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Comparison of the total cross sections for positron (electron) collisions with alkali-metal atoms*

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Abstract. The total cross sections for electron and positron collisions with sodium and potassium are calculated in the modified Glauber (MG) approximations, employing the Szazs–McGinn wavefunctions within the frozen-core approach. While the present values of total cross sections for electron and positron collisions are found to be consistent with those previously obtained in the model-potential approach, the positron and electron MG cross sections of the present calculation merge with each other at a rather low energy, as was observed in experiments by Stein *et al.*

1. Introduction

Recently, Stein *et al* (1988, 1990) have, for the first time, performed the measurement of total cross sections for positron (and electron) collisions with alkali-metal atoms (Na, K, and Rb). They found that the total cross sections for electron and positron collisions with alkali-metal atoms at non-room temperatures, unlike the results of total cross section for collision with inert gases at room temperature, merge with each other at a rather low energy around 40 eV. In recent works (Gien 1989a, b, 1990), we have performed the calculation of total cross section for $e^{\pm}$ scatterings from Li, Na, K and Rb, employing the modified Glauber (MG) approximations (Gien 1987b; see also Gien 1988). For scattering from Li, Na, and K (Gien 1989a, b), we considered the model-potential approach (Gien 1987a, b), in which the polarization terms of the core potential were not neglected, while for scattering from Rb (Gien 1990), we employed the frozen-core approach to deduce the core potential from the wavefunctions of the core electrons, which were already made available by Szazs and McGinn (1967). Our MG total cross sections for $e^{\pm}$ collisions with Na, K, and Rb were found to agree reasonably well with experimental data (Stein *et al* 1988, 1990), if the uncertainty existing in experimental data, due to the inability of distinguishing the elastically scattered positrons (electrons) from the incident ones near the forward direction, is taken into consideration. While the MG values for electron and positron collisions with Rb were found to merge with each other (within 5%), those calculated within the model potential approach for $e^{\pm}$ collisions with Na and K were found not to merge. The MG electron cross sections in the latter case consistently lie above the positron cross sections for about 10–15%. We then tentatively explained the non-merging of our electron and

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positron MG total cross sections as rooting from the very strong core polarization potential of the alkali targets, which made the core potential react to oppositely charged projectiles differently. On the other hand, the absence of the core polarization term from the frozen-core potential, which was employed in our calculation of total cross section for rubidium, made it possible for our MG $e^{\pm}$ total cross sections to merge with each other. Since the wavefunctions of Szazs and McGinn (1967) are also available for K and Na, it would, therefore, be interesting to also calculate, for a comparison, the total cross sections for electron and positron collisions with sodium and potassium in the frozen-core approach. This work is, therefore, intended to provide a self-consistency check for the model-potential and frozen-core approaches which have been considered for electron (positron) collisions with alkali atoms in the literature. It will also, hopefully, reveal to us how seriously the use of different types of wavefunction would affect the results of calculation. On the other hand, we would like to find out as well whether or not the strong core-polarization term of the model potential was, indeed, the source for the non-merging of the electron and positron MG total cross sections obtained earlier (Gien 1989a, b) within the model-potential approach.

2. Results and discussion

As has already been discussed in previous publications (Gien 1989a, 1990), it has been generally believed that a Glauber-related approximation, such as the MGA, may start to work well only at a scattering energy greater than a couple of times the ionization threshold energy of the target (for potassium, the threshold energy is 4.339 eV, while for sodium, it is 5.138 eV). We have, therefore, performed the calculation at scattering energies down to around 10 eV, although we believe that the MG values of the total cross sections will probably be reliable only at energies above around 20 eV or even higher.

As was also already stressed (Gien 1989a, 1990), while the positronium formation channel was implicitly taken into consideration in our calculation of total cross sections through the use of the optical theorem, the effect of the positronium formation channel on the total cross sections, especially at higher energies, in our opinion, is expected to be negligible, since while the positronium formation in positron collisions with alkali atoms is an exothermic process, the scattering energy in this range (10–1000 eV) is far from the region of significance for positronium formation.

For various reasons (see our related discussion in Gien 1988, pp 150, 171), in both MG calculations (previously in the model-potential approach and here in the frozen-core approach), we chose to ignore the exchange effect which may somewhat alter the electron results at low energies. The inclusion of exchange will most likely move the electron cross sections at low energies away from (or closer to) the positron cross sections which were observed to stay apart from each other in experiments. However, at an energy as high as 40 eV or above, where the positron and electron total cross sections were observed to merge, the exchange effect, if any, will almost certainly be small and its effect on the MG electron cross sections (and hence on the merging) can safely be expected to be insignificant.

In table 1 we exhibit the total cross sections for electron and positron collisions with K and Na at high energies above 150 eV. While experimental data are still not available, the MG positron and electron values are too close in this range of energy to be exhibited with clarity on a figure. The results at energies below 100 eV, where

Table 1. Total cross sections in πa_0^2 for electron and positron scattering from sodium and potassium. MG2, modified Glauber approximation (frozen-core approach) with the contribution from the 3s (4s) and 3p (4p) intermediate states to the second-Born term of the valence-electron–atom scattering evaluated exactly. VMG, valence-electron–atom scattering (inert-core) modified Glauber approximation.

	Na			K		
Energy (eV)	e^- MG2	e^+ MG2	$e^\pm$ VMG	e^- MG2	e^+ MG2	$e^\pm$ VMG
150	17.26	16.70	16.02	27.60	26.87	24.72
200	13.79	13.38	12.63	22.30	21.70	19.45
300	10.01	9.733	8.975	16.44	15.99	13.79
400	7.955	7.739	7.017	13.21	12.84	10.76
500	6.645	6.468	5.787	11.12	10.82	8.865
800	4.525	4.410	3.841	7.705	7.509	5.872
1000	3.760	3.668	3.157	6.458	6.300	4.822

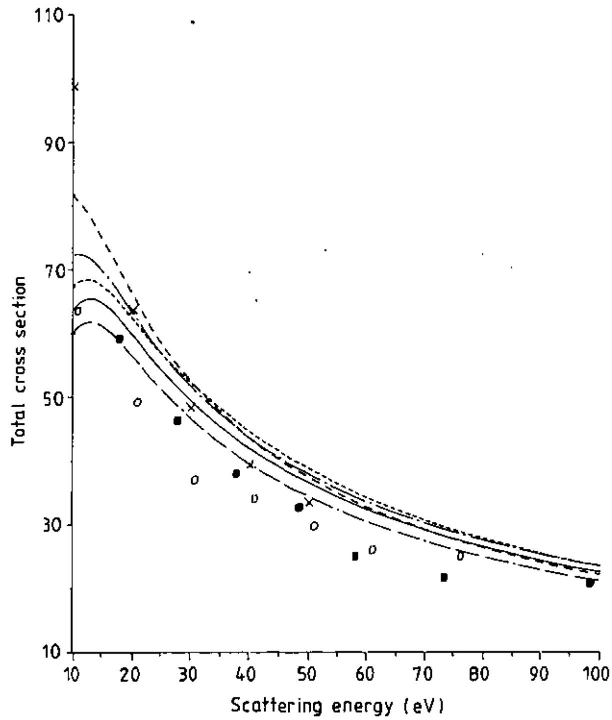

Figure 1. Total cross sections in πa_0^2 for electron and positron collisions with Na. - - - -: MG2, modified Glauber (see definition in the caption of table 1), electron scattering, frozen-core; ——: MG2, modified Glauber, positron scattering, frozen-core; – – –: VMG, inert-core modified Glauber; — · —: MG2, modified Glauber, model-potential approach (Gien 1989ab), electron scattering; —— · ——: MG2, modified Glauber, model-potential approach (Gien, 1989a, b), positron scattering; ×: close-coupling (Ward *et al* 1989), positron scattering; ●: positron experimental data (Stein *et al* 1990); ○: electron experimental data (Stein *et al* 1990).

experimental data are available (Stein *et al* 1988, 1990), are presented in figure 1 (Na) and in figure 2 (K). These results are to be compared with those previously obtained (Gien 1989a, b) in the calculations within the model potential approach and with those of the close-coupling approximation (Ward *et al* 1989).

The values of total cross section for both electron and positron collisions, in the frozen-core approximation as well as in the inert-core approximation, are consistent with those calculated in the model potential approach. The consistency of these results, which were obtained with two completely different methods of approach, reaffirms the reliability of the model-potential approach developed for use in electron (positron) collisions with alkali atoms. The slight difference between the two sets of values (in the model-potential and frozen-core approaches) is as expected. In fact, this is partly due to the presence of the strong core polarization potentials in the model potential approach, and partly due to the difference in the wavefunctions used for the two calculations. For electron scattering, the absence of the polarization term from the frozen-core potential tends to slightly decrease the values of total cross section, while this absence tends to slightly increase the values of total cross section for positron scattering. This is also as expected, since the polarization terms of the core potentials are the same for both charged projectiles, while the static parts are of opposite signs. Thus, for electron scattering, these two interaction effects (polarization and static) add up. They tend, therefore, to increase the scattering power of the potential and, thereby, the resulting total cross sections. In the case of positron scattering, these two effects cancel each other. They tend, therefore, to usually decrease the scattering power of the potential and, thereby, the resulting total cross sections.

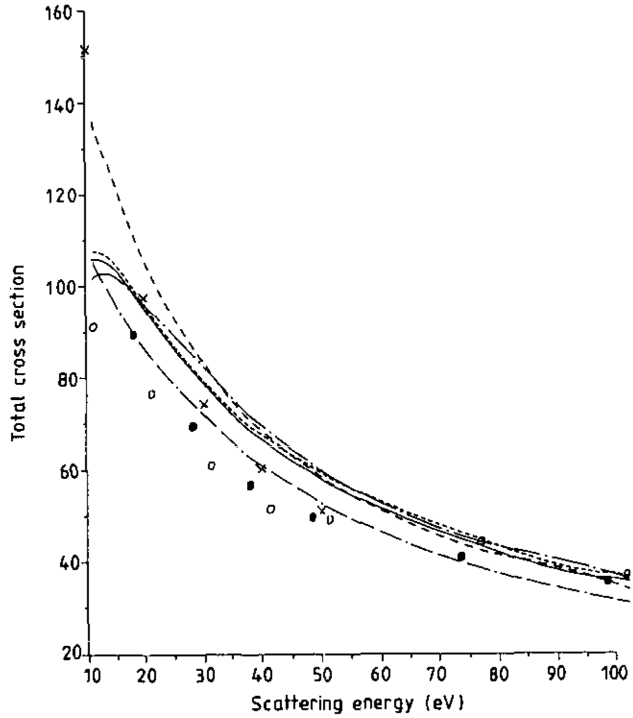

Figure 2. Total cross sections in πa_0^2 for electron and positron collisions with K. Details are the same as in figure 1.

It should be noted that the core polarization influences the electron and positron total cross sections not only through the scattering amplitude of the pure core scattering, but also through the distortion of the scattering wave in the scattering by the valence-electron atom (see, for example, Gien 1990). As for the pure core scattering alone, the effect of the polarization term of the model core potential is to decrease the strength of the phaseshifts of the lowest-order partial waves (which, as usual, are the predominant contribution to the scattering amplitude) in positron scattering and to increase their strength in electron scattering, in comparison with the strength of the corresponding phaseshifts in the scattering by the frozen-core potential. This correctly reflects the effect of the core polarization on the electron and positron total cross sections, as discussed above.

This slight increase (and decrease) of the cross sections makes the two values of total cross section for electron and positron collisions in the frozen-core approach merge with each other (within 5%) at a rather low energy below 40 eV. This work, therefore, confirms the validity of our earlier speculation (Gien 1989a, b, 1990) about the source of the non-merging of our results of total cross section for electron and positron collisions calculated in the model potential approach. The merging of the MG electron and positron total cross sections in the frozen-core approximation is more compatible with what was observed experimentally. However, this compatibility does not seem to be explainable in the case of scattering from Na and K, whose core polarizations are known to be rather large (Peach 1982) to be negligible. The physical insight gained from this work is that despite the non-negligible large core polarization of the alkali targets, the effects of the core polarization on the total cross sections for electron and positron collisions are, relatively speaking, rather small. Indeed, this effect is to only slightly worsen the merging of the total cross sections (from within 5% to within 10–15%).

While the results of this work are useful for a needed self-consistency check of the model-potential and frozen-core approaches, we do not intend, here, to advocate the preference of the frozen-core approach over the model-potential approach. Despite the seemingly better merging of the cross sections, the former method of approach seems to be somewhat less 'physical' than the latter and, furthermore, the agreement between the positron frozen-core MG cross sections and experimental data seems to somewhat worsen at low energies. In our opinion, the results of the two methods of approach, as far as the comparison with experimental data is concerned, are both acceptable, in view of the uncertainty existing in the experimental data (Stein *et al* 1989, 1990), due to the inability to discriminate against the elastically scattered electrons (positrons) near the forward direction (also see our discussion in Gien 1989a, b, 1990). It should be stressed that the merging of the positron and electron cross sections, as observed in experiments, might also be understood for this very same reason. This, combined with the fact that new experimental data by Stein *et al* (1990) seem to consistently lie somewhat below our MG values (see figures 1 and 2), prompts us to speculate that a more proper comparison should perhaps be made with the so-called 'effective' cross sections (Ward *et al* 1988a, b, 1989). The estimate of the effective total cross sections in the MG approximations requires the availability of values of a high degree of accuracy for the elastic differential cross sections at small scattering angles. The accurate evaluation of the terms which constitute the MG scattering amplitude at these small angles is, however, extremely difficult and rather time consuming. These calculations usually consume an exorbitant amount of computer time to achieve a desired accuracy. Fortunately, with the availability of some very cheap and fast microcomputers and workstations on the market at present, we hope that, with time, we shall be able to obtain these effective total cross sections in the MG calculation. We are vigorously pursuing this course for both the frozen-core and the model-potential approach.

3. Conclusion

The MG total cross sections calculated in the frozen-core approach for electron and positron collisions with K and Na are found to be consistent with those previously calculated in the model potential approach (Gien 1989a, b). The new MG values are, therefore, also in fair agreement with experimental data. The MG electron and positron total cross sections obtained in the frozen-core approach merge with each other (within 5%) at a rather low energy. The consideration of the large core-polarization terms of the potential in the model-potential approach does seem to be the source for the non-merging of the modified Glauber total cross sections previously obtained for electron and positron collisions with sodium and potassium.

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