Elastic scattering of electrons by helium and lithium in the two-potential eikonal approximation

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The two-potential eikonal approximation proposed by Ishihara and Chen has been used to calculate the elastic differential scattering cross section of helium and lithium by electrons at intermediate energies. A significant improvement over the conventional Glauber cross section is achieved.

Absolute measurements of the differential cross section for the elastic scattering of electrons by helium[1-7] and lithium[8] at intermediate and high energies have revived theoretical interest to look for an accurate and computationally feasible theoretical approach. The Glauber approximation,[9] which has been extensively applied in the recent past to study the electron-atom collision problems at intermediate energies, is well known for its shortcomings (appreciable under estimation of the cross section except at small angles where it logarithmically diverges). Various methods have been suggested to improve upon the Glauber approximation, such as the Glauber angle approximation,[10] eikonal-optical model,[11] eikonal-Born series (EBS) method,[12] the modified Glauber (MG) approach,[13] and the two-potential eikonal (TPE) approach of Ishihara and Chen.[14] Included among other successful methods are the second-order potential (SOP) method of Winters *et al.*,[15] the distorted-wave second Born approximation of Dewangan and Walters,[16] two-potential treatment of Singhal and Srivastava,[17] and the second-order Born calculation including coupling to all channels by Bonham and Konaka.[18] The situation (up to 1976) regarding various theoretical approaches for electron-atom collisions has been reviewed recently by Bransden and McDowell.[19]

The simplicity of the TPE approach of Ishihara and Chen[14] has prompted us to apply it to study the elastic electron-helium and lithium scattering. The basic idea underlying this approach is to treat properly the close-encounter collisions where the electron-atom interaction is $-(Z/r)(r\to 0)$ and the condition $|V|\ll E$ does not hold good even for high energies. The method essentially consists of pulling out a static potential V_{st}, incorporating the singularity of the total interaction V, and evaluating its contribution by solving the radial Schrödinger equation. The rest of the interaction $V_0=V-V_{st}$, which is smooth enough, is treated in the Glauber approximation.

Consider the scattering of an electron from a Z-electron atom. The interaction potential, in atomic units, is given by

$$V(\vec{r},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)=-\frac{Z}{r}+\sum_{j=1}^{Z}\frac{1}{|\vec{r}-\vec{r}_j|}\,, \qquad (1)$$

where $\vec{r}$ and $\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z$ are, respectively, the coordinates of the incident and the target electrons relative to the nucleus. A short-range central potential V_{st}, which is taken to be the static potential of the ground state of the target atom, is substracted from the interaction V, so that the remaining part

$$V_0(\vec{r},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)=V(\vec{r},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)-V_{st}(r) \qquad (2)$$

is slowly varying and satisfies the semiclassical condition $|V_0|\ll E$ for all $\vec{r}$. The contribution of V_0 is obtained in the Glauber approximation and that of V_{st} is calculated quantum mechanically by taking a few partial waves. The transition amplitude from the initial state $|\Phi_i\rangle$ of the target to the final state $|\Phi_f\rangle$ is given by[14]

$$F_{fi}(q)=\frac{ik_i}{2\pi}\int d^2b\,e^{i\vec{q}\cdot\vec{b}}[1-\Gamma_{fi}(\vec{b})] +\frac{1}{k_i}\sum_l(2l+1)P_l(\cos\theta)e^{i\delta_l}\sin\delta_l \times\int\frac{d\varphi_b}{2\pi}\Gamma_{fi}(\vec{b}_l)\,, \qquad (3)$$

where $\vec{q}=\vec{k}_i-\vec{k}_f$ is the momentum transfer, $\vec{k}_i$ and $\vec{k}_f$ are, respectively, the momenta of the incident and scattered electrons, $\vec{b}$ is the impact parameter, and δ_l is the phase shift of the lth partial wave for the central potential V_{st}. $\Gamma_{fi}(\vec{b})$ is the Glauber phase function and is given by

$$\Gamma_{fi}(\vec{b})=\langle\Phi_f|\exp[i\chi(\vec{b},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)]|\Phi_i\rangle\,, \qquad (4)$$

where

$$\chi(\vec{b},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)=\chi_0(\vec{b},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)+\Delta\chi(\vec{b},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)\,, \qquad (5)$$

$$\chi_0(\vec{b},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)=-\frac{1}{k_i}\int_{-\infty}^{\infty}dz\,V_0(\vec{r},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)\,, \tag{6a}$$

$$\Delta\chi(\vec{b},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Z)=\frac{2}{k_i}V_0(z=0)\int_0^{\infty}dz\left(1-\frac{z}{[z^2-(V_{st}/E)r^2]^{1/2}}\right), \tag{6b}$$

and

$$b_l=(l+\tfrac{1}{2})/k_i\,. \tag{6c}$$

The correction $\Delta\chi$ to the Glauber phase function is expected to contribute very little and can therefore be ignored.

For the ground state of helium, we have used the Hartree-Fock orbitals ϕ_{1s} of Byron and Joachain[20] of the form

$$\phi_{1s}=(4\pi)^{-1/2}(Ae^{-\alpha r}+Be^{-\beta r})\,, \tag{7}$$

where $A=2.605\,05$, $B=2.081\,44$, $\alpha=1.41$, and $\beta=2.61$, and for lithium we have used those of Clementi[21] of the form

$$\phi(r)=R(r)Y_0^0(\theta,\varphi)\,, \tag{8a}$$

$$R(r)=\sum_{i=1}^{2}A_ie^{-\xi_ir}+\sum_{i=3}^{6}A_ire^{-\xi_ir}\,. \tag{8b}$$

The values of the parameters A_i and ξ_i are given by Clementi.[21]

The effect of exchange is taken into account in the Ochkur approximation and through the exchange pseudopotential of Furness and McCarthy[22,23,24] for helium and lithium:

$$V_{ex}=\tfrac{1}{2}\left(\tfrac{1}{2}k^2-V_{st}(r)-\{[\tfrac{1}{2}k^2-V_{st}(r)]^2+8\pi|\phi_{1s}|^2\}^{1/2}\right), \tag{9}$$

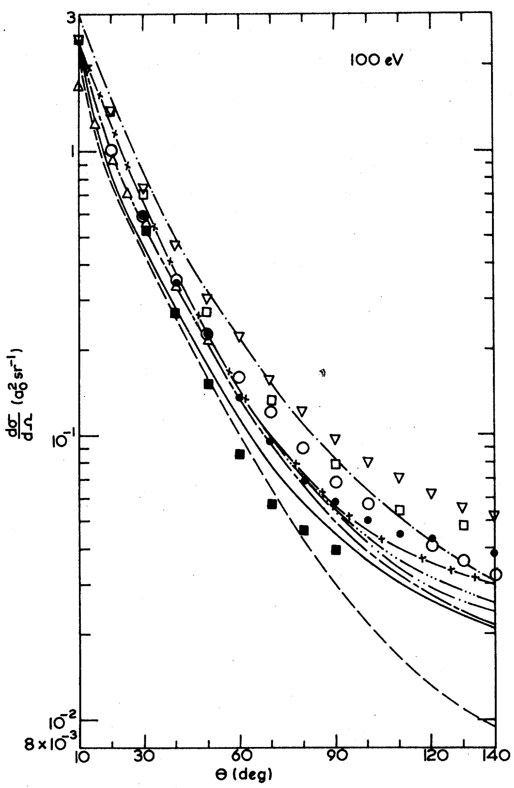

FIG. 1. Differential cross section for e-He elastic scattering at 100 eV. Solid curve: Present calculation in TPE approximation with Furness and McCarthy exchange; long dash-small dash curve: Present calculation in TPE approximation with Ochkur exchange; dashed curve: Present calculation in the Glauber approximation with Ochkur exchange; dash-dot curve: MG results (Ref. 13); dash-cross curve: EBS results (Ref. 12); dash-double-dot curve: Distorted-wave second Born approximation results (Ref. 16); dash-triple-dot curve: SOP results (Ref. 15). Experimental data; Δ: Jansen *et al.* (Ref. 1); ▽: Kurepa and Vuskovic (Ref. 5); ○: Gupta and Rees (Ref. 2); □: Crooks and Rudd (Ref. 7); ●: Sethuraman *et al.* (Ref. 6); ■: McConkey and Preston (Ref. 4).

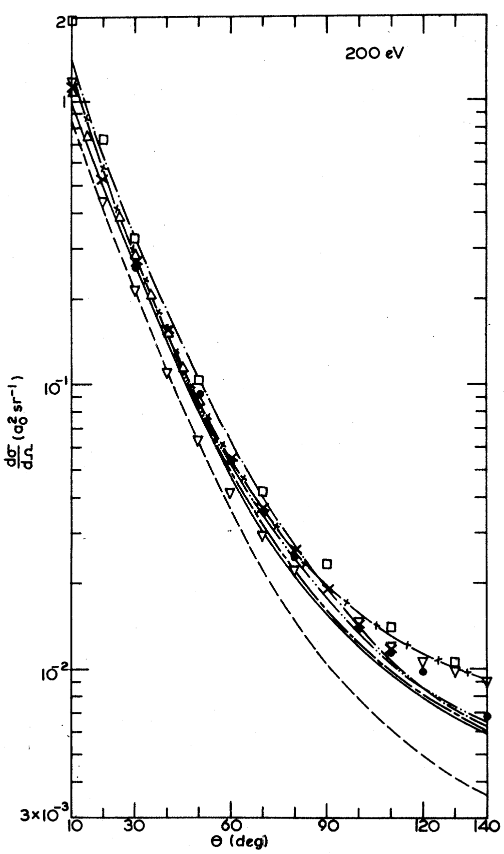

FIG. 2. Same as Fig. 1 but at 200 eV. ×: Experimental results of Bromberg (Ref. 3).

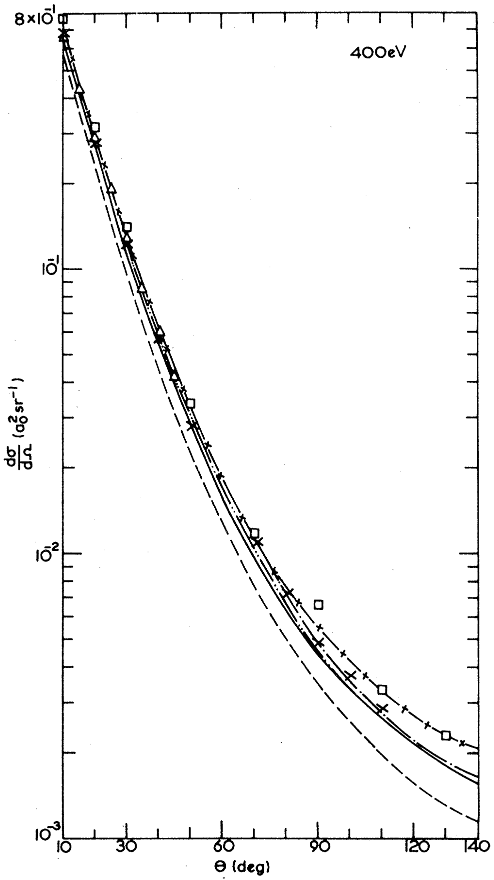

FIG. 3. Same as Fig. 2 but at 400 eV.

$$V_{ex}^{(\pm)}=\tfrac{1}{2}\left(\tfrac{1}{2}k^2-V_{st}(r)-\left\{\left[\tfrac{1}{2}k^2-V_{st}(r)\right]^2+2\left|R_{1s}\right|^2\mp\left|R_{2s}\right|^2\right\}^{1/2}\right), \tag{10}$$

where R_{1s} and R_{2s} denote the radial Hartree-Fock orbitals of lithium. (+) denotes singlet states and (−) triplet states of the system.

The partial-wave summation in Eq. (3) is done up to $l=10$. The integrals involved in the evaluation of Γ_{fi} and in Eq. (3) are done numerically following the prescriptions of Franco[25] and Kumar and Srivastava.[26]

e-He elastic scattering. We have calculated e-He elastic scattering differential cross sections (DCS) at 100, 200, 400, and 700 eV. The results are shown in Figs. 1–4. The present TPE results have been compared with those in the conventional Glauber approximation and many other approaches. Also shown are the measurements of various experimental research groups. The results with Furness-McCarthy exchange and in the Ochkur approximation differ only a little from each other. At all the energies considered here, one of the

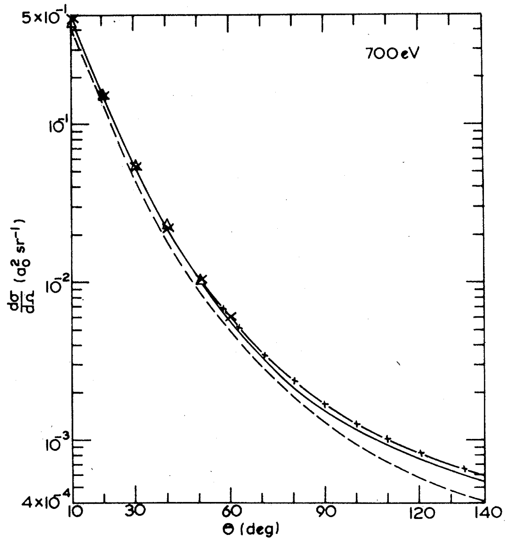

FIG. 4. Same as Fig. 2 but at 700 eV.

noticeable features is that the present TPE approximation remarkably improves the conventional Glauber results at all scattering angles and particularly so at large ones. The reason is that (i) the singularity of the interaction contained in V_{st} is accurately taken into account by partial-wave summation and (ii) the semiclassical condition necessary for the applicability of the Glauber approximation is actually satisfied for the remaining interaction. As a test of the latter we compare in Fig. 5 for helium, the real and imaginary parts of

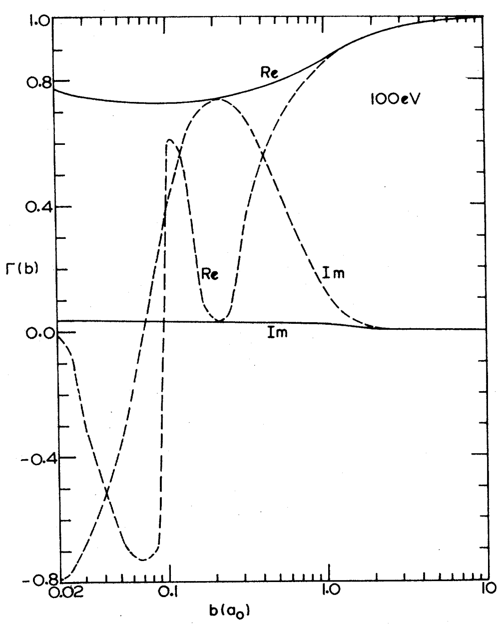

FIG. 5. Real and imaginary parts of Γ (b) for the potential V_0 (solid curve) and for the total interaction V (dashed curve) for elastic e-He scattering at 100 eV.

the eikonal-phase function Γ for the potential V_0 with those for the full interaction V. The former, as anticipated, shows a very smooth variation as a function of b.

Figure 1 displays our results at 100 eV. A substantial improvement over ordinary Glauber results is obtained. Nevertheless, the present TPE results continue to underestimate the cross sections compared to those obtained by other approaches. Figures 2 and 3 display differential cross sections at 200 and 400 eV, respectively. The present TPE results show a good agreement with those of Winters *et al.*[15] (not shown) and Dewangan and Walters[16] at all scattering angles. They do not significantly differ from those obtained by EBS calculation of Byron and Joachain[12] at the small and intermediate scattering angles ($\lesssim 60°$). As far as comparison with the experimental measurements is concerned, we observe that they compare well with the data of Jansen *et al.*[1] and Bromberg[3] in the region of 10–50°. For large scattering angles, Bromberg's data lie higher than our results by about 15–20%. This difference narrows down considerably at 400 eV. The data of Kurepa and Vuskovic[5] at 200 eV are smaller at small scattering angles, i.e., up to ~70° compared to other measurements as well as the present TPE results, but at large scattering angles they merge with the data of Bromberg.[3] The experimental measurements of Crooks and Rudd[7] continue to remain higher even at 400 eV. Figure 4 shows the situation at 700 eV. Our results compare very well with the data of Jansen *et al.*[1] and are almost identical to those of Dewangan and Walters.[16] The EBS results show a difference only at larger scattering angles.

e-Li elastic scattering. Figures 6 and 7 show the results of present calculation in TPE approximation and in the conventional Glauber approximation along with experimental data of Williams *et al.*[8] for incident electron energies of 20 and 60 eV, respectively. At 20 eV, the improvement (over the conventional Glauber results) obtained here by using TPE approximation leads to an overall qualitative agreement with the shape of the experimental curve. Quantitatively the TPE results underestimate DCS by almost an order of magnitude and lie below those of Issa[27] in two-state close-coupling approximation. The overall shape is also well reproduced at 60 eV but the present TPE results overestimate DCS and also lie above those of Vanderpoorten[24] in the local-optical potential model. It should be pointed out that the overall error in normalization of the data of Williams *et al.*[8] is about ±35%. The disagreement at 60 eV is therefore not very discouraging.

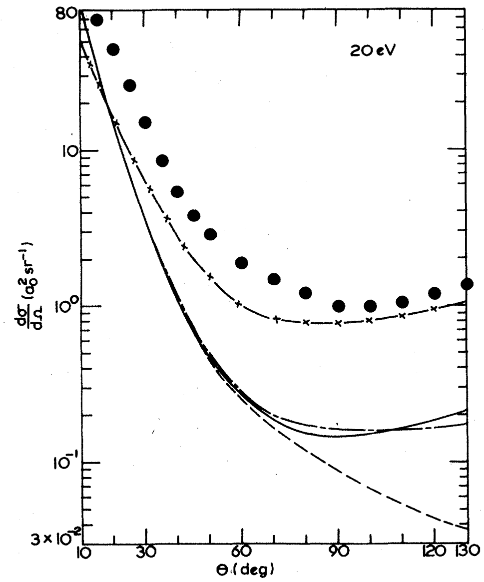

FIG. 6. Differential cross section for e-Li elastic scattering at 20 eV. Solid curve: Present calculation in TPE approximation with Furness and McCarthy exchange; long dash-small dash curve: Present calculation in TPE approximation with Ochkur exchange; dashed curve: Present calculation in the Glauber approximation with Ochkur exchange; dash-cross curve: Issa two-state close-coupling results. Solid circles are data points of Ref. 8.

To summarize: The comparison of our results with the experimental data and other theoretical results shows that the TPE approximation of Ishihara and Chen[14] leads to substantial improvement over the ordinary Glauber approximation. Never-

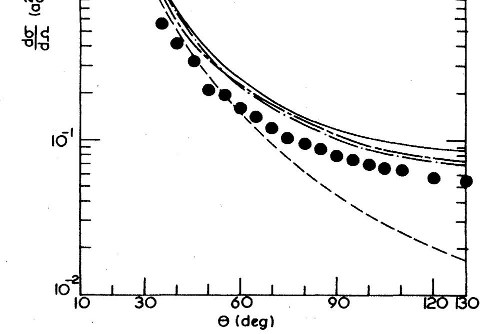

FIG. 7. Same as in Fig. 6 but at 60 eV. Dashed-dot curve: Results of Ref. 24.

theless, the improvement so obtained is much less than that which is observed in the case of e-H elastic scattering. It is perhaps a reflection of the limitations of this method rather than the choice of the target wave function.

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[1]R. H. J. Jansen, F. J. deHeer, H. J. Lurken, B. Van Wingerden, and H. J. Blaauw, J. Phys. B 9, 185 (1976).
[2]S. C. Gupta and J. A. Rees, J. Phys. B 8, 1267 (1975).
[3]J. P. Bromberg, J. Chem. Phys. 61, 963 (1974), and results taken from Ref. 12.
[4]J. W. McConkey and J. A. Preston, J. Phys. B 8, 63 (1975).
[5]M. V. Kurepa and L. Vuskovic, J. Phys. B 8, 2067 (1975).
[6]S. K. Sethuraman, J. A. Rees, and J. R. Gibson, J. Phys. B 7, 1941 (1974).
[7]G. B. Crooks and M. E. Rudd, Bull. Am. Phys. Soc. 17, 131 (1972).
[8]W. Williams, S. Trajmar, and D. Bozinis, J. Phys. B 9, 1529 (1976).
[9]R. J. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin (Interscience, New York, 1959), Vol. 1, p. 315.
[10]J. C. Y. Chen and L. Hambro, J. Phys. B 5, L199 (1972); L. Hambro, J. C. Y. Chen, and T. Ishihara, Phys. Rev. A 8, 1283 (1973).
[11]C. J. Joachain and M. H. Mittleman, Phys. Rev. A 4, 1492 (1971); F. W. Byron Jr. and C. J. Joachain, *ibid.* 6, 2559 (1974).
[12]F. W. Byron Jr. and C. J. Joachain, Phys. Rev. A 8, 1267 (1973); J. Phys. B 10, 207 (1977).
[13]F. W. Byron Jr. and C. J. Joachain, J. Phys. B 8, 1284 (1975); T. T. Gien, *ibid.* 9, 3203 (1976); Phys. Rev. A 16, 1793 (1977).
[14]T. Ishihara and J. C. Y. Chen, Phys. Rev. A 12, 370 (1975).
[15]K. H. Winters, C. D. Clark, B. H. Bransden, and J. P. Coleman, J. Phys. B 7, 788 (1974).
[16]D. P. Dewangan and H. R. J. Walters, J. Phys. B 10, 637 (1977).
[17]R. Singhal and B. B. Srivastava, J. Phys. B 10, 3725 (1977).
[18]R. A. Bonham and S. Konaka, J. Chem. Phys. 69, 525 (1978).
[19]B. H. Bransden and M. R. C. McDowell, Phys. Rep. 30, C207 (1977).
[20]F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. 146, 1 (1966).
[21]E. Clementi, IBM J. Res. Dev. 9, 2 (1965).
[22]J. B. Furness and I. E. McCarthy, J. Phys. B 6, 2280 (1973).
[23]R. Vanderpoorten, J. Phys. B 8, 926 (1975).
[24]R. Vanderpoorten, J. Phys. B 9, L535 (1976).
[25]V. Franco, Phys. Rev. Lett. 26, 1088 (1971).
[26]S. Kumar and M. K. Srivastava, Phys. Rev. A 12, 801 (1975).
[27]M. R. Issa, thesis, Durham, 1977 (unpublished); B. H. Bransden and M. R. C. McDowell, Phys. Rep. 46, C249 (1978).