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# Elastic scattering of electrons and positrons by lithium

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The differential cross sections for the elastic scattering of electrons and positrons by lithium are calculated for energies $\geq 10$ eV in the corrected static approximation and in an approximation which combines the contribution of the nonstatic parts of the higher-order ($n \geq 3$) terms in the Glauber sense with the corrected static contribution. The latter approach yields results which are better when compared to those in the eikonal-Born–series approximation in the entire angular range for the energies where data are available. Results for the total elastic-scattering cross sections in the energy ranges of 10–200 eV, have also been reported. The present results are in reasonably good agreement with the absolute measurements of Williams *et al.* and other theoretical results.

## I. INTRODUCTION

During the last few years the scattering of electrons by lithium has received a good deal of attention by various authors. Recent direct measurements of angular distribution for elastic scattering of electrons by lithium by Williams *et al.*[1] in the medium energy range has further stimulated the study. The early works due to Burke and Taylor,[2] Dai and Stauffer,[3] Walters,[4] Sarkar *et al.*,[5] and Inokuti and McDowell[6] for the total elastic-scattering cross section are not in good agreement with the experimental findings. Walters[7] investigated this problem afresh and calculated the total elastic-scattering cross section by generalizing the Inokuti and McDowell model and allowing explicitly for the open channels and other nonadiabatic effects. He obtained cross sections which are consistent with the earlier calculations.[2,4] Vanderpoorten[8] studied this process using a local optical potential model, accounting for the polarization, excitation, and exchange effects, and calculated the differential cross section (DCS) at 60 eV. His results are not different from the frozen-core Glauber results of Walters.[4] Guha and Ghosh[9] have used an integral form of the close-coupling treatment including the effect of polarization potential in the sense of Temkin's[10] approach.

Apart from these studies, the problem of elastic scattering at medium energies may also be described by the eikonal-optical model (EOM), the second-order potential (SOP) model, eikonal-Born–series (EBS) approach, modified Glauber (MG) approach, and the two-potential approximation (TPA). These have been found to be quite successful in describing the elastic and inelastic scattering of electrons by hydrogen and helium. A recent review article by Bransden and McDowell[11] deals very exhaustively with various theoretical procedures.

Let us look at the EBS approach. This approach, due to Byron and Joachain,[12] basically combines the Born and Glauber series to obtain a consistent approximation to the scattering amplitude valid through order $k_i^{-2}$ ($k_i$ being the wave number of the incident particle) and relies on the convergence of the Born series. Recently it has been found[13] that for the intermediate-energy elastic scattering from the $2s$ state of hydrogen, the convergence of the Born series is much slower, particularly at large momentum transfers. Higher-order Born terms should therefore be included in some sense. One may exactly calculate the contribution of the static interaction to all orders and add to it the nonstatic part of $f_{B2}$ (second-order Born term) to obtain the so-called corrected static (CS) approximation of Buckley and Walters[14]

$$f_{cs} = f_{st} + (f_{B2} - f_{B2}^{st}) . \tag{1}$$

This approach does not include the contribution from the nonstatic part of the third- and higher-order terms which may be quite important. In the case of elastic scattering from the $2s$ state of atomic hydrogen, the real part of the scattering amplitude is found to be dominated by $f_{G3}$ (third-order Glauber term) in the intermediate- and large-angle region. The corrected static approximation may be improved upon by adding to it the contribution from the nonstatic parts of the third- and higher-order terms in (say) the Glauber approximation:

$$f = f_{st} + (f_{B2} - f_{B2}^{st}) + (f_G - f_{G2} - f_G^{st} + f_{G2}^{st}) . \tag{2}$$

Equation (2) should lead to an improvement over both the EBS and the CS approximations.

In this paper we study the elastic scattering of electrons and positrons by lithium using Eq. (2) along with the EBS, the static, and CS approximations [Eq. (1)]. The lithium atom is taken as a one-electron system with inert core. In Sec. II,

 

we give a brief description of the details of calculation. The results are presented and discussed in Sec. III.

## II. CALCULATION

The wave function of the lithium atom may be expressed as

$$\Psi_i = \frac{1}{\sqrt{6}} \sum_{\text{cyc}} \beta_1\alpha_2\alpha_3\phi_{1s}(1)[\phi_i(2)\phi_{1s}(3) - \phi_i(3)\phi_{1s}(2)], \tag{3}$$

where $\phi$ is the spatial part of the one-electron orbital and $\alpha$ and $\beta$ refer to the components of the spin part. These one-electron orbitals have been taken from the table of Clementi and Roetti.[15] However, for the calculation of the second Born term we have considered the lithium atom as a one-electron system with inert core. The absolute square of $\phi_{2s}$ atomic orbitals comes out to be

$$\phi_{2s}^*\phi_{2s} = \frac{1}{4\pi}\left(\sum_{j=1}^{3} A_j e^{-\alpha_j r} + \sum_{j=4}^{11} A_j r e^{-\alpha_j r} + \sum_{j=12}^{21} A_j r^2 e^{-\alpha_j r}\right). \tag{4}$$

Using Eq. (4) and following Byron and Joachain, one can easily evaluate the simplified second-Born ($f_{SB2}$) (Eq. 2.8, Ref. 12) and corrected second-Born ($f_{B2}$) (Eq. 2.10, Ref. 12) terms. The excitation energy $\bar{w}$ has been taken as 0.0754 by using the polarizability sum rule $\bar{\alpha} = (\langle\Psi_i|Z^2|\Psi_i\rangle)/\bar{w}$ which asymptotically satisfies the long-range behavior $V(r) \sim -\bar{\alpha}/2r^4$ with $\bar{\alpha} = 164.68$ a.u. (Ref. 16). The higher-order terms of the Glauber series, i.e., $f_{G2}$ and $f_{G3}$, are evaluated following Yates.[17] The scattering amplitude $f_{st}$ in the static approximation is obtained by solving the radial Schrödinger equation ($l \leq 20$) for the static interaction which is defined as

$$V_{st} = \langle\Psi_i|V|\Psi_i\rangle. \tag{5}$$

Finally, the effect of exchange is taken into account through the exchange pseudopotential of Furness and McCarthy[18]:

$$V_{ex}^{(\pm)} = \frac{1}{2}\left\{\frac{k_i^2}{2} - V_{st}(r) - \left[\left(\frac{k_i^2}{2} - V_{st}(r)\right)^2 + 8\pi|\phi_{1s}|^2 \mp 4\pi|\phi_{2s}|^2\right]^{1/2}\right\}. \tag{6}$$

It is included in the Schrödinger equation along with the static interaction. The (+) denotes singlet states and (−) triplet states. No account of exchange is taken in the correction terms in Eqs. (1) and (2). The exchange contribution in the EBS approach is taken in the Ochkur approximation.

## III. RESULTS AND DISCUSSION

### A. Electron-lithium scattering

We have shown in Fig. 1 the variation of various components of the elastic-scattering amplitude with scattering angle at 20 eV. It is seen that $\mathrm{Re}f_{B2}$ falls off rapidly with the increase in the scattering angle compared to other amplitudes ($f_{B1}$, $\mathrm{Im}f_{B2}$, and $f_{G3}$). Further it is found that $\mathrm{Re}f_{SB2}$ differs from $\mathrm{Re}f_{B2}$ by 5% in the small-angle region and quite a bit for large scattering angles. On the average this difference is approximately 50% beyond 80°. The situation is not very much different at 60 eV. The scattering amplitude at large angles is dominated by $f_{G3}$. This feature is also observed by Joachain *et al.*[13] in the case of intermediate-energy elastic scattering of electrons from 2*s*-state atomic hydrogen and is an indication of poor convergence of the Born series. In order to probe as to whether this poor convergence is mainly due to the nonstatic or the static parts of the higher-order terms, we have looked at the real and imaginary parts of the third term in Eq. (2). Figure 2 shows that their contribution to the total scattering amplitude is very little beyond about 60°. In the case of elastic scattering from the 2*s* state of atomic hydrogen at $E = 200$ eV, their contribution drops to insignificant values beyond about 20° (Fig. 3). This indicates that fairly good convergence could be obtained if the static-interaction contribution is taken out and evaluated exactly. Equation (2) should tend to

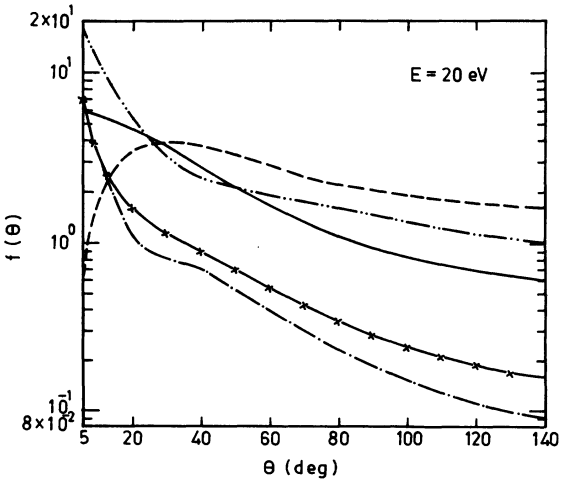


FIG. 1. The elastic scattering amplitude for electron-lithium scattering at 20 eV. Solid curve; $f_{B1}$; dash-dot curve: $\mathrm{Re}f_{B2}$: Dash-cross curve: $\mathrm{Re}f_{SB2}$; dash-double dot curve: $\mathrm{Im}f_{B2}$; broken curve: $-f_{G3}$.

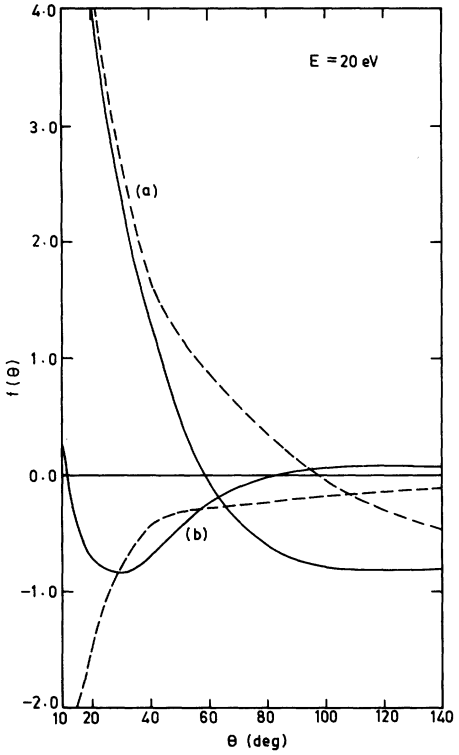


FIG. 2. The elastic scattering amplitude for electron-lithium scattering at 20 eV. (a) Contribution of $f_{st}$ + $(f_{B2} - f_{B2}^{st})$. (b) Contribution of $(f_G - f_{G2} - f_G^{st} + f_{G2}^{st})$. Solid curve: real part; broken curve: imaginary part.

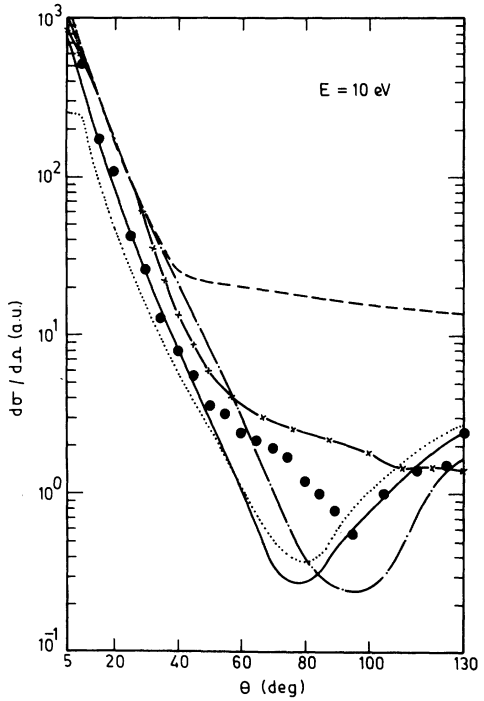


FIG. 4. The elastic differential cross section for electron-lithium scattering at 10 eV. Solid curve: present calculation; dash-dot curve: results in corrected static approximation; dotted curve: results in static approximation; broken curve: EBS results; dash-cross curve: results of Guha and Ghosh (Ref. 9); ●: experimental data of Williams *et al.* (Ref. 1).

reasonably good results at large scattering angles even in situations where the EBS method does not work.

Figures 4–7 show our differential cross sections for elastic scattering of electrons from the ground state of lithium at 10, 20, 60, 100, and

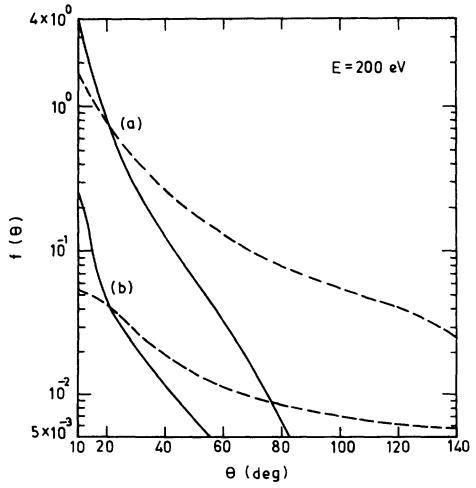


FIG. 3. The elastic scattering amplitude for electron-2*s* atomic hydrogen at 200 eV. Same as Fig. 2.

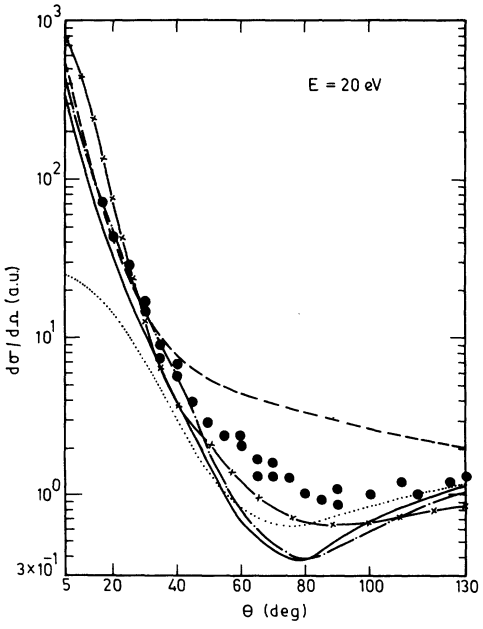


FIG. 5. Same as Fig. 4 but at 20 eV.

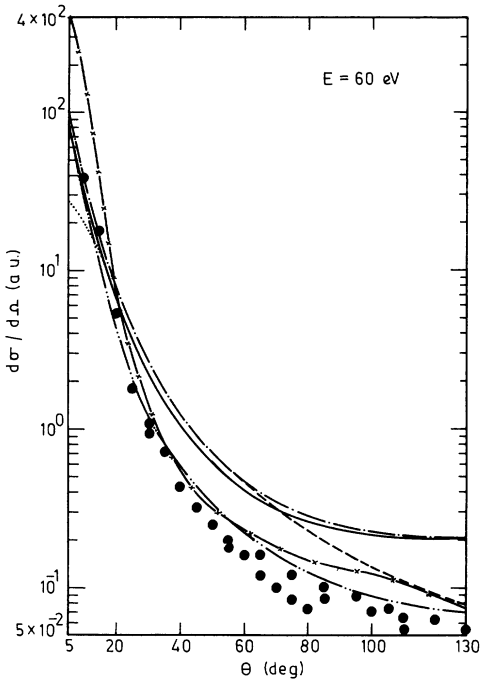


FIG. 6. Same as Fig. 4 but at 60 eV. Dash-double dot curve: results of Vanderpoorten (Ref. 8).

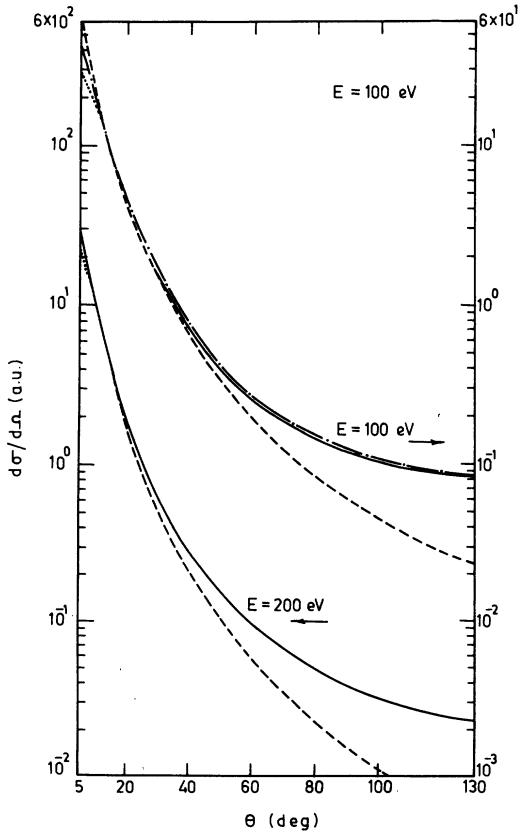


FIG. 7. Same as Fig. 4 but at 100 and 200 eV.

200 eV, along with the available experimental data and other theoretical results. It is worth mentioning that Williams *et al.*[1] have normalized their elastic- and inelastic-scattering data to the difference between the total cross section of Kasdan *et al.*[19] and the ionization cross section of Aleksakhin *et al.*[20] at each impact energy. This introduces an overall error of about ±35% in their normalization. Recently Tino *et al.*[21] measured electron-lithium total cross sections up to 10 eV and found an excellent agreement with the close-coupling calculations. The data of Tino *et al.*[21] are about 35% lower than the earlier data of Kasdan *et al.*[19] This would affect the Williams *et al.*[1] cross sections definitely at 10 eV and perhaps at 20 and 60 eV as well.

It is evident from Figs. 4 and 5 that the present calculations using Eq. (2) and the CS approximation, Eq. (1), are quite successful in reproducing the shape of the experimental curve. It is seen that, at 10 eV, the present results show a very good agreement with the experimental data up to 50°; thereafter at intermediate angles they deviate from the experimental data but again yield a good agreement in the region of large scattering angles. The minimum is predicted at 80°, whereas the experimental data show it at 90°. The CS results closely follow the results of Eq. (2). They overestimate the experimental result by a factor of 3 in the region beyond 10°, although the minimum is reproduced in agreement with the experimental data. The results of Guha and Ghosh[9] overestimate the DCS in the entire angular region. The situation at 20 eV is very much similar. The results obtained from Eq. (2) and the CS approximation compare very well with each other at all scattering angles. The shallow experimental minimum is well reproduced by both the results. We have also displayed the results obtained in the static approximation. It is seen that it gives a good account as expected at large angles, both at 10 and 20 eV. The results of Guha and Ghosh overestimate the DCS for scattering angle less than about 20° but show a better agreement with experimental data compared to the present results in the region of scattering angle 50° to 100°. The trend of results at 60 eV (Fig. 6) is very different compared to that at 10 and 20 eV. All the results remain higher in magnitude beyond 20°. Among these, the local optical-potential results of Vanderpoorten[8] are very close to the experimental data. However, the present results give a reasonably good agreement below 20°. Further it is observed that the EBS results show a poor agreement as expected at 10 and 20 eV. The situation improves as one goes to higher energies, i.e., $\geq$ 60 eV. Figure 7 shows the DCS at 100 and 200

eV. As there is no data available at these energies, it is rather difficult to assess the reliability of the EBS procedure.

### B. Positron-lithium scattering

The study of positron-lithium scattering is simpler compared to electron-lithium scattering because of the absence of exchange contribution. Although the experimental data for this process are not available for comparison, nevertheless our calculation would provide a new set of theoretical results which are differenct from those obtained in other models. Thus we believe that intercomparison of the results of different approximations would be meaningful on lines similar to electron-lithium scattering.

Figure 8 displays our results for $e^+$-lithium DCS at 10 and 60 eV. We have also shown the theoretical results of Sarkar *et al.*[5] obtained in eikonal and polarized first-Born approximation at 10 eV. It is seen in the present calculations that both the CS approximation and Eq. (2) show a smoother behavior for the DCS. This feature is in agreement with the results of $e^+$-hydrogen and -helium elastic scatterings. The CS results overestimate the DCS on the average by a factor of 2 compared to the results from Eq. (2) in the entire angular region. However, this difference narrows down considerably at 60 eV but still remains quite distinct at large scattering angles. Further, it is also seen in the region of 5 to 20° that the present calculations are smaller compared to the eikonal and polarized first-Born-approximation results of Sarkar *et al.*[5] Their results show peaks in contrast to the present calculations. The present calculations differ considerably when compared with $e^-$-lithium scattering results (Figs. 4 and 7) at all scattering angles.

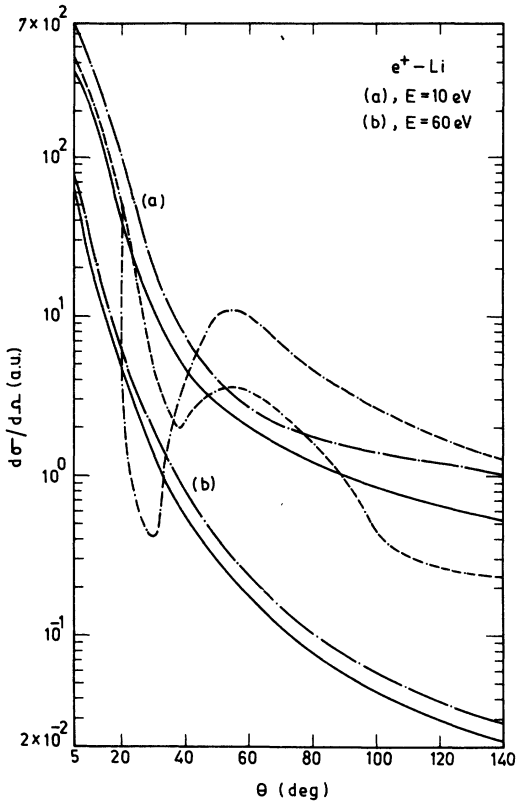


FIG. 8. The elastic differential cross sections for positron-lithium scattering at (a) $E = 10$ eV and (b) $E = 60$ eV. Solid curve: present calculation; dash-dot curve: results in corrected static approximation; double dash-dot curve: results of Sarkar *et al.* in polarized first-Born approximation at 10 eV, triple dash-dot curve: results of Sarkar *et al.* in eikonal approximation at 10 eV (Ref. 5).

### C. Total elastic cross section

Tables I and II show our total elastic cross-section results at 10, 20, 60, 100 and 200 eV. The measured values of Williams *et al.*[1] along with other theoretical results are also included for comparison. It is seen that our results [Eq. (2)] compare well with the experimental data. The extent of agreement may, however, have to be revised in light of the recent measurements

TABLE I. Total elastic cross sections (in units of $\pi a_0^2$ for elastic scattering of electrons by lithium: GG, results of Guha and Ghosh (Ref. 9); MS, results of Mukherjee and Sural (Ref. 22); TS, two-state close coupling results of M. R. Issa (unpublished, see Ref. 11).

| Energy (eV) | Present results Eq. (2) | Present results in CS approximation | GG | MS | TS | Experimental data of Williams *et al.*[1] |
|---|---|---|---|---|---|---|
| 10 | 52.33 | 87.32 | 84.91 | 29.5 | 22.0 | 45.6 |
| 20 | 19.22 | 27.50 | 48.11 | 12.7 | 12.0 | 21.7 |
| 60 | 5.42 | 6.37 | 15.72 | | 4.7 | 5.1 |
| 100 | 3.18 | 3.54 | | 2.16 | | |
| 200 | 1.54 | 1.64 | | 1.13 | | |

TABLE II. Total elastic cross sections (in units of $\pi a_0^2$) for elastic scattering of positrons by lithium. MS; results of Mukherjee and Sural (Ref. 22).

| Energy (eV) | Present results Eq. (2) | Present results in CS approximation | MS |
|---|---|---|---|
| 10 | 23.95 | 53.44 | 21.80 |
| 20 | 9.14 | 16.87 | 9.63 |
| 60 | 3.33 | 4.20 | |
| 100 | 2.13 | 2.45 | 2.15 |
| 200 | 1.14 | 1.22 | 1.17 |

of Tino *et al.*[21] The CS results are higher than those from Eq. (2) but approach them as the energy increases. A similar trend exists for positron-lithium scattering. The overall magnitude of the positron elastic scattering is smaller by a factor of 2 compared to the electron scattering. The present results for positron-lithium scattering are in fairly good accord with the theoretical results of Mukherjee and Sural[22] using an integral approach to the second-order potential method.

In summary, we have analyzed the electron- and positron-lithium elastic scattering in corrected static and in an improved approximation which includes nonstatic parts (in the Glauber approximation) of the higher-order terms. At lower energies, i.e., around 10 eV, the convergence of the Born series is poor and hence it must be summed up in some sense. The correction terms in Eq. (2) do this job. At higher energies the results obtained from Eq. (2) and the CS approximation are very close to each other. This is indicative of a better convergence, as expected, of the multiple-scattering series at higher energies. Above 20 eV, therefore, the CS approximation is good enough. The results, of course, may be further improved if the two core electrons of lithium are also included in the calculation of $f_{B2}$. It should improve the contribution from close-encounter collisions. We find that the present approximation is quite successful in predicting the elastic differential cross sections for a wide range of energy.

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