Total cross sections for $e^{\pm}$—alkali-metal-atom collisions

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The total cross sections for electron and positron scatterings by lithium, sodium, and potassium in the intermediate energy range from 40 to 1000 eV are calculated using the modified Glauber and second Born approximations. A model potential approach is developed to enable an exact inclusion of the core-interaction effects. Within this approach, the positron cross sections are predicted to be somewhat smaller than those of electron scattering. Calculations have also been performed with the consideration of the inert-core and frozen-core assumption and the use of the Clementi wave function to represent the target electrons. Comparison to existing experimental data is made.

I. INTRODUCTION

Alkali-metal atoms have been a subject of interest in several recent theoretical and experimental investigations in $e^{\pm}$-atom collisions because of their various interesting properties: relatively simple structure, low ionization potentials (3.9—5.4 eV), and existence of resonance lines in the visible or quartz ultraviolet part of the electromagnetic spectrum (which make the alkali metals interesting as components of stellar atmosphere and other plasmas). The total collisional cross sections have been measured or estimated by various experimental research groups[1–3] for electron impact on these atoms. Only very recently, some pioneering work by Stein *et al.*[4] has provided a set of total cross sections for positron scattering on potassium at low scattering energies from 5.2 to 48.6 eV. Similar to the case of collision by inert-gas atoms, the positron total cross sections on potassium are found to lie somewhat below those of electron scattering. The availability of this new set of positron data (other sets of data of e^+ collision at higher scattering energies and on other alkali-metal-atom targets, undoubtedly, will soon become available) has inspired us to carry out the theoretical calculation of total cross section for $e^{\pm}$—alkali-metal-atom scatterings. For positron collision on potassium, some theoretical estimates have been available[5–7] using the integrated cross section of elastic scattering in place of the actual total cross section. These estimates therefore left out the contribution from the excitation and ionization processes which may be quite significant to be negligible at higher scattering energies. Some of these estimates are found to be significantly smaller than the corresponding experimental values at low energies. Thus, the availability of the theoretical values for total cross section of electron and especially of positron collision on alkali-metal atoms would be very much desirable.

In this work, we shall therefore carry out the calculation of total cross section for $e^{\pm}$—alkali-metal-atom (Li, Na, and K) scatterings, using the second Born (SB) and modified Glauber[8] (MG) approximations. We shall particularly be interested in the results of the latter method of approximation which has been known to provide the total cross sections for positron collision with helium[9] in very good agreement with experimental data[10] at intermediate energies from 100 to 1000 eV. For electron-lithium scattering, Khare and Vijayshri[11] have carried out the calculation of total cross section in the MG approximation. However, these authors had to use the less accurate wave functions by Veselov *et al.*[12] in their work to make the calculation become manageable. Very recently,[11] Khare also reported some results of total cross section for $e^{\pm}$-Na and -K collisions. While no detailed description of the calculation was given, Khare had to consider some further approximation [inert-core (IC) or single-particle scattering model (SPSM)] to avoid the complexity which is to be encountered in the calculation of the multiple-scattering terms of the Glauber amplitude in these cases. In Sec. II, we shall, therefore, describe in some detail the modified Glauber theory within the framework of electron and positron collision on these (more complex) atomic targets and derive as well the analytic expressions for the relevant scattering amplitudes which are needed for the subsequent calculation of total cross section. The results obtained for electron and positron collisions with potassium, sodium, and lithium will be displayed with discussion in Sec. III.

II. THEORY

In one of our earlier works,[13] we proposed that the conventional Glauber amplitude which has been found to work remarkably well for $e^{\pm}$-atom scatterings at intermediate energies[14] could be improved by correcting its second-order eikonal term with the second-Born-approximation counterpart,

$$f_{\mathrm{MG}}=f_G-f_{G2}+f_{B2}\ . \tag{1}$$

The conventional Glauber approximation, modified in a very simple fashion like this, has been known in the literature as the modified Glauber approximation (MGA).

It has also been well known that if the Hartree-Fock wave functions by Clementi[15] are used to represent the bound states of alkali-metal atoms, the calculation of the scattering amplitudes in an eikonal-related approximation such as the modified Glauber one becomes very difficult

and almost unmanageable because of the presence of a great number of the so-called multiple-scattering terms in these amplitudes. These terms originate from the scattering between the scattered electron and the core of the atom (which includes the nucleus and a great number of core electrons). The calculation of these terms is quite a tedious job and becomes an almost impossible task in scatterings by a heavy atomic target despite the fact that one has succeeded in putting these multiple-scattering terms of the conventional Glauber amplitude into some simple (one-variable) integral forms.[16,17] To overcome this difficulty, we have recently[18] developed a method of approach (which, henceforth, will be referred to as the model potential approach) which enables an "exact" inclusion of the core-interaction effects while the calculation of the scattering amplitude can be handled with much less hardship even in the case of scattering by a multielectron atomic target such as sodium and potassium. Thus, with this method of approach, it is the first time that the core-interaction effects in $e^{\pm}$—alkali-metal-atom scatterings can be included "exactly" to the scattering amplitude. As was already described in some detail elsewhere,[18] the essential idea of the method is to employ some very accurate model potential existing at present for the relevant e^-—positive-ion system[19] to generate the wave function of the "equivalent one-electron" atom whose dynamics is governed by this model potential. The correlation effect between the valence electron and the core ones as well as any other effect which may originate from the core are all implicitly contained in the core potential. Thus, the bound states of the actual atom may now be represented by those of the "equivalent one-electron atom." Within this approach, the electron (positron) scattering by the complex core of the atom is represented by the various terms of the model potential. Unlike the Hartree-Fock orbital of the valence electron, the wave function of a bound state of the equivalent one-electron atom in the model potential approach may be seen as being already fully correlated by the core electrons through the core potential of the atom. In Table I, we display the model potentials by Peach[20] of the e^--Li^+, e^--Na^+, and e^--K^+ systems. Employing these model potentials, we have been able to generate the wave functions of the $2s$ (Li), $3s$ (Na), and $4s$ (K) ground states of these equivalent one-electron atoms. These wave functions are tabulated in Table II. They are expected to be rather accurate as the corresponding eigenenergies obtained by this procedure are found to be almost exactly the same as those supplied by Peach along with her model potentials (see Table II). With the model potential approach, the calculation of the scattering amplitude becomes much easier as we now have to deal only with a one-electron wave function. Although we now have to face a more complex model potential in the reduction of a scattering amplitude, we have in fact succeeded in putting all the relevant amplitudes of the modified Glauber and second Born approximations in forms which can be accessed for numerical computation without any difficulty.

The conventional Glauber amplitude of $e^{\pm}$—alkali-metal-atom scattering in the model potential approach can be separated into two terms,

$$f_G = f_G^a + f_G^c \ , \tag{2}$$

where f_G^a and f_G^c are, respectively, the Glauber amplitude of scattering by the "valence-electron atom" whose scattering potential is $V_a = z(1/r - 1/|\mathbf{r}-\mathbf{r}'|)$ and that involving both the valence-electron atom and the residual core potential V_c (with $V_c = V - z/r$). We obtain for these amplitudes

$$f_G^a = \hat{D}(\alpha_\mu) f_G^a(\alpha_\mu) \tag{3a}$$

and

$$f_G^c = \hat{D}(\alpha_\mu) f_G^c(\alpha_\mu) \ , \tag{3b}$$

where $\hat{D}(\alpha_\mu)$ is an appropriate differential operator which generates the various terms of the product of the initial- and final-state wave functions $u_f^*(r)u_i(r)$,

$$\hat{D}(\alpha_\mu) = \sum_\mu A_\mu (-1)^\mu \frac{\partial^\mu}{\partial(\alpha_\mu)^\mu} \ . \tag{4}$$

TABLE I. Model potentials of the e^-—positive-ion system of alkali-metal atoms:

$$V = \frac{z}{r} + \frac{Z}{r}(1+\delta r + \delta' r^2)e^{-\gamma r} + \frac{\alpha_d}{2r^4}\omega_2(\beta r) + \frac{\alpha_q'}{2r^6}\omega_3(\beta' r)$$

where $\omega_n(x) = [1 - e^{-x}\sum_{m=0}^{n}(x^m/m!)]^2$.

Atom	Li	Na	K
z	−1	−1	−1
Z	−2	−10	−18
γ	4.049 451 698	2.703 497 450	7.040 979 814
α_d	−0.192 23	−0.923 89	−5.145 8
δ	2.446 920 908	−0.385 624 507 4	4.064 463 84
δ'	0.249 578 031	0.344 886 205 7	−0.095 953 348 76
β	3.911 542 198	4.668 977 902	4.945 957 718
β'		3.157 998 45	2.289 741 79
α_q'		−0.857 368 812 1	−25.558 643 67

A_μ are expressed in terms of the coefficients of the wave functions. $F_G^a(\alpha_\mu)$ and $f_G^c(\alpha_\mu)$ are, respectively, given by

$$f_G^a(\alpha_\mu)=\frac{ik_i}{8\pi^2}\int d^2\mathbf{b}\,d\mathbf{r}\,e^{i\mathbf{q}\cdot\mathbf{b}}(1-e^{i\chi_0})e^{-\alpha_\mu r} \tag{5a}$$

and

$$f_G^c(\alpha_\mu)=ik_i\int_0^\infty ds\int_0^\infty db\,s^2bJ_0(qb)K_1(\alpha_\mu s)\times\left[\frac{2s}{bY}\right]^{i\eta}(1-Y^2)^{i\eta+1/2}\times F(\tfrac{1}{2}+\tfrac{1}{2}i\eta,\tfrac{1}{2}i\eta+1;1;Y^2)\times(1-e^{i\chi_c})\,. \tag{5b}$$

χ_0 is the Glauber phase of the valence-electron–atom scattering. $Y=2bs/(b^2+s^2)$, $\eta=-z/k_i$, and $z=-1$ for electron and $+1$ for positron scattering. χ_c is the Glauber phase of the core potential scattering,

$$\chi_c(b)=-\frac{1}{k_i}\int_{-\infty}^{+\infty}V_c(r')dz'\,. \tag{6}$$

With the model potential by Peach (see Table I), $\chi_c(b)$ can be put in the following form:

$$\chi_c(b)=-\frac{Z}{k_i}[(1+\delta' b^2)K_0(\gamma b)+b(\delta+\delta'/\gamma)K_1(\gamma b)]-\frac{1}{k_i}\int_{-\infty}^{+\infty}V_c^{\rm pol}(r')dz'\,. \tag{7}$$

Z is a negative number for electron and a positive number for positron scattering. $V_c^{\rm pol}$ is the polarization part of the core potential. In the case of Li scattering, $V_c^{\rm pol}$ is

$$V_c^{\rm pol}=\frac{\alpha_d}{2r^4}\left[1-e^{-\beta r}\sum_{m=0}^{2}\frac{(\beta r)^m}{m!}\right]^2, \tag{8a}$$

while in the case of Na and K scattering, $V_c^{\rm pol}$ is in the following form:

$$V_c^{\rm pol}=\frac{\alpha_d}{2r^4}\left[1-e^{-\beta r}\sum_{m=0}^{2}\frac{(\beta r)^m}{m!}\right]^2+\frac{\alpha_q'}{2r^6}\left[1-e^{-\beta' r}\sum_{m=0}^{3}\frac{(\beta' r)^m}{m!}\right]^2. \tag{8b}$$

It is well known that $f_G^a(\alpha_\mu)$ is reducible to a closed form.[21]

On the other hand, the second-order eikonal term of the conventional Glauber expansion can be separated into three terms,

$$f_{G2}=f_{G2}^a+f_{G2}^{ac}+f_{G2}^c\,. \tag{9}$$

In the forward direction ($\mathbf{q}=0$), the second-order eikonal amplitude which corresponds to the valence-electron–atom scattering is divergent logarithmically.

TABLE II. Wave functions of alkali-metal atoms in the model potential approach: $R(r)=a_0e^{-\alpha_0 r}+a_1re^{-\alpha_1 r}+a_2r^2e^{-\alpha_2 r}+a_3r^3e^{-\alpha_3 r}+a_4e^{-\beta r}$, $\beta=\sqrt{\varepsilon}$.

State	Energy ε (supplied[a]) in Ry	Energy ε (generated) in Ry	a_0	a_1	a_2	a_3	a_4	α_0	α_1	α_2	α_3
Li 2s	0.395 918	0.395 920	5.333 873 9	−1.833 167 2	0.320 336 29	0	−3.652 355 6	1.026 370	2.491 871	1.017 959	
Na 3s	0.377 466	0.377 471	0	24.585 984	−33.797 186	0.761 041 76	−2.727 990 7		2.354 095	3.528 590	1.535 323
K 4s	0.318 164	0.318 193	7.441 357 5	17.184 090	−11.825 597	0.251 117 10	−3.972 510 4	10.956 78	1.531 749	2.173 498	1.129 665

[a] References 19 and 20.

Therefore, to calculate this term of the modified Glauber amplitude in the forward direction, one has usually evaluated it concurrently with the Glauber amplitude of the valence-electron–atom scattering f_G^a. f_{G2}^c is the second-order eikonal amplitude corresponding to the pure core-potential scattering. f_{G2}^c is found to be

$$f_{G2}^c=\frac{ik_i}{2}\int_0^\infty b\,db\,J_0(qb)\chi_c^2 . \tag{10}$$

The second-order eikonal amplitude which involves both the valence-electron–atom and the core-potential scattering is shown to be

$$f_{G2}^{ac}=\hat{D}(\alpha_\mu)f_{G2}^{ac}(\alpha_\mu) , \tag{11}$$

where

$$f_{G2}^{ac}(\alpha_\mu)=\frac{ik_i}{8\pi^2}\int d^2\mathbf{b}\,d\mathbf{r}\,e^{-\alpha_\mu r}\chi_0\chi_c e^{i\mathbf{q}\cdot\mathbf{b}} . \tag{12}$$

After some algebra, $f_{G2}^{ac}(\alpha_\mu)$ can also be put in a double-integral form whose numerical calculation can be carried out easily.

The second-order Born amplitude can also be separated into three parts,

$$f_{B2}=f_{B2}^a+f_{B2}^{ac}+f_{B2}^c , \tag{13}$$

where f_{B2}^a, f_{B2}^{ac}, and f_{B2}^c are the counterparts of f_{G2}^a, f_{G2}^{ac}, and f_{G2}^c, respectively. The second-order Born term corresponding to the pure core-potential scattering is independent of the form of the wave function of the target and can be expressed in terms of a triple-integral form

$$f_{B2}^c=\frac{2}{\pi^2}\int\frac{d\mathbf{k}}{k^2-k_i^2-i\epsilon}h(K_i)h(K_f) , \tag{14}$$

where $h(K_{i,f})$ are given by

$$h(K_{i,f})=\frac{1}{K_{i,f}}\int_0^\infty r'V_c(r')\sin(K_{i,f}r')dr' \tag{15}$$

and $\mathbf{K}_{i,f}=\mathbf{k}_{i,f}-\mathbf{k}$. With Peach's model potentials in the forms shown in Table I, we have also succeeded in reducing $h(K_{i,f})$ to a closed form after some very tedious analytical calculations. Thus, the numerical calculation of f_{B2}^c reduces to that of a triple integral in the general case. The procedure of calculating this triple integral has been well known. However, for the imaginary part of f_{B2}^c in the forward direction (which is in fact the only part of the amplitude needed to be evaluated to obtain the total cross section of the process via the optical theorem), the numerical calculation reduces to that of a simple (one-variable) integral. Thus, the calculation of $\mathrm{Im}f_{B2}^c(0)$ can be carried out quite easily and fast. In a similar fashion, we can put the second Born amplitude which involves the scattering by both the core potential and the valence-electron atom in the following form:

$$f_{B2}^{ac}=4\int d\mathbf{k}\frac{\langle u_f,\mathbf{k}_f\mid V_a\mid u_i,\mathbf{k}\rangle}{k^2-k_i^2-i\epsilon}h(K_i)+4\int d\mathbf{k}\frac{\langle u_f,\mathbf{k}\mid V_a\mid u_i,\mathbf{k}_i\rangle}{k^2-k_f^2-i\epsilon}h(K_f) . \tag{16}$$

f_{B2}^{ac} can, therefore, be calculated *exactly* without having to consider the usual average closure approximation. This is in fact another advantage for using the model potential approach. The transition amplitudes $\langle u_f,\mathbf{k}_f\mid V_a\mid u_i,\mathbf{k}\rangle$ and $\langle u_f,\mathbf{k}\mid V_a\mid u_i,\mathbf{k}_i\rangle$ are also reducible to closed forms,

$$\langle u_f,\mathbf{k}_f\mid V_a\mid u_i,\mathbf{k}\rangle=-\frac{z}{2\pi^2}\left[\hat{D}(\alpha_\mu)\left[\frac{2\alpha_\mu}{(\alpha_\mu^2+K_f^2)^2}\right]-1\right]\frac{1}{K_f^2} \tag{17a}$$

and

$$\langle u_f,\mathbf{k}\mid V_a\mid u_i,\mathbf{k}_i\rangle=-\frac{z}{2\pi^2}\left[\hat{D}(\alpha_\mu)\left[\frac{2\alpha_\mu}{(\alpha_\mu^2+K_i^2)^2}\right]-1\right]\frac{1}{K_i^2} . \tag{17b}$$

$z=-1$ for electron and $z=+1$ for positron scattering. Thus, the calculation of f_{B2}^{ac} in the most general case reduces to that of a triple integral. Again, to calculate $\mathrm{Im}f_{B2}^{ac}(0)$ in the forward direction, one is actually required to perform only a simple integration which can again be carried out quite easily and fast.

As for the second Born term corresponding to the valence-electron–atom scattering, we use, as usual, the closure approximation in which the term corresponding to the elastic intermediate-state transition ($2s$ for Li, $3s$ for Na, and $4s$ for K) will be calculated exactly. We obtain

$$\bar{f}_{B2}=\bar{f}_{\mathrm{SB2}}+8\pi^2\int d\mathbf{k}\frac{\langle u_i,\mathbf{k}_f\mid V_a\mid u_i,\mathbf{k}\rangle\langle u_i,\mathbf{k}\mid V_a\mid u_i,\mathbf{k}_i\rangle}{k^2-k_i^2-i\epsilon}-8\pi^2\int d\mathbf{k}\frac{\langle u_i,\mathbf{k}_f\mid V_a\mid u_i,\mathbf{k}\rangle\langle u_i,\mathbf{k}\mid V_a\mid u_i,\mathbf{k}_i\rangle}{k^2-p^2-i\epsilon} , \tag{18}$$

where

$$\bar{f}_{\mathrm{SB2}}=\hat{D}(\alpha_\mu)F(\alpha_\mu) \tag{19}$$

with

$$F(\alpha_\mu)=4\alpha_\mu\frac{d}{d\alpha_\mu^2}\left[-\frac{2}{\alpha_\mu^2}I(\alpha_\mu^2)+I(\alpha_\mu=0)\frac{q^2}{\alpha_\mu^2(\alpha_\mu^2+q^2)}\right] , \tag{20}$$

where $I(\alpha_\mu^2)$ is the well-known Dalitz integral. Thus, the calculation of the second Born term in the simplified closure approximation, $\bar{f}_{\mathrm{SB2}}$, can, as was well known, be carried out either in closed forms or by a simple (one-variable) numerical integration.[22] The calculation of the imaginary parts in the forward direction of the two extra terms in Eq. (18) can also be reduced to that of an easy one-variable integration. In order to obtain the total cross sections via the optical

theorem, one also needs to calculate the imaginary part of the Glauber amplitude of valence-electron—atom scattering. This term, as was pointed out above, should be evaluated concurrently with $f_{G2}^{a}(0)$ (Refs. 9 and 23) and for our complex wave functions, we can easily obtain a closed form for the difference of these two terms as follows:

$$f_G^a(0)-f_{G2}^a(0)=-8ik_i\left[\frac{i\eta}{1-i\eta}+2\eta^2+\sum_{n=1}^{\infty}\left[\frac{(-i\eta)_n}{n!}\right]^2\frac{1}{1-i\eta+n}-\sum_{n=2}^{\infty}\left[\frac{(-i\eta)_n}{n!}\right]^2\frac{1}{1-n}\right]\hat{D}(\alpha_\mu)\frac{1}{\alpha_\mu^5}\,. \tag{21}$$

It should be stressed that Eqs. (18), (19), and (21) are quite general and applicable to any type of wave function. We have, in fact, also employed them (see Sec. III) to calculate the total cross sections in the inert-core approximation with the Clementi wave functions. Finally, the total cross sections of $e^{\pm}$ collision are derived through the consideration of the optical theorem,

$$\sigma=\frac{4\pi}{k_i}\mathrm{Im}f(0)\,, \tag{22}$$

where f will be either the modified Glauber or the second Born amplitude.

III. NUMERICAL RESULTS AND DISCUSSION

The analytic expressions derived in Sec. II have been employed to obtain the total cross sections for electron— and positron—alkali-metal-atom collisions in the modified Glauber and second Born approximations. $f_G^a(0)-f_{G2}^a(0)$ can be evaluated quite easily with the use of its closed form [Eq. (21)]. The imaginary part of the pure core-potential scattering term f_{G2}^c is calculated with Eq. (10). The calculation of f_G^c and of f_{G2}^{ac} requires us to carry out some double integration. We have carefully checked and tested our computer program written to calculate these double integrals and made sure that the convergence of the double numerical integration has been attained. The calculation of $\bar{f}_{B2}$ in the forward direction can be carried out without any difficulty with the employment of Eqs. (18) and (19). Following a method suggested by Bonham,[24] we choose the average excitation energy Δ in $p^2=k_i^2-2\Delta$ to be

$$\Delta=\tfrac{1}{2}\exp\left[\frac{L(-1)}{S(-1)}\right]\,, \tag{23}$$

where $L(-1)$ and $S(-1)$ are characteristics of the target atom. We used the values of $L(-1)$ and $S(-1)$ by Zeiss *et al.*[25] to obtain a value of Δ equal to 0.088 75 a.u. for the Li target. For Na and K, we used the values of $L(-1)$ and $S(-1)$ by Dehmer *et al.*[26] and Inokuti *et al.*[26] to obtain the value of Δ equal to 0.1401 and 0.1295 a.u., respectively. It may be worth noting that although the second Born term was calculated here using the form of Eq. (18) for the closure approximation instead of the simplified one of Eq. (19), we found that the results of total cross section are, relatively speaking, rather insensitive to whether $\bar{f}_{B2}$ or $\bar{f}_{SB2}$ was chosen for the calculation.

The total cross sections of the valence-electron—atom approximation in which the core potential scattering is neglected have also been obtained. We have also obtained for comparison the total cross sections in the inert-core approximation of the conventional modified Glauber and second Born methods using the Hartree-Fock wave functions by Clementi[15] to represent the valence electron. In the case of Li scattering, the inert-core values will also be obtained with the employment of a less accurate wave function by Veselov *et al.*[12]

In Table III, we present the total cross sections of $e^{\pm}$-Li collision in the modified Glauber and second Born approximations.[27] Comparing the results calculated in the valence-electron—atom approximation of the model potential approach to those calculated in the inert-core approximations with the use of the Clementi and Veselov *et al.* wave functions, we find some expected slight variation among the results obtained with different wave functions. At scattering energies where Khare and Vijayshri also evaluated, our results with the use of the Veselov *et al.* wave functions (not shown) agree with theirs. The inert-core values calculated with the simple Veselov *et al.* wave function are, however, found to differ from the inert-core values calculated with the Clementi wave function much more considerably than the values obtained in the valence-electron—atom approximation of the model potential approach. The very close agreement of the valence-electron—atom results to those of the inert-core approximation calculated with the Hartree-Fock wave function by Clementi (even much closer than those calculated with the same inert-core approximation but with the use of a different and less accurate wave function) indicates that our model potential approach for $e^{\pm}$-atom scatterings is rather reliable. Since the wave function acquired for the valence electron in the model potential approach contains implicitly all the correlation effects caused by other core electrons, the results calculated with the wave function obtained for the valence electron in the model potential approach, to some extent, may even be preferred over the inert-core results calculated with the Clementi wave function. The rather slight difference between the two sets of values indicates that the correlation effect in the case of a light alkali-metal atom (Li) is rather small. Of course, the main advantage of the model potential approach over the direct calculation still is its ability of including "exactly" the core scattering effects to the scattering amplitude. The direct "exact" calculation of the core scattering in an eikonal-related approximation in the case of a heavy alkali-metal-atom target (such as Na and K) is obviously out of the question.

TABLE III. Total cross sections (πa_0^2 units) of $e^{\pm}$-Li collisions in the modified Glauber (MG) and second Born (SB) approximations.

Energies (eV)	SB inert-core Clementi wave fn.	SB valence-e^- atom (mod. pot.)	SB e^- full model potential	SB e^+ full model potential	MG inert-core Clementi wave fn.	MG valence-e^- atom (mod. pot.)	MG e^- full model potential	MG e^+ full model potential
40.0	4.183[1][a]	4.121[1]	4.506[1]	4.362[1]	3.671[1]	3.618[1]	3.591[1]	3.553[1]
50.0	3.497[1]	3.444[1]	3.763[1]	3.647[1]	3.154[1]	3.108[1]	3.113[1]	3.075[1]
54.4	3.266[1]	3.217[1]	3.513[1]	3.406[1]	2.972[1]	2.928[1]	2.942[1]	2.905[1]
60.0	3.015[1]	2.970[1]	3.242[1]	3.144[1]	2.770[1]	2.729[1]	2.752[1]	2.716[1]
70.0	2.658[1]	2.618[1]	2.854[1]	2.771[1]	2.473[1]	2.436[1]	2.471[1]	2.436[1]
80.0	2.381[1]	2.345[1]	2.555[1]	2.481[1]	2.237[1]	2.203[1]	2.244[1]	2.211[1]
90.0	2.159[1]	2.126[1]	2.315[1]	2.250[1]	2.044[1]	2.013[1]	2.059[1]	2.027[1]
100.0	1.978[1]	1.948[1]	2.119[1]	2.060[1]	1.884[1]	1.855[1]	1.903[1]	1.873[1]
150.0	1.407[1]	1.385[1]	1.503[1]	1.463[1]	1.364[1]	1.343[1]	1.392[1]	1.368[1]
200.0	1.102[1]	1.085[1]	1.174[1]	1.145[1]	1.077[1]	1.061[1]	1.107[1]	1.087[1]
300.0	7.785	7.665	8.266	8.071	7.673	7.554	7.937	7.789
400.0	6.072	5.977	6.431	6.285	6.008	5.914	6.236	6.118
500.0	5.001	4.923	5.288	5.171	4.960	4.883	5.159	5.061
600.0	4.266	4.199	4.504	4.407	4.237	4.171	4.412	4.328
800.0	3.316	3.263	3.493	3.420	3.299	3.248	3.439	3.374
1000.0	2.724	2.681	2.865	2.807	2.714	2.671	2.830	2.777

[a]Numbers in square brackets are powers of ten.

In Tables IV, V, and VI, we display the total cross sections of electron and positron collisions on Na and K atoms which are calculated in the modified Glauber and second Born approximations. These total cross sections are obtained both in the valence-electron—atom scattering and in the full-atom scattering where the core scattering effect is included via the core potential. The total cross sections calculated with the consideration of the inert-core assumption, using the Hartree-Fock wave function by Clementi for the valence electron, have also been obtained and are shown along for comparison together with some experimental data available for electron scattering at low intermediate energies. Our total cross sections obtained in the inert-core MG approximation for both $e^{\pm}$-K and $e^{\pm}$-Na scatterings agree with the few values presented by Khare.[11] Khare and his associate's values of SPSM, where the multiple-scattering terms are neglected, are, however, much higher than those calculated in the inert-core approximation.

For a light atomic target (Li) and within the modified Glauber approximation, we find that the contribution from the core scattering in electron scattering is negligible

TABLE IV. Total cross sections (πa_0^2 units) of e^--Na collision in the modified Glauber and second Born approximations.

Energies (eV)	SB inert-core Clementi wave fn.	SB valence-e^- atom (mod. pot.)	SB full model pot.	MG inert-core Clementi wave fn.	MG valence-e^- atom (mod. pot.)	MG full model pot.	Expt. data Kasdan *et al.*	Expt. data Vuskovic and Srivastava
40.0	3.888[1][a]	3.688[1]	6.996[1]	3.290[1]	3.131[1]	2.474[1]		4.761[1]
50.0	3.286[1]	3.114[1]	5.864[1]	2.886[1]	2.742[1]	2.373[1]	6.477[1]	
54.4	3.080[1]	2.919[1]	5.480[1]	2.738[1]	2.599[1]	2.315[1]		3.432[1]
60.0	2.856[1]	2.706[1]	5.061[1]	2.570[1]	2.439[1]	2.237[1]		
70.0	2.534[1]	2.399[1]	4.459[1]	2.318[1]	2.198[1]	2.101[1]		
80.0	2.281[1]	2.159[1]	3.990[1]	2.114[1]	2.003[1]	1.975[1]		
90.0	2.078[1]	1.966[1]	3.614[1]	1.944[1]	1.841[1]	1.861[1]		
100.0	1.911[1]	1.807[1]	3.305[1]	1.801[1]	1.705[1]	1.759[1]		
150.0	1.377[1]	1.301[1]	2.332[1]	1.326[1]	1.254[1]	1.383[1]		
200.0	1.087[1]	1.027[1]	1.813[1]	1.058[1]	9.998	1.147[1]		
300.0	7.760	7.322	1.265[1]	7.628	7.200	8.676		
400.0	6.091	5.745	9.781	6.017	5.676	7.053		
500.0	5.041	4.753	8.000	4.993	4.708	5.980		
600.0	4.316	4.068	6.784	4.282	4.036	5.213		
800.0	3.372	3.177	5.225	3.353	3.159	4.180		
1000.0	2.782	2.620	4.263	2.769	2.609	3.510		

[a]Numbers in square brackets are powers of ten.

at low energies and gradually increases to only about 10% at 1000 eV. This contribution is greater for heavier (with a more complex core) targets and becomes rather large for potassium. At scattering energy around 100 eV where an eikonal-related approximation is expected to begin to work well,[9] the scattering seems to be insensitive to the core-interaction effect. Above this range of energy, the consideration of the core interaction increases the total cross section and modifies more and more the cross section as the scattering energy is greater. The core interaction at low energies below 100 eV actually cancels out a part of the scattering capacity of the atom as a whole and thereby decreases the total collisional cross sections in comparison to those obtained with the core interaction excluded. It should, however, be warned that an eikonal-related approximation such as the modified Glauber one is not expected to work very well at these low scattering energies. In the case of scattering by potassium, the inclusion of the core-interaction effects may enhance (at high energy) or depress (at low energy) the total cross section up to 50%. Thus contrary to popular belief and unlike Li, the core scattering in the case of a heavy alkali-metal-atom target is quite significant, and is not negligible.

The second Born values in both the valence-electron and the full-atom scattering are greater than those of the MGA counterparts in the whole range of scattering energy and for all alkali-metal-atom targets under consideration. The second Born values may exceed the MGA ones up to 80% at low energies. Since the difference between the second Born and the modified Glauber approximations is that in the MG approximation, scattering terms of higher than the second order are not totally neglected, the significant difference between the collisional cross sections obtained in the two approximations reconfirms that the contributions to the scattering amplitude from these higher-order scattering terms are quite significant at lower energies and should therefore not be neglected. This is exactly the same situation that one has experienced with in the case of electron and positron scattering by an inert gas (He).[9] The difference between the two cross sections in the valence-electron—atom scattering decreases as the scattering energy increases to an insignificant value at 1000 eV and above as expected. On the other hand, the significant difference between the two cross sections in the full-atom scattering which remains considerable at as high as an energy of 1000 eV in the case of Na and K indicates that the contributions from higher-order scattering terms originating from the core-potential scattering remain rather significant at a considerably high energy for heavy atomic targets and cannot be neglected therein even at high energy. The contribution from these terms is especially important in scattering by the K atom where both the static potential coupling strength and dipole and quadrupole polarizabilities of the core are great.

For positron scattering, most of the remarks made above in electron scattering remain valid. The core potential in positron scattering also affects the total cross section less significantly than in electron scattering. This difference from the electron scattering case probably arises from the fact that the core static potential in the

TABLE V. Total cross sections (πa_0^2 units) of e^--K collision in the modified Glauber and second Born approximations.

Energies (eV)	SB inert-core Clementi wave function	SB valence-electron atom (mod. pot.)	SB full model potential	MG inert-core Clementi wave function	MG valence-electron atom (mod. pot.)	MG full model potential	Expt. data Kasdan *et al.*	Expt. data Vuskovic *et al.*	Experimental data of Stein *et al.* Energy (eV)	Cross sec.
40.0	5.627[1][a]	5.117[1]	1.704[2]	4.716[1]	4.312[1]	2.438[1]		6.818[1]	41.4	7.692[1]
50.0	4.764[1]	4.327[1]	1.417[2]	4.155[1]	3.789[1]	2.702[1]	8.523[1]		51.6	6.655[1]
54.4	4.469[1]	4.058[1]	1.320[2]	3.947[1]	3.596[1]	2.735[1]				
60.0	4.148[1]	3.764[1]	1.214[2]	3.712[1]	3.378[1]	2.740[1]		5.000[1]		
70.0	3.683[1]	3.340[1]	1.064[2]	3.356[1]	3.050[1]	2.689[1]				
80.0	3.320[1]	3.008[1]	9.471[1]	3.065[1]	2.783[1]	2.603[1]			76.75	5.922[1]
90.0	3.027[1]	2.741[1]	8.541[1]	2.822[1]	2.561[1]	2.506[1]				
100.0	2.785[1]	2.521[1]	7.781[1]	2.618[1]	2.373[1]	2.408[1]		3.182[1]	102.5	5.328[1]
150.0	2.013[1]	1.819[1]	5.409[1]	1.936[1]	1.751[1]	1.987[1]				
200.0	1.592[1]	1.438[1]	4.163[1]	1.548[1]	1.399[1]	1.691[1]				
300.0	1.139[1]	1.027[1]	2.868[1]	1.119[1]	1.009[1]	1.320[1]				
400.0	8.957	8.069	2.197[1]	8.844	7.968	1.097[1]				
500.0	7.422	6.681	1.786[1]	7.349	6.617	9.461				
600.0	6.359	5.722	1.506[1]	6.308	5.677	8.364				
800.0	4.975	4.473	1.151[1]	4.946	4.448	6.856				
1000.0	4.108	3.692	9.335	4.089	3.675	5.857				

[a]Numbers in square brackets are powers of ten.

TABLE VI. Total cross sections (πa_0^2 units) of e^+-Na and e^+-K collisions in the modified Glauber and second Born approximations. [The values of the second Born and modified Glauber approximations in the inert-core approximation calculated with the Clementi wave function and those of the valence-electron—atom scattering in the model potential approach are the same as those of electron scattering (see Tables V and VI).]

	Sodium		Potassium			
Energies (eV)	SB full model potential	MG full model potential	SB full model potential	MG full model potential	Expt. data by Stein *et al.* Energy (eV)	Cross sections e^+-K
40.0	4.922[1][a]	2.394[1]	4.589[1]	2.443[1]	38.4	6.456[1]
50.0	4.170[1]	2.238[1]	3.926[1]	2.326[1]	48.6	5.981[1]
54.4	3.912[1]	2.168[1]	3.701[1]	2.269[1]		
60.0	3.630[1]	2.080[1]	3.456[1]	2.197[1]		
70.0	3.223[1]	1.936[1]	3.105[1]	2.074[1]		
80.0	2.904[1]	1.808[1]	2.829[1]	1.963[1]		
90.0	2.646[1]	1.696[1]	2.607[1]	1.862[1]		
100.0	2.433[1]	1.596[1]	2.423[1]	1.772[1]		
150.0	1.749[1]	1.239[1]	1.821[1]	1.429[1]		
200.0	1.377[1]	1.018[1]	1.477[1]	1.202[1]		
300.0	9.758	7.603	1.087[1]	9.177		
400.0	7.613	6.126	8.658	7.458		
500.0	6.267	5.160	7.225	6.304		
600.0	5.341	4.475	6.216	5.475		
800.0	4.143	3.562	4.882	4.357		
1000.0	3.398	2.976	4.037	3.637		

[a]Numbers in the square brackets are powers of ten.

positron scattering is a repulsive one while that of electron scattering is an attractive one. For potassium, the polarization term of the core potential which, with a significantly great strength, remains an attractive one would cancel a part of the static potential effect in the case of positron scattering and would thereby make the modification in the collisional cross section less dramatic. Unlike those obtained in the conventional modified Glauber[9] and second Born approximations, the total cross sections of positron scattering obtained in the model potential approach are found to be somewhat smaller than those of electron scattering. This is a rather interesting result of the model potential approach since this property has also been observed in experiments. Within the modified Glauber approximation, this difference which tends to be negligible at very low energy (40 eV) increases with scattering energy up to an intermediate one around 200 eV and then declines at higher energies. The difference is also more significant for heavier atomic targets (potassium) whose core polarizabilities are greater. Thus, the difference existing between the positron and electron total cross sections may be understood, at least within the model potential approach, as originating from the core potential which reacts in different ways to electron and positron scattering. As was well known, a weak point of the conventional MG approximation in the calculation of total cross section is its inability to treat the polarization effect in electron and positron scatterings on some different footing, and as a result, the same total cross sections are obtained for both electron and positron scattering. With the employment of the model potential approach in the modified Glauber approximation, the core polarization effect can now be handled more appropriately. In this context, the use of the model potential ap-

TABLE VII. Total cross sections of $e^{\pm}$-Li, $e^{\pm}$-Na, and $e^{\pm}$-K collisions (in πa_0^2 units) in the frozen-core (FC) approximation calculated within the modified Glauber and second-Born approximations and with the use of the Clementi wave functions.

	Li		Na		K	
Energy (eV)	SB FC	MG FC	SB FC	MG FC	SB FC	MG FC
40	4.350[1][a]	3.623[1]	5.814[1]	2.520[1]	1.366[2]	2.807[1]
50	3.636[1]	3.129[1]	4.919[1]	2.389[1]	1.143[2]	2.941[1]
100	2.056[1]	1.895[1]	2.846[1]	1.736[1]	6.401[1]	2.462[1]
200	1.144[1]	1.096[1]	1.593[1]	1.116[1]	3.491[1]	1.699[1]
500	5.176	5.087	7.160	5.701	1.523[1]	9.299
1000	2.813	2.789	3.849	3.302	8.056	5.577

[a]Numbers in square brackets are powers of ten.

proach in MGA may even be preferred to some extent.

In Table VII, we present also the MG and SB total cross sections obtained in the frozen-core approximation with the employment of the Clementi wave functions to represent the bound states of the target electrons. Our values of electron scattering in the frozen-core approximation are found to be consistent to those obtained in the model potential approach.

Finally, our theoretical MG values of electron scattering, when compared to the few presently existing experimental data at low energy, are found to be appreciably smaller. This disagreement should not, however, be taken very seriously since the modified Glauber approximation is expected, as in the case of the He target, to work well only at higher energies. Furthermore, the significantly great error of experimental data as well as the discrepancy existing among the values measured by different research groups[1-4] make the comparison less meaningful. For positron scattering, the unique set of data available at present in the literature is that of potassium at low energies.[4] Some of these data[28] are shown in Table VI. We find that the modified Glauber values around 40—50 eV also seem to be lower than these data points. Therefore, it would be very desirable to have these total collisional cross sections measured at higher energies for comparison.

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