K-shell excitation in Ca ions by neutral atoms in the intermediate velocity range

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Electron excitation cross sections of Ca^{19+} and Ca^{18+} ions by impact of neutral atoms are calculated with the symmetric eikonal theoretical model. Theoretical results agree with recent experiments.

In a recent paper (hereafter referred to as I), Xiang-Yuan Xu *et al.*[1] have measured excitation cross sections of one- and two-electron ions, Ca^{19+} and Ca^{18+}, respectively, incident on various gas targets ranging from H_2 to Xe, at impact velocity $v=18.5$ (8.6 MeV/amu). For the present theoretical analysis, Ca ions will be considered as the targets (the projectile in the experiment) while the neutral atoms will be the projectiles. As usual, Z_T and Z_P denote the target and projectile Coulomb charges, respectively. As referred to in I, this collision belongs to the intermediate velocity region, i.e., $Z_T/v=1.08$. From the point of view of the distortion created by the projectile, those measurements cover from the perturbative region (i.e., the case of H_2 impact where $Z_P/v=0.054$) to the nonperturbative regime (for Xe impact where $Z_P/v=2.9$). The authors of I restricted the theoretical analysis to the simplest case, i.e., Ca^{19+}, the one-electron system. They essayed an explanation of the experiments in terms of the correction to the binding energy introduced by Basbas[2] in the context of ionization. Although the tendency of the data was explained, a significant deviation for the higher Z_P was noted (even when compared with the Glauber theory). It should be noted that binding correction formulations are based on an expansion in terms of $r_Z=Z_P/Z_T$, so they are expected to work when $r_Z \ll 1$. For Kr impact, $r_Z=1.8$, and it is not too surprising to find that binding corrections break down. The set of Ca^{18+} data was not analyzed in I.

In our group we have developed a theoretical method, called symmetric eikonal[3,4] (SE), which has been very successful in explaining a similar experience with Fe^{24+} ions.[5] In the present report we want to show that this method can explain the experimental data quite properly, without resorting to a binding effect. The SE theory is based on two properties: the correct orthonormalization, and proper Coulomb conditions of the distorted wave functions used.

For Ca^{19+} ions the theory is straightforward, and there are no complications since it is a one-electron system. The projectiles (the neutral gases) were considered as point particles with effective charges given by the nuclear charge Z_{PN} minus the screening of the K-shell electrons

$$Z_{\rm eff}=Z_{PN}-2\frac{16}{\{4+[P/(Z_{PN}-\frac{5}{16})]^2\}^2}\ , \qquad (1)$$

where P is the momentum transfer.[6] Screenings from outer shells can be neglected for the present impact energy.[6] Results are shown in Fig. 1 and compared with the experimental K x-ray production cross sections. As in Ref. 1, we add the excitation cross sections to all states up to $n=7$, excepting the metastable one ($2s$), since it does not decay within view of the detector. We have not made corrections due to cascades into the $2s$ state; corrections can be evaluated by using the corresponding branching ratios,[7] however, they introduce small modifications, and can be neglected.[1] The theory gives a good account of the experiments. Two deviations should be noted: the theoretical value for Ar lies 40% above the data, while for Xe it rests 50% below the data. In the Ar case, the discrepancy may not be significant, since the measurements have a relative uncertainty of 30%. For the Xe case, we may have some problems such as the omission of the screening of the Xe outer shells, or simply the failure of the theory at very large perturbations.

For Ca^{18+}, the theory needs an extension to account

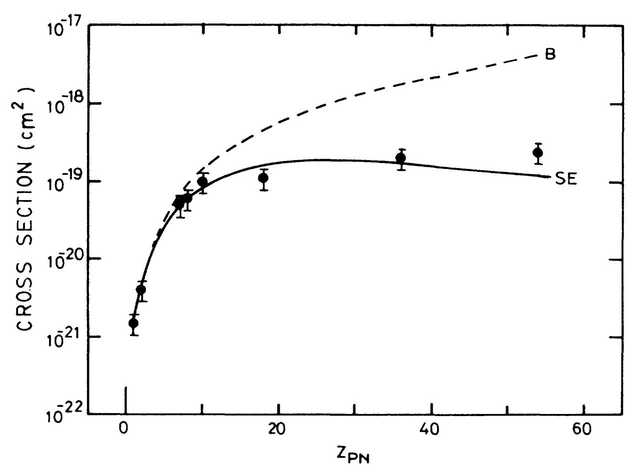

FIG. 1. Excitation cross sections of Ca^{19+} by impact of neutral atoms at 18.5 a.u. impact velocity as a function of the projectile nuclear charge. The results involve excitation from $1s$ to $n=2$–7 except for the metastable state $2s$. The solid line denotes the SE theoretical results; the dashed one, the first Born approximation. The experiments are from Xu *et al.* (Ref. 1).

for the two-electron system. For the initial electronic state we considered a product of triple ζ orbitals of Clementi and Roetti's Table 3.[8] For the final one, we have used the singlet-state description used by Bell *et al.*[9]

$$\psi_{nl}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[\varphi_{nlm}(19|\mathbf{r}_1)\varphi_{1S}(20|\mathbf{r}_2)+\varphi_{nlm}(19|\mathbf{r}_2)\varphi_{1S}(20|\mathbf{r}_1)]\ , \qquad (2)$$

where $\varphi_{nlm}(Z|\mathbf{r})$ represents a hydrogenic wave function in a Coulomb charge Z. We have considered neither second-order double-excitation processes nor excitation to triplet states.[10] We have not evaluated excitations to the $n\ ^1S$ $(n=3-7)$ states for this case because the contributions of the calculations can be estimated to be less than 5%.[11] The new formulation can be reduced to a combination of single-electron excitation T-matrix elements times orbital overlaps which are very close to unity.[12] Thus, the theory presents no additional complication. Results are shown in Fig. 2 and compared with the experiments. Due to the fact that Z_T is very large, the present results are close to two times the value of the cross section corresponding to an excitation of a one-electron atom of effective charge $Z_T-\frac{5}{16}$. Discrepancies between our two-electron model and the single-electron one are within 2%. The agreement with the experiments is very good except for the Ar value.

We can conclude that the SE theory provides good performance when compared with these kinds of measurements in the intermediate energy range. In accordance with the Xe value, the theory seems to underestimate the experiments at very high perturbations.

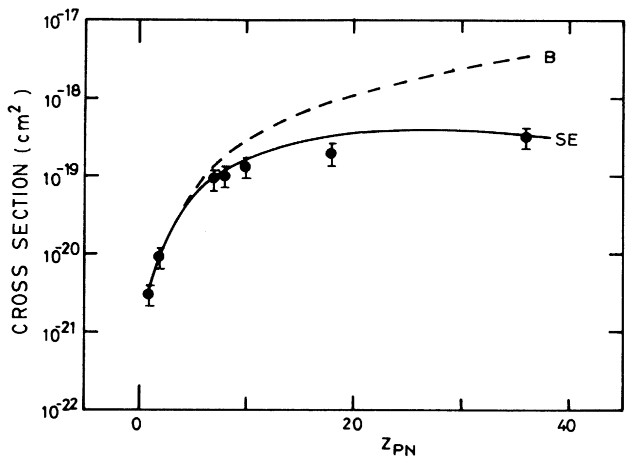

FIG. 2. Similar to Fig. 1 for Ca^{18+}. For this case the results involve excitation from $1s^2\ ^1S$ to $1snl\ ^1L$ $(n=2-7;\ l=p,d,\ldots;\ L=P,D,\ldots)$.

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[6]See Appendix 2 of Ref. 3 for details.

[7]K. Omidvar, At. Data Nucl. Data Tables **28**, 1 (1983).

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[10]If LS-coupling approximation is valid for the excited ion, in the absence of spin-dependent perturbations, only transitions with $\Delta S=0$ can be induced.

[11]For these final states the calculations are a bit more complicated since the simple wave function given by Eq. (2) cannot be used, as it does not satisfy the necessary condition of orthogonality to the approximate initial (ground-state) wave function.

[12]Details of the formulation will be published elsewhere.