron transitions with relatively high probability. The results presented below have been calculated with the following twelve intermediate states: $[1s^2]2s^2\ ^1S$, $2s2p\ ^1P$, $2p^2\ ^1S$, $2p^2\ ^1D$, $2s3s\ ^1S$, $2s3p\ ^1P$, $2p3s\ ^1P$, $2p3p\ ^1S$, $2p3p\ ^1D$, $2s3d\ ^1D$, $2p3d\ ^1P$, $2s4d\ ^1D$. The inclusion of additional intermediate states of $|1s^2 3l 3l'\rangle$ type does not change the result significantly.

Table 1. Double excitation cross section (in units of 10^{-17} cm^2) of the beryllium atom ($1s^2 2s^2\ ^1S$–$1s^2 2p^2\ ^1D$) by proton and antiproton impact.

E (keV)	σ_{first}	σ_{proton}	$\sigma_{antiproton}$
100	7.52	12.5	11.1
250	3.11	4.06	3.85
500	1.57	1.83	1.78
750	1.05	1.17	1.15
1000	0.790	0.856	0.848
1500	0.527	0.558	0.554

The resulting cross section (equation (5)) for the double-electron excitation of beryllium by proton and anitiproton impact is given in table 1. In the second column of the table we also present the result of the first-order calculation (in the first Born approximation) which is independent of projectile charge. The calculation demonstrates that the dependence of the cross section on the sign of projectile charge is more pronounced at intermediate collision energy where the correlative and two-step mechanisms are comparable. As collision energy increases the role of the two-step mechanism becomes less important and as a result the distinction between the cross section for proton and antiproton impact becomes less evident. The cross section for double excitation of the $1s^2 2p^2\ ^1D$ state of beryllium by proton impact exceeds that for antiproton impact in the considered energy range.

In the present work we have shown the existence of the effect of the sign of projectile charge for double-electron excitation of the $1s^2 2p^2\ ^1D$ stationary discrete state of the beryllium atom by proton and antiproton impact. This effect is more pronounced at intermediate collision energies where the correlative and two-step mechanisms are comparable. The electron correlations play a significant role in the two-electron excitation of the beryllium atom over all the energy range considered. The calculation also demonstrates the relatively high value of the cross section for the excitation process studied. It facilitates the experimental measurement of the double-excitation cross section of beryllium.

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