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An integral approach to the second-order potential method: electron and positron scattering by hydrogen, helium and lithium

Arunima Mukherjee† and D P Sural
Department of Physics, Jadavpur University, Calcutta-700032, India

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Abstract. The differential equations of the second-order potential model are converted into a set of integral equations for the scattering amplitudes. After making a partial-wave decomposition and retaining only the physical amplitudes in the kernel, the resulting equations are used to calculate the cross sections for elastic scattering of electrons and positrons by hydrogen, helium and lithium within the energy ranges of 20–500 eV, 40–500 eV and 10–200 eV, respectively. The results are compared with the calculations of other workers.

1. Introduction

A useful approach to the study of electron (positron)–atom scattering problems is to expand the total wavefunction in terms of the eigenfunctions of the target atom. In practice, only a few target states can be retained in the expansion, and the effect of the other states has to be incorporated in some approximate way. This has been successfully done by Bransden and Coleman (1972) who have introduced a second-order potential which is calculated by using a closure approximation. An average energy parameter occurring in the second-order potential can be chosen suitably to get the proper long-range behaviour for the real part of the potential. The second-order potential (SOP) method has been applied to different systems and a discussion can be found in the recent review by Bransden and McDowell (1977). In the wave formalism, a partial-wave decomposition converts the equations in the SOP model into sets of coupled second-order integro-differential equations for the radial wavefunctions, the number of equations in a set for each partial wave depending upon the number of channels explicitly retained. Even in the one-channel case, the numerical solution of the integro-differential equations is laborious (Winters *et al* 1974). Another procedure in use is to employ the semiclassical impact-parameter approximation and get a set of first-order integro-differential equations for the probability amplitudes. Ambiguity may, however, occur in the definition of the classical trajectory of the incident particle. Most of the calculations have been made with straight-line trajectories and using an impact-parameter approximation to the scattering amplitude. For light particles like the electron and positron, the straight-line trajectory assumption can be valid only for

† UGC teacher fellow on leave from Lady Brabourne College, Calcutta, India.

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high velocities. The angular range over which the differential cross sections may be accurate decreases with the decrease in the velocity of incidence.

In the present work, we have converted the equations in the SOP model (in the wave formalism) into integral equations incorporating the boundary conditions of the problem and have obtained equations satisfied by the scattering amplitudes. The relation between the scattering amplitude in the SOP method and that obtained in an approximate form of the second Born approximation can be explicitly seen in this approach. The equations for the partial-wave amplitudes have been obtained after making an angular momentum analysis. An approximation in the kernels, which leads to considerable simplification, is used to calculate the cross sections for elastic scattering of electrons and positrons by hydrogen, helium and lithium atoms. The results are compared in § 3 with those available from other workers.

The integral form of the conventional close-coupling approximation for electron (positron)–atom scattering has been used earlier by Sloan and Moore (1968), Ghosh and Basu (1973) and Chaudhuri *et al* (1974).

Atomic units will be used in this paper unless stated otherwise.

2. Theory

If $\boldsymbol{r}$ represents the coordinates of the incident electron (positron) and $\boldsymbol{r}_1$ represents, collectively, the coordinates of the electrons in the target atom, then the equations for the channel wavefunctions $F_n(\boldsymbol{r})$ in the SOP model (Bransden and Coleman 1972) can be written as

$$(E-\epsilon_n+\tfrac{1}{2}\nabla^2)F_n(\boldsymbol{r})=\sum_{m=0}^{N}(V_{nm}(\boldsymbol{r})+K_{nm})F_m(\boldsymbol{r}) \qquad n=0,1,2,\ldots,N \tag{1}$$

with

$$F_n(\boldsymbol{r}) \xrightarrow[r\to\infty]{} (2\pi)^{-3/2}\exp(\mathrm{i}\boldsymbol{k}_0\cdot\boldsymbol{r})\delta_{n0}+f_{n0}(\hat{\boldsymbol{k}}'_n,\hat{\boldsymbol{k}}_0)(2\pi)^{-3/2}r^{-1}\exp(\mathrm{i}k'_n r) \tag{2}$$

for open channels. Here E is the total energy of the system, $\boldsymbol{k}_0$ is the momentum of the incident particle, $\boldsymbol{k}'_n$ is the momentum of the scattered particle with the target atom left in the nth eigenstate of energy ϵ_n, and $V_{nm}(\boldsymbol{r})$ is the direct local potential

$$V_{nm}(\boldsymbol{r})=\int \phi_n^*(\boldsymbol{r}_1)V(\boldsymbol{r}_1,\boldsymbol{r})\phi_m(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1 \tag{3}$$

where $\phi_n(\boldsymbol{r}_1)$ represents the normalised target eigenfunctions and $V(\boldsymbol{r}_1,\boldsymbol{r})$ is the interaction between the incident particle and the target. K_{nm} is a non-local potential operator, which, in the closure approximation, is given by

$$K_{nm}F_m(\boldsymbol{r})=2\int\left(\int \phi_n^*(\boldsymbol{r}_1)V(\boldsymbol{r}_1,\boldsymbol{r})V(\boldsymbol{r}_1,\boldsymbol{r}')\phi_m(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1-\sum_{j=0}^{N}V_{nj}(\boldsymbol{r})V_{jm}(\boldsymbol{r}')\right)$$
$$\times G_0(\bar{k}^2;\boldsymbol{r},\boldsymbol{r}')F_m(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}' \tag{4}$$

where $G_0(\bar{k}^2;\boldsymbol{r},\boldsymbol{r}')$ is the free-particle Green's function for an average energy $\frac{1}{2}\bar{k}^2$ with the outgoing wave boundary condition. The value of $\bar{k}^2$ can be chosen to suit some physical requirement of the problem under consideration. In particular, a choice may

be made so as to make the real part of the second-order potential behave correctly at large distances.

We now convert the set of equations (1), together with the boundary conditions (2), into a set of integral equations

$$F_n(\boldsymbol{r}) = (2\pi)^{-3/2} \exp(\mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{r})\delta_{n0} + \lim_{\eta \to 0^+} \sum_{m=0}^{N} \int \frac{1}{(2\pi)^3} \frac{\exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{r} - \boldsymbol{x})]}{E - \epsilon_n - \frac{1}{2}q^2 + \mathrm{i}\eta} \times (V_{nm}(\boldsymbol{x}) + K_{nm})F_m(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{q} \qquad n = 0, 1, 2, \ldots, N. \tag{5}$$

The scattering amplitude in the SOP model for a transition from a state $(\boldsymbol{k}_0, 0)$ to a state $(\boldsymbol{k}'_n, n)$ is

$$f_{n0}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{k}}_0) = -(2\pi)^{1/2} \sum_{m=0}^{N} \int \exp(-\mathrm{i}\boldsymbol{k}'_n \cdot \boldsymbol{r})(V_{nm}(\boldsymbol{r}) + K_{nm})F_m(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r}. \tag{6}$$

Using equations (5) and (6), we get the integral equations satisfied by the scattering amplitudes:

$$f_{n0}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{k}}_0) = f_{n0}^{\mathrm{ASB}}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{k}}_0) - \frac{1}{4\pi^2} \lim_{\eta \to 0^+} \sum_{m=0}^{N} \int \frac{f_{nm}^{\mathrm{ASB}}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{q}}) f_{m0}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{k}}_0)\, \mathrm{d}\boldsymbol{q}}{E - \epsilon_m - \frac{1}{2}q^2 + \mathrm{i}\eta} \qquad n = 0, 1, 2, \ldots, N \tag{7}$$

where

$$f_{n0}^{\mathrm{ASB}}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{k}}_0) = -\frac{1}{2\pi} \int \exp(-\mathrm{i}\boldsymbol{k}'_n \cdot \boldsymbol{r})(V_{n0}(\boldsymbol{r}) + K_{n0}) \exp(\mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{r})\, \mathrm{d}\boldsymbol{r}. \tag{8}$$

The contribution of $V_{n0}(\boldsymbol{r})$ to $f_{n0}^{\mathrm{ASB}}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{k}}_0)$ is the scattering amplitude in the first Born approximation. Together with the contribution of the integral operator K_{n0}, $f_{n0}^{\mathrm{ASB}}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{k}}_0)$ can be seen to differ from the corrected simplified second Born approximation (Buckley and Walters 1975, see also Holt and Moiseiwitsch 1968) in that the close-coupling scattering amplitude has been replaced by the Born amplitude. The equations (7) thus bring out explicitly the relation between the SOP model and the approximate form of the second Born approximation (ASB).

The kernels of the set of integral equations (7) contain terms like $f_{nm}^{\mathrm{ASB}}(\hat{\boldsymbol{k}}'_n, \hat{\boldsymbol{q}})$ representing the ASB amplitude for scattering to the state $(\boldsymbol{k}'_n, n)$ from the state $(\boldsymbol{q}, m)$ in which energy need not be conserved. Great simplification occurs if one restricts the q values to force energy conservation, and ignores the unphysical amplitudes. This approximation has been exploited by Sloan and Moore (1968) and by Sil and coworkers (Saha *et al* 1975, Mandal *et al* 1975) for several atomic scattering problems. We, also, shall use this approximation in the present work. A discussion about its validity for the problem under consideration will be given in § 3.

Introducing the partial-wave amplitudes (for atomic s states)

$$T^{n0}_{lk'_nk_0} = \tfrac{1}{2}k_0 \int_{-1}^{+1} f_{n0}(\hat{\boldsymbol{k}}'_n \cdot \hat{\boldsymbol{k}}_0) P_l(\hat{\boldsymbol{k}}'_n \cdot \hat{\boldsymbol{k}}_0)\, \mathrm{d}(\hat{\boldsymbol{k}}'_n \cdot \hat{\boldsymbol{k}}_0) \tag{9}$$

and

$$T^{Anm}_{lk'_nk'_m} = \tfrac{1}{2}k'_m \int_{-1}^{+1} f_{nm}^{\mathrm{ASB}}(\boldsymbol{k}'_n \cdot \hat{\boldsymbol{k}}'_m) P_l(\hat{\boldsymbol{k}}'_n \cdot \hat{\boldsymbol{k}}'_m)\, \mathrm{d}(\hat{\boldsymbol{k}}'_n \cdot \hat{\boldsymbol{k}}'_m) \tag{10}$$

and utilising the set of equations (7), we get, with the on-shell approximation mentioned above, the following equations satisfied by the $T^{n0}_{lk'_nk_0}$:

$$T^{n0}_{lk'_nk_0} = T^{An0}_{lk'_nk_0} + i\sum_{m=0}^{N} T^{Anm}_{lk'_nk'_m} T^{m0}_{lk'_mk_0} \qquad n = 0, 1, 2, \ldots, N. \tag{11}$$

After evaluating the ASB partial-wave amplitudes $T^{An0}_{lk'_nk_0}$ from equations (8) and (10) and similarly obtaining the $T^{Anm}_{lk'_nk'_m}$, the set of equations (11) can be solved to yield the required amplitudes $T^{n0}_{lk'_nk_0}$. The scattering amplitudes $f_{n0}(\hat{\boldsymbol{k}}'_n \cdot \hat{\boldsymbol{k}}_0)$ and the differential and integrated cross sections for the transitions may then be obtained in the usual manner.

We have employed this procedure to work out the cross sections, in the one-channel approximation, for elastic scattering of electrons and positrons by hydrogen, helium and lithium. We first need to calculate $f^{ASB}_{00}(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0)$ which, from equation (8), can be written as

$$f^{ASB}_{00}(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0) = f^{B}_{00}(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0) + f^{S}_{00}(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0) \tag{12}$$

where the first term on the right is the first Born elastic scattering amplitude, and the second term is, explicitly,

$$f^{S}_{00}(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0) = \frac{1}{8\pi^4} \lim_{\eta \to 0^+} \int \frac{\exp[i(\boldsymbol{q} - \boldsymbol{k}'_0) \cdot \boldsymbol{r}]}{q^2 - \bar{k}^2 - i\eta} \times (V^{(2)}_{00}(\boldsymbol{r}, \boldsymbol{r}') - V_{00}(\boldsymbol{r}) V_{00}(\boldsymbol{r}')) \exp[i(\boldsymbol{k}_0 - \boldsymbol{q}) \cdot \boldsymbol{r}'] \, d\boldsymbol{r} \, d\boldsymbol{r}' \, d\boldsymbol{q} \tag{13}$$

with

$$V^{(2)}_{00}(\boldsymbol{r}, \boldsymbol{r}') = \int \phi^*_0(\boldsymbol{r}_1) V(\boldsymbol{r}_1, \boldsymbol{r}) V(\boldsymbol{r}_1, \boldsymbol{r}') \phi_0(\boldsymbol{r}_1) \, d\boldsymbol{r}_1. \tag{14}$$

For $e^{\pm}$–H scattering, the interaction potential $V(\boldsymbol{r}_1, \boldsymbol{r})$ is given by

$$V(\boldsymbol{r}_1, \boldsymbol{r}) = \frac{ZZ'}{r} - \frac{Z'}{|\boldsymbol{r} - \boldsymbol{r}_1|} \tag{15}$$

where Z is the atomic number of the target atom (+1 for hydrogen) and Z' is +1 and −1 for incident positrons and electrons, respectively. We have, in this case,

$$\phi_0(\boldsymbol{r}_1) = \varphi_{1s}(r_1) = (\alpha^3/\pi)^{1/2} \exp(-\alpha r_1) \qquad \alpha = 1{\cdot}0 \tag{16}$$

and

$$f^{S}_{00}(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0) = \frac{32Z'^2\alpha^4}{\pi^2} \lim_{\eta \to 0^+} \int \frac{d\boldsymbol{q}}{(q^2 - \bar{k}^2 - i\eta)(\boldsymbol{q} - \boldsymbol{k}'_0)^2 (\boldsymbol{k}_0 - \boldsymbol{q})^2} \times \left(\frac{1}{[(\boldsymbol{k}_0 - \boldsymbol{k}'_0)^2 + 4\alpha^2]^2} - \frac{16\alpha^4}{[(\boldsymbol{q} - \boldsymbol{k}'_0)^2 + 4\alpha^2]^2 [(\boldsymbol{k}_0 - \boldsymbol{q})^2 + 4\alpha^2]^2} \right). \tag{17}$$

The integrals occurring in (17) are converted (after splitting up into partial fractions, if necessary) into one-dimensional integrals by the Dalitz method (Dalitz 1951) and evaluated numerically for different values of k_0 and scattering angle. The numerical integrations have been done by using variations of the Gaussian quadrature method suitable for the behaviour of the individual integrands. A sufficient number of quadrature points have been taken to ensure convergence.

The ASB partial-wave amplitudes are then generated by another numerical integration of $f^{S}_{00}(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0) P_l(\hat{\boldsymbol{k}}'_0 \cdot \hat{\boldsymbol{k}}_0)$ and addition of the Born partial-wave amplitudes

for elastic scattering (see equation (10)). The latter amplitudes can be expressed analytically and their numerical values have been carefully determined. Using equation (11), we next determine $T^{00}_{lk'_0k_0}(k'_0 = k_0)$ and hence the elastic cross sections. Our results, along with those for helium and lithium atoms, are presented in the next section.

For $e^{\pm}$–He scattering, the interaction potential is

$$V(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}) = \frac{ZZ'}{r} - \frac{Z'}{|\boldsymbol{r}-\boldsymbol{r}_1|} - \frac{Z'}{|\boldsymbol{r}-\boldsymbol{r}_2|} \tag{18}$$

and we have used the following helium ground-state wavefunction (Byron and Joachain 1966)

$$\phi_0(\boldsymbol{r}_1, \boldsymbol{r}_2) = \varphi_{1s}(r_1)\varphi_{1s}(r_2) \tag{19}$$

with

$$\varphi_{1s}(r_1) = (N_1/\pi)^{1/2}[\exp(-\alpha r) + B\exp(-\beta r)] \tag{20}$$

$$N_1 = 1{\cdot}6966 \qquad B = 0{\cdot}7990 \qquad \alpha = 1{\cdot}41 \qquad \beta = 2{\cdot}61.$$

The interaction potential in the case of scattering by a lithium atom is, similarly,

$$V(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{r}) = \frac{ZZ'}{r} - \sum_{i=1}^{3} \frac{Z'}{|\boldsymbol{r}-\boldsymbol{r}_i|}. \tag{21}$$

The ground-state (2s) wavefunction for lithium has been chosen to be a single Slater determinant consisting of one-electron spin orbitals, the space parts of which are (Walters 1973)

$$\varphi_{1s}(r_i) = (\alpha^3/\pi)^{1/2}\exp(-\alpha r_i) \tag{22}$$

$$\varphi_{2s}(r_i) = Ar_i\exp(-\beta r_i) + B\varphi_{1s}(r_i) \tag{23}$$

$$A = 0{\cdot}1125 \qquad B = -0{\cdot}1686 \qquad \alpha = 2{\cdot}7 \qquad \beta = 0{\cdot}65.$$

The evaluation of $V^{(2)}_{00}(\boldsymbol{r}, \boldsymbol{r}') - V_{00}(\boldsymbol{r})V_{00}(\boldsymbol{r}')$ in this case is more involved. Its expression is given below:

$$2Z'^2\Bigg(\int \frac{\varphi^2_{1s}(r_1)}{|\boldsymbol{r}-\boldsymbol{r}_1||\boldsymbol{r}'-\boldsymbol{r}_1|}\,d\boldsymbol{r}_1 + \frac{1}{2}\int \frac{\varphi^2_{2s}(r_1)}{|\boldsymbol{r}-\boldsymbol{r}_1||\boldsymbol{r}'-\boldsymbol{r}_1|}\,d\boldsymbol{r}_1 - \int \frac{\varphi^2_{1s}(r_1)}{|\boldsymbol{r}-\boldsymbol{r}_1|}\,d\boldsymbol{r}_1 \int \frac{\varphi^2_{1s}(r_2)}{|\boldsymbol{r}'-\boldsymbol{r}_2|}\,d\boldsymbol{r}_2$$
$$- \int \frac{\varphi_{1s}(r_1)\varphi_{2s}(r_1)}{|\boldsymbol{r}-\boldsymbol{r}_1|}\,d\boldsymbol{r}_1 \int \frac{\varphi_{1s}(r_2)\varphi_{2s}(r_2)}{|\boldsymbol{r}'-\boldsymbol{r}_2|}\,d\boldsymbol{r}_2 - \frac{1}{2}\int \frac{\varphi^2_{2s}(r_1)}{|\boldsymbol{r}-\boldsymbol{r}_1|}\,d\boldsymbol{r}_1 \int \frac{\varphi^2_{2s}(r_2)}{|\boldsymbol{r}'-\boldsymbol{r}_2|}\,d\boldsymbol{r}_2\Bigg). \tag{24}$$

The rest of the procedure is similar to that for hydrogen and helium but the calculations are lengthy.

In all the cases of average energy parameter $\bar{k}^2$ has been chosen to yield the actual dipole polarisability of the target.

3. Results and discussion

We have calculated the elastic cross sections for $e^{\pm}$–H and $e^{\pm}$–He collisions with the incident energy varying between 20 eV (40 eV for helium target) and 500 eV. The $e^{\pm}$–Li elastic cross sections have been determined for an energy range of 10 to 200 eV. The results are discussed in the following subsections.

3.1. Elastic scattering of electrons and positrons by hydrogen

Our results for the integral cross sections for elastic scattering of electrons by hydrogen atoms are presented in table 1. These are compared with the one-channel results of Bransden *et al* (1972) and of Winters *et al* (1974) obtained, respectively, in the impact-parameter and wave formalisms of the second-order potential method. It may be noted that if the contribution of the continuum states of the target atom is properly included, then the electron exchange effect is taken care of. In the SOP theory, the continuum contribution has been taken into account approximately. However, Winters *et al* have introduced in their partial-wave equation another term which comes from the static exchange approximation. They presented integrated cross section values with the exchange effect incorporated in this manner. They have also given the $|T_l|^2$ values without the additional exchange term for $l = 0$ to 7. We have utilised these latter values and the estimated contribution for $l > 7$ (obtained from the impact-parameter results presented in the same paper) to compute the cross sections shown in the fourth column of table 1. It is these results with which our cross sections should be compared to see how far our on-shell approximation works. It is seen that the present cross sections are somewhat closer to the exact SOP results than are the values obtained in the impact-parameter (IP) method. The difference between our cross sections and those of Winters *et al* decreases with increasing energy.

Table 1. Integrated cross sections (in units of πa_0^2) for elastic scattering of electrons by hydrogen. IP, impact-parameter results of Bransden *et al* (1972); WNE, wave formulation results (without exchange, see text) of Winters *et al* (1974); 1s–2s–2p (on-shell), results of Saha *et al* (1975).

Incident energy (eV)	Present results	IP	WNE	1s–2s–2p (on-shell)	
				With exchange	Without exchange
20	2·303			1·05	0·819
54·4	0·650	0·609	0·819		
100	0·327	0·310	0·380		
200	0·157	0·150	0·168	0·150	0·136
400	0·0771				
500	0·0619			0·0621	0·0593

In the last two columns of table 1, we have included e^-–H elastic scattering cross sections determined by Saha *et al* (1975) who, in effect, have used an on-shell approximation to the 1s–2s–2p close-coupling equations with and without exchange. It can be seen that, at the high-energy end, the cross sections with exchange are close to our results obtained in the one-channel approximation. At low energy, however, the two sets of cross sections are found to differ.

Table 2 shows our integrated cross sections for positron–hydrogen elastic scattering within the energy range 20 to 500 eV. In the absence of any other SOP results for the problem, we have made comparison with the results of Mandal *et al* (1975) and Basu *et al* (1976). Mandal *et al* have used a 1s–2s–2p on-shell approximation similar to that of Saha *et al* for e^-–H scattering. The difference between their 1s–2s–2p cross sections without the inclusion of the positronium formation (column 3) and our one-channel SOP

Table 2. Integrated cross sections (in units of πa_0^2) for elastic scattering of positrons by hydrogen. 1s–2s–2p (on-shell), results of Mandal *et al* (1975); CCA, close-coupling calculations of Basu *et al* (1976) including 1s states of H and Ps.

Incident energy (eV)	Present results	1s–2s–2p (on-shell)		CCA
		Without Ps formation	With Ps formation	
20	0·803	0·819	0·927	0·676
54·4	0·375			0·433
100	0·234	0·245	0·245	0·256
200	0·132	0·136	0·136	0·139
400	0·0712			
500	0·0583			

results is small at all energies. Mandal *et al* have found that, above 40 eV, the cross sections remain practically unaltered when the Ps channel is taken into account (see column 4). Basu *et al* have employed the integral form of the close-coupling approximation (CCA) retaining only the 1s states of hydrogen and positronium, but have not made the on-shell approximation. The cross sections found by them are shown in the fifth column of the table. A comparison of these results indicates that the on-shell approximation to the one-channel SOP model may be reasonable for e^+–H scattering at the higher end of the energy region studied.

3.2. Elastic scattering of electrons and positrons by helium

We present the integrated elastic scattering cross sections for e^-–He collisions in table 3. Our results are compared with two other sets of SOP cross sections. The first is that of Berrington *et al* (1973) who have used the impact-parameter formulation and have explicitly retained the 1^1S, 2^1S and 2^1P states of helium (the second-order potential has been taken only in the elastic channel). The other results are those obtained using the one-channel wave formalism (without the additional exchange term) by Winters *et al*

Table 3. Integrated cross sections (in units of πa_0^2) for elastic scattering of electrons by helium. IP, impact-parameter results of Berrington *et al* (1973) retaining 1^1S, 2^1S and 2^1P states of He and the second-order potential in the elastic channel; W, wave formulation results of Winters *et al* (1974); UBA, unitarised Born approximation results.

Incident energy (eV)	Present results	IP	W	UBA
40	1·26			0·564
50	0·949	0·813	1·38[a]	0·484
100	0·421	0·415	0·581[a]	0·294
200	0·225	0·215	0·263[a]	0·172
300	0·161	0·147	0·195[b]	0·124
400	0·127	0·107	0·138[b]	0·0974
500	0·105	0·088	0·107[b]	0·0804

[a] Without exchange, see text.
[b] With exchange.

(1974). They have been worked out from the tabulated $|T_l|^2$ values without exchange and by using the published exchange results to get an estimate for the contribution of the higher partial waves. However, for incident energies above 200 eV, the $|T_l|^2$ values without exchange were not available to us, and the integrated cross sections are those found by Winters *et al* with the additional exchange term taken into account. In any case, the exchange effect progressively diminishes at higher energies. As in the case of hydrogen, our cross section values lie in between the IP and the wave formalism results. At 500 eV, when the exchange effect should be small, the present cross section is almost the same as that of Winters *et al.* The unitarised Born approximation (Seaton 1961) results, obtained by us as a by-product, are shown in the last column.

Table 4 contains the integral cross sections for elastic scattering of positrons by helium calculated by the present method. This table also shows the cross sections obtained by Dewangan and Walters (1977) in an approximate form of the distorted-wave second Born approximation. The method used by these authors to approximate the Green's function is similar to ours (see also Sloan and Moore 1968). However, while the procedure followed by Dewangan and Walters is a perturbative one for one part of the potential, the present approach, like that of the original SOP method, attempts to consider terms of all orders in the effective potential. A discussion on this distinction has been given by Bransden and McCarthy (1977). As expected, the difference between the two sets of cross sections shown in table 4 becomes small as the energy increases.

Table 4. Integrated cross sections (in units of πa_0^2) for elastic scattering of positrons by helium. ADWSBA, results of Dewangen and Walters (1977) in an approximate form of the distorted-wave second Born approximation.

Incident energy (eV)	Present results	ADWSBA
40	0·156	
50	0·160	
100	0·193	0·177
200	0·151	0·134
300	0·112	0·105
400	0·0881	0·0865
500	0·0728	0·0734

3.3. Elastic scattering of electrons and positrons by lithium

The $e^{\pm}$–Li elastic cross sections (integral) of the present work are shown in table 5. The scattering of electrons by lithium (and sodium) has been investigated earlier by M R Issa (1977, unpublished results) with the SOP formalism. He has employed one-electron wavefunctions for the target and has explicitly included the 2s and 2p states of lithium, besides taking the second-order potential into account. We reproduce in table 5, Issa's results from calculations of the following two types:

(i) The impact-parameter calculation with the inclusion of the 2s and 2p states of lithium and the second-order potential in the elastic channel.

(ii) The wave formulation calculation with exchange and the inclusion of the states and potential mentioned in (i).

Table 5. Integrated cross sections (in units of πa_0^2) for elastic scattering of electrons and positrons by lithium. IP, impact-parameter results of M R Issa (1977, unpublished) retaining the 2s and 2p states of Li and the second-order potential in the elastic channel; W, wave formalism calculations of Issa with the same states and potential as in IP.

Incident energy (eV)	Electron impact			Positron impact (present results)
	Present results	IP	W	
10	29·5	21·3	26·2	21·8
20	12·7		13·3	9·63
50	4·44	4·90	5·33	3·86
100	2·16	2·72		2·15
150	1·47			1·47
200	1·13	1·61		1·17

Since we have used the determinantal wavefunction explained in § 2 and have made a one-channel calculation, it is difficult to make a definite conclusion from a comparison between the two works. However, allowing for the difference due to these reasons, the on-shell approximation appears to give results of the right magnitude. A few years ago, Walters (1973) used the Glauber approximation and the wavefunction shown in equations (22) and (23) to study the e^-–Li scattering problem. In a later work (Walters 1976), he generalised an earlier model of Inokuti and McDowell (1974) by taking into account the non-adiabatic effect and calculated the elastic cross sections for incident energies up to 50 eV. Walters presented his results graphically and we are unable to include their cross section values in the table. However we note that our cross sections are comparable to those obtained in the two works of Walters at the higher ends of the respective energy regions studied. The few recent experimental data of Williams *et al* (1976) do not agree with the present calculation or with Issa's results at the lower energy end. However the disagreement seems to have decreased at 60 eV.

The positron results cannot be compared as no other calculations are available to us.

4. Conclusion

Judging by the results obtained for different targets and from the fact that only algebraic equations need be handled, we feel that, in the present method, it will be easy to get reasonably accurate cross sections for general electron (positron)–atom scattering problems (in the intermediate- and high-energy regions) when rearrangement and excitation channels are included. We expect to explore such possibilities in the future.

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