Comparison of integral-equation approximations for $e^{\pm}$-H scattering at intermediate energies

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It has been shown that the approximate solutions of the Fredholm integral equation for the scattering amplitude obtained by demanding that $f_{\text{out}}=f_{\text{in}}=\lambda_{p,n}f_{Bn}$ on the mass shell in the integral equation (where f_{Bn} is the scattering amplitude in the nth Born approximation, n and p are nonzero positive integers, and $\lambda_{p,n}$ is a scattering-angle- and energy-dependent complex multiplying factor) are identical to those obtained from the Schwinger variational principle with incoming and outgoing trial wave functions which are correct to $(p-1)$th and $(n-1)$th order in the interaction potential in a Born approximation. Further, the scattering amplitude obtained from the Schwinger variational principle, with outgoing and incoming scattering waves correct up to first order in the interaction potential in the Born approximation, has been employed to calculate total collisional cross sections for $e^{\pm}$-H scattering in the 20—500-eV energy range. The results are in good agreement with the adopted cross section of de Heer *et al.* and those obtained in the modified Glauber approximation and the [2,2] Padé approximant for $E \geq 30$ eV.

I. INTRODUCTION

In a recent investigation, Khare and Lata[1] have modified a method proposed by Das[2] and have employed their modified method to investigate elastic scattering of electrons and positrons by atomic hydrogen. It may be recalled that Das used an input scattering amplitude f_{in} in the Fredholm integral equation to obtain a better output scattering amplitude f_{out} as an approximate solution of the integral equation. He took f_{in} as a complex multiple of the first Born scattering amplitude f_{B1}. The real and imaginary parts of the complex multiple a^D+ib^D were determined by minimizing $|f_{\text{out}}-f_{\text{in}}|^2$ integrated over the whole angular region with respect to the parameters a^D and b^D. Thus the parameters, although dependent upon the incident energy, are independent of the scattering angle θ. f_{out} so obtained was utilized by Das and his associates[3–7] to study elastic as well as inelastic scattering of the electrons and positrons by the hydrogen and helium atoms in the intermediate energy range. They claimed that the method was quite successful. However, Jhanwar *et al.*[8] and Khare and Lata[1] have pointed out a number of shortcomings of the method proposed by Das (henceforth to be referred as the Das method).

To remove some of the deficiencies of the Das method, Khare and Lata[1] took f_{in} as $(a^P+ib^P)(f_{B1}+\bar{f}_{B2})$, where $\bar{f}_{B2}$ is the second Born term, in the Fredholm integral equation to obtain a better f_{out}. The parameters a^P and b^P were determined in exactly the same manner as suggested by Das. However, following the spirit of the eikonal-Born-series (EBS) method,[9] Khare and Lata neglected from the expression for f_{out} all the terms which fall asymptotically faster than k_i^{-2}, k_i being the wave number of the incident particle. Thus in their method (henceforth to be referred to as the KL method) the imaginary part of the third Born term $\bar{f}_{B3I}$ and b^P were taken as zero because they fall asymptotically as k_i^{-3}. They also replaced the real part of the third Born term $\bar{f}_{B3R}$ by the third term of the Glauber series, f_{G3}. Their results are found to be better when compared with those obtained by the Das method for the real part of the forward scattering amplitude, total collisional cross sections (calculated with the help of the optical theorem), and the differential cross sections for the elastic scattering of electrons and positrons by the hydrogen atom over the energy range varying from 50 to 1000 eV. However, like the Das parameters, a^P is also independent of the scattering angle, which is not supposed to be.[8] Furthermore, the KL method does not distinguish between electrons and positrons as far as the total collisional cross sections are concerned. On the other hand, the Das method yields unrealistic large differences between the two cross sections (see Table III of Ref. 1). It has also been noticed by Khare and Lata[10] that the KL method underestimates total collisional cross sections for e^--He and e^--H_2 scatterings. Hence further improvement in the input trial wave function is desired.

In the present investigation we have obtained the parameters $\lambda_{p,n}$ by demanding f_{out} be equal to f_{in} on the mass shell in the Fredholm integral equation. We have demonstrated that such solutions for the scattering amplitude $[f_{p,n}]$, where p and n are positive integers excluding zero, are identical to those obtained from the Schwinger variational principle[11] with incoming and outgoing trial wave functions which are correct to $(p-1)$th and $(n-1)$th order in the interaction potential in the Born approximation. Since these solutions are obtained from a variational principle, they are likely to yield better results. In recent years a number of investigators[9,12–15] have employed the Schwinger variational principle to investigate scattering of electrons and positrons by atoms. However, in almost all the cases zeroth-order wave functions were employed as the trial wave functions for both outgoing and incoming scattered waves and the resultant $[f]$ was the same as given by the [1,1] Padé approximant. The results so obtained were not satisfactory. Buckley and Walters[15] took sufficiently flexible one-state trial wave func-

tions and concluded that for s-s transition, $[f]$ obtained from the Schwinger variational principle does not account for the long-range polarization effects. We note that the trial wave functions employed by the above-mentioned authors[15] were separable and the distortion of the wave function of the target was not included, which is required for the proper account of the polarization effects.

For the first time, in this paper, we employ trial wave functions for the outgoing and incoming scattering waves correct up to first order in the interaction potential in the Schwinger variational principle. $[f]$ so obtained, which explicitly includes polarization effects, is expected to yield better results in comparison with those obtained from the [1,1] Padé approximant and nonvariational f_{out} utilized by Das[2] and Khare and Lata.[1] As a test case the calculations have been carried out for the total collisional cross sections for the scattering of the electrons and positrons by the hydrogen atom in the intermediate-energy range. The results are compared with those obtained from [1,1], [1,2], and [2,2] Padé approximants, the Das method, the Khare-Lata method, the EBS method,[9] the modified Glauber approximation[16] (MGA), and also with the adopted cross sections of de Heer *et al.*[17] For comparison, calculations have also been carried out after taking the imaginary part of $[f]$ equal to $\bar{f}_{B2I}+f_{G4}$, where $\bar{f}_{B2I}$ is the imaginary part of the second Born term and f_{G4} is the fourth-order Glauber term.

II. THEORY

The scattering amplitude for the $e^{\pm}$-atom scattering from the initial state i to the final state f is given by the Fredholm integral equation[1]

$$f^{fi}(\mathbf{k}_f,\mathbf{k}_i)=f_{B1}^{fi}(\mathbf{k}_f,\mathbf{k}_i)+\frac{1}{2\pi^2}\sum_m\int\frac{f_{B1}^{fm}(\mathbf{k}_f,\mathbf{q})f^{mi}(\mathbf{q},\mathbf{k}_i)}{q^2-k_m^2-i\epsilon}d\mathbf{q}\,, \tag{1}$$

where f^{mi} and f_{B1}^{fm} are the exact and first Born scattering amplitudes, respectively. $\mathbf{k}_f$ is the momentum vector of the projectile after the scattering and $k_m^2=k_i^2-2(E_m-E_i)$, E_i and E_m being the initial and intermediate target energies. We iterate Eq. (1), p times and obtain

$$f^{fi}(\mathbf{k}_f,\mathbf{k}_i)=f_{Bp}^{fi}(\mathbf{k}_f,\mathbf{k}_i)+\frac{1}{2\pi^2}\sum_m\int\frac{\bar{f}_{Bp}^{fm}(\mathbf{k}_f,\mathbf{q})f^{mi}(\mathbf{q},\mathbf{k}_i)}{q^2-k_m^2-i\epsilon}d\mathbf{q}\,, \tag{2}$$

where

$$f_{Bp}=\sum_{j=1}^{p}\bar{f}_{Bj} \tag{3}$$

is the scattering amplitude in the pth Born approximation and $\bar{f}_{Bj}$ is the jth Born term. We note that (2) is still exact. To obtain approximate solutions we take

$$f^{mi}(\mathbf{q},\mathbf{k}_i)=\lambda_{p,n}f_{Bn}^{mi}(\mathbf{q},\mathbf{k}_i) \tag{4}$$

for all values of m (including $m=i$ and f), where n is an integer and $\lambda_{p,n}$ is a complex multiplying factor. Putting (4) into (2) we obtain

$$f_{\text{out}}^{fi}=f_{Bp}^{fi}+\lambda_{p,n}(\bar{f}_{Bp+1}^{fi}+\bar{f}_{Bp+2}^{fi}+\cdots+\bar{f}_{Bp+n}^{fi})=f_{Bp}^{fi}+\lambda_{p,n}(f_{Bp+n}^{fi}-f_{Bp}^{fi})\,. \tag{5}$$

From (4) we also have for $m=f$

$$f_{\text{in}}^{fi}=\lambda_{p,n}f_{Bn}^{fi}\,. \tag{6}$$

To obtain the expressions utilized by Das[2] and Khare and Lata,[1] the multiplying factor $\lambda_{p,n}$ (to be denoted by $a_{p,n}+ib_{p,n}$) is determined by minimizing $\int|f_{\text{out}}-f_{\text{in}}|^2d\Omega$ with respect to $a_{p,n}$ and $b_{p,n}$ (we drop the superscript fi to simplify the notation). Such a procedure yields

$$a_{p,n}=\frac{\int\{f_{BpR}(f_{BpR}+f_{BnR}-f_{Bp+nR})+f_{BpI}(f_{BpI}+f_{BnI}-f_{Bp+nI})\}\sin\theta\,d\theta}{\int\{(f_{BpR}+f_{BnR}-f_{Bp+nR})^2+(f_{BpI}+f_{BnI}-f_{Bp+nI})^2\}\sin\theta\,d\theta} \tag{7a}$$

and

$$b_{p,n}=\frac{\int\{f_{BpI}(f_{BpR}+f_{BnR}-f_{Bp+nR})-f_{BpR}(f_{BpI}+f_{BnI}-f_{Bp+nI})\}\sin\theta\,d\theta}{\int\{(f_{BpR}+f_{BnR}-f_{Bp+nR})^2+(f_{BpI}+f_{BnI}-f_{Bp+nI})^2\}\sin\theta\,d\theta}\,, \tag{7b}$$

where f_{BmR} and f_{BmI} are the real and imaginary parts of the mth Born scattering amplitude f_{Bm}, respectively. Remembering that the first Born term is purely real it is easy to verify that for $p=n=1$ we get

$$a_{1,1}=a^D \quad\text{and}\quad b_{1,1}=b^D\,.$$

Similarly, for $p=1$ and $n=2$ we obtain

$$a_{1,2}=a^P \quad\text{and}\quad b_{1,2}=b^P\,,$$

where a^D,b^D are given by (6) of Ref. 1 and a^P,b^P are given by (9) of Ref. 1. Thus we obtain from (5)

$$f_{\text{out}}^{D}=f_{B1}+(a^D+ib^D)\bar{f}_{B2} \tag{8}$$

and

$$f_{\text{out}}^{\text{KL}}=f_{B1}+(a^P+ib^P)(\bar{f}_{B2}+\bar{f}_{B3})\,. \tag{9}$$

Let us now obtain a different type of approximate solution of the Fredholm integral equation by demanding $f_{\text{out}}=f_{\text{in}}=\lambda_{p,n}f_{Bn}$ on the mass shell in (5). Such a procedure yields

$$\lambda_{p,n}=\frac{f_{Bp}}{f_{Bp}-(f_{Bp+n}-f_{Bn})} \tag{10}$$

and the scattering amplitude $[f_{p,n}]$ is given by

$$[f_{p,n}]=f_{\text{out}}=f_{\text{in}}=\frac{f_{Bp}f_{Bn}}{f_{Bp}-(f_{B\overline{p+n}}-f_{Bn})} . \tag{11}$$

It should be noted that $\lambda_{p,n}$ given by (10) depends on energy as well as scattering angle. On the other hand, $\lambda_{p,n}$ given by Eqs. (7) depends only on energy. Equation (11) may be rewritten as

$$[f_{p,n}]=f_{Bn}\sum_{m=0}^{\infty}\left[\frac{f_{B\overline{p+n}}-f_{Bn}}{f_{Bp}}\right]^m . \tag{12}$$

Hence asymptotically $[f_{p,n}]$ agrees with the first $p+n$ terms of the Born series.

Now we proceed to demonstrate that (11) can also be obtained from the Schwinger variational principle. The fractional form for the direct scattering amplitude $[f]$ as obtained from the Schwinger variational principle in terms of the outgoing $\psi_{\mathbf{k}_i}^{+}(\mathbf{r},\mathbf{x})$ and incoming $\psi_{\mathbf{k}_f}^{-}(\mathbf{r},\mathbf{x})$ wave functions is given by[11]

$$[f]=-2\pi^2\frac{\langle\psi_{\mathbf{k}_f}^{-}\mid U\mid\phi_{\mathbf{k}_i}\rangle\langle\phi_{\mathbf{k}_f}\mid U\mid\psi_{\mathbf{k}_i}^{+}\rangle}{\langle\psi_{\mathbf{k}_f}^{-}\mid(U-UG_0^{+}U)\mid\psi_{\mathbf{k}_i}^{+}\rangle} , \tag{13}$$

where $\phi_{\mathbf{k}_i}(\mathbf{r},\mathbf{x})$ and $\phi_{\mathbf{k}_f}(\mathbf{r},\mathbf{x})$ are the initial and final wave functions of the system (projectile plus atom), respectively; $\mathbf{r}$ and $\mathbf{x}$ are the coordinates of the projectile and the atomic electrons, respectively. $G_0^{+}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}')$ is the outgoing free-particle Green's function of the system and U is the reduced interaction energy. Let us now take $\mid\psi_{\mathbf{k}_i}^{+}\rangle$ and $\mid\psi_{\mathbf{k}_f}^{-}\rangle$ as the scattering wave functions in the $(n-1)$th and $(p-1)$th Born approximation, respectively, i.e.,

$$\mid\psi_{\mathbf{k}_i}^{+}\rangle=\left[\sum_{m=0}^{n-1}(G_0^{+}U)^m\right]\mid\phi_{\mathbf{k}_i}\rangle$$

$$\equiv\mid X_{\mathbf{k}_i}^{n-1}\rangle , \tag{14a}$$

where there are n terms operating on $\mid\phi_{\mathbf{k}_i}\rangle$. Similarly,

$$\langle\psi_{\mathbf{k}_f}^{-}\mid=\langle\phi_{\mathbf{k}_f}\mid\left[\sum_{m=0}^{p-1}(UG_0^{+})\right]$$

$$\equiv\langle X_{\mathbf{k}_f}^{p-1}\mid , \tag{14b}$$

where there are p terms operating on $\langle\phi_{\mathbf{k}_f}\mid$. Putting (14) in (13) we get

$$[f_{p,n}]=\frac{f_{Bp}f_{Bn}}{f_{B1}+\bar{f}_{B2}+\cdots+\bar{f}_{Bp}-(\bar{f}_{B\overline{n+1}}+\bar{f}_{B\overline{n+2}}+\bar{f}_{B\overline{n+3}}+\cdots+\bar{f}_{B\overline{n+p}})} \tag{15}$$

which is identical to (11). Thus we establish that the approximate solutions of the Fredholm integral equation for the scattering amplitude $[f_{p,n}]$ which are obtained by demanding $f_{\text{out}}=f_{\text{in}}=\lambda_{p,n}f_{Bn}$ on the mass shell are identically the same as those obtained from the Schwinger variational principle with incoming and outgoing trial wave functions which are correct to $(p-1)$th and $(n-1)$th order in the interaction potential in a Born approximation. Taking $p=n=1$ in (11) we get

$$[f_{1,1}]=\frac{f_{B1}f_{B1}}{f_{B1}-\bar{f}_{B2}} . \tag{16}$$

Similarly, the combinations $(n=2,\ p=1)$ and $(n=p=2)$ yield, respectively,

$$[f_{1,2}]=\frac{f_{B1}(f_{B1}+\bar{f}_{B2})}{f_{B1}-\bar{f}_{B3}} \tag{17}$$

and

$$[f_{2,2}]=\frac{(f_{B1}+\bar{f}_{B2})^2}{f_{B1}+\bar{f}_{B2}-\bar{f}_{B3}-\bar{f}_{B4}} . \tag{18}$$

Let us now consider the scattering amplitudes in the form of Padé approximants. Using the table given by Macdonald[18] for the epsilon algorithm, the expression for the scattering amplitudes $f_{[p,n]}$ in the $[p,n]$ Padé approximant can be obtained. We find that $f_{[1,1]}$ is exactly the same as given by (16). However, $f_{[1,2]}$ and $f_{[2,2]}$ are given by

$$f_{[1,2]}=f_{B1}+\frac{\bar{f}_{B2}\bar{f}_{B2}}{\bar{f}_{B2}-\bar{f}_{B3}} \tag{19}$$

and

$$f_{[2,2]}=f_{[1,2]}+\frac{(\bar{f}_{B2}\bar{f}_{B4}-\bar{f}_{B3}^{2})(f_{B1}\bar{f}_{B3}-\bar{f}_{B2}^{2})}{(\bar{f}_{B2}-\bar{f}_{B4}-2\bar{f}_{B3})(f_{B1}\bar{f}_{B3}-\bar{f}_{B2}^{2})-(\bar{f}_{B2}\bar{f}_{B4}-\bar{f}_{B3}^{2})(f_{B1}+\bar{f}_{B3}-2\bar{f}_{B2})} . \tag{20}$$

Thus higher Padé approximants do not yield the same expressions as given by the Schwinger variational principle. Nevertheless, if we take $\bar{f}_{B3I}$ equal to zero and replace $\bar{f}_{B3R}$ by f_{G3} in (17) as well as in (19) then both of them asymptotically reduce to the eikonal Born series which is correct up to order k_i^{-2} at higher energies.

It is evident that (8) and (16) have been derived with the same inputs, i.e., plane waves for $\mid\psi_{\mathbf{k}_i}^{+}\rangle$ and $\mid\psi_{\mathbf{k}_f}^{-}\rangle$. However, (16) does not explicitly contain $\bar{f}_{B2}$ in the numerator; hence, as pointed out by Buckley and Walters, it is not ex-

pected to represent long-range effects properly. On the other hand, in (8), a^D+ib^D is just a number; hence, $f^D_{\rm out}$ contains polarization effects through $\bar{f}_{B2}$, explicitly in the numerator. Hence, at relatively lower energies, (8) is expected to yield better results in comparison with those obtained from (16). At high energies both (8) and (16) tend to f_{B2}. Similarly, (9) and (17) are obtained when $|\psi^+_{\mathbf{k}_i}\rangle$ is taken as the scattered wave function correct to first order but with $|\psi^-_{\mathbf{k}_f}\rangle$ as a plane wave. However, now both (9) and (17) contain $\bar{f}_{B2}$ in the numerator, but (17) has $\bar{f}_{B3}$ in the denominator whereas in (9) $\bar{f}_{B3}$ appears in the numerator. Hence the difference between the results obtained from (9) and (17) is expected to be less than the difference between the results obtained from (8) and (16). At high energies both of them tend to f_{B3}.

Equation (18) employs trial inputs which are better than those employed in the derivation of (8), (9), (16), and (17). Hence $[f_{2,2}]$ is expected to yield better results than those given by $[f_{1,1}]$, $[f_{1,2}]$, and nonvariational amplitudes $f^D_{\rm out}$, $f^{\rm KL}_{\rm out}$, $f_{[1,2]}$, and $f_{[2,2]}$.

As remarked in the Introduction, in the present paper we have calculated $Q_T(e^{\mp})$ for the hydrogen atom in the intermediate-energy range using (16)—(20) and the optical theorem which is given as

$$Q_T=\frac{4\pi}{k_i}\mathrm{Im}[f(0)]\ , \tag{21}$$

where $\mathrm{Im}[f(0)]$ is the imaginary part of the scattering amplitude in the forward direction. Utilization of (16)—(20) in (21) requires the evaluation of $\bar{f}_{Bn}(0)$ for $n=1,2,3,4$ for the hydrogen atom. The evaluation of $f_{B1}(0)$ is trivial and usually closure is employed to evaluate $\bar{f}_{B2}$. However, as yet no tractable method is available to evaluate $\bar{f}_{B3}$ and $\bar{f}_{B4}$. Nevertheless, if we employ closure to evaluate $\bar{f}_{B3}(0)$ then it is well known that the $\bar{f}_{B3}(0)$ is equal to zero.[13] This reduces (17) and (19) to

$$[f_{1,2}(0)]=f_{B1}(0)+\bar{f}_{B2}(0)\ . \tag{22}$$

Thus $\mathrm{Im}[f(0)]$ is equal to $\bar{f}_{B2I}$, and $Q_T(e^{\mp})$ so obtained is exactly equal to those given by EBS method. On the other hand, under the above condition (18) and (20) reduce, respectively, to

$$[f_{2,2}(0)]=\frac{\{f_{B1}(0)+\bar{f}_{B2}(0)\}^2}{f_{B1}(0)+\bar{f}_{B2}(0)-\bar{f}_{B4R}(0)-i\bar{f}_{B4I}(0)} \tag{23}$$

and

$$f_{[2,2]}(0)=f_{B1}(0)+\bar{f}_{B2}(0)+\frac{\bar{f}_{B4}(0)}{1+\dfrac{\{f_{B1}(0)-\bar{f}_{B2}(0)\}\bar{f}_{B4}(0)}{\bar{f}^2_{B2}(0)}}\ . \tag{24}$$

Now, $\bar{f}_{B4I}$ asymptotically varies[20] as k_i^{-3} but $\bar{f}_{B4R}$ goes as k_i^{-4}. Hence if we neglect all those terms which fall asymptotically faster than k_i^{-3}, then (23) and (24) reduce to

$$[f_{2,2}(0)]=\frac{\{f_{B1}(0)+\bar{f}_{B2}(0)\}^2}{f_{B1}(0)+\bar{f}_{B2}(0)-i\bar{f}_{B4I}(0)} \tag{25}$$

and

$$f_{[2,2]}(0)=f_{B1}(0)+\bar{f}_{B2}(0)+\frac{i\bar{f}_{B4I}(0)}{1+\dfrac{\{f_{B1}(0)-\bar{f}_{B2}(0)\}}{\bar{f}^2_{B2}(0)}i\bar{f}_{B4I}(0)}\ , \tag{26}$$

respectively. The above equations include all the terms up to k_i^{-3} asymptotically. We further note that the purely imaginary fourth term of the Glauber series, f_{G4}, also varies as k_i^{-3} and is expected to be a good representation of $\bar{f}_{B4I}$. Hence in (25) and (26) we replace $i\bar{f}_{B4I}$ by f_{G4} and finally obtain

$$[f_{2,2}(0)]=\frac{\{f_{B1}(0)+\bar{f}_{B2}(0)\}^2}{f_{B1}(0)+\bar{f}_{B2}(0)-f_{G4}(0)} \tag{27}$$

and

$$f_{[2,2]}(0)=f_{B1}(0)+\bar{f}_{B2}(0)+\frac{f_{G4}(0)}{1+\{f_{B1}(0)-\bar{f}_{B2}(0)\}\dfrac{f_{G4}(0)}{\bar{f}^2_{B2}(0)}}\ . \tag{28}$$

The above equations along with (21) are utilized to calculate $Q_T(e^{\mp})$. For further comparison we expand

$$\left[1-\frac{f_{G4}(0)}{f_{B1}(0)+\bar{f}_{B2}(0)}\right]^{-1}$$

in powers of $f_{G4}(0)$ and take terms only up to the first power in $f_{G4}(0)$. Thus we get from (27)

$$\mathrm{Im}[f_{2,2}(0)]=\bar{f}_{B2I}(0)+f_{G4}(0)\ . \tag{29}$$

The same expression up to first power in $f_{G4}(0)$ is obtained from (28). The above equation is also utilized to calculate $Q_T(e^{\mp})$. It is evident that (22) and (29) when used with (21) will not distinguish between $Q_T(e^-)$ and $Q_T(e^+)$. On the other hand (16), (27), and (28), like the Das method, will yield different values for $Q_T(e^-)$ and $Q_T(e^+)$.

The evaluation of $\bar{f}_{B2}$ is carried out exactly in the same manner as done by Jhanwar *et al.*[21] For the evaluation of $f_{G4}(0)$ we note that for the hydrogen atom[21]

$$f_G(0)-f_{G2}(0)=-ik_i\left[\frac{i\eta}{i-i\eta}+2\eta^2+J(\eta)\right]\ , \tag{30}$$

where

$$J(\eta)=\sum_{m=1}^{\infty}\left[\frac{(-i\eta)_m}{m!}\right]^2\frac{1}{1+m-i\eta}-\sum_{m=2}^{\infty}\left[\frac{(-i\eta)_m}{m!}\right]^2\frac{1}{(1-m)}\ , \tag{31}$$

f_{G2} is the second term of the Glauber series f_G, $(a)_m$ is the Pochhammer symbol given by

$$(a)_m=a(1+a)(2+a)\cdots(m-1+a)=\frac{\Gamma(a+m)}{\Gamma(a)}\ ,$$

with $(a)_0=1$, and $\eta=-Q/k_i$, Q being charge of the pro-

jectile. Now we expand the right-hand side of (30) and collect the terms of η^4, which is nothing but $f_{G4}(0)$. Following the above procedure we obtain

$$f_{G4}(0)=-ik_i\eta^4\left\{\frac{9}{8}+\sum_{m=2}^{\infty}\left[\frac{1}{m^2(m+1)^3}-\frac{2S_{m-1}}{m^2(m+1)^2}+\frac{8S_{m-1}^2}{m(m^2-1)}-\frac{8}{m(m^2-1)}\sum_{l=1}^{m-1}\frac{S_l}{l}+\frac{2T_{m-1}}{m(m^2-1)}\right]\right\}, \tag{32}$$

where

$$S_m=\sum_{l=1}^{m}\frac{1}{l}$$

and

$$T_m=\sum_{l=1}^{m}\frac{1}{l^2}\ . \tag{33}$$

III. RESULTS AND DISCUSSION

Table I shows the values of $f_{G4}(0)$ and $\mathrm{Im}[f_G(0)-f_{G2}(0)]$ for $e^{\mp}$-H elastic scattering in the energy range 20–500 eV. At 20 eV the two values differ by about 55% indicating a fairly good contribution of the higher-order imaginary terms of the Glauber series, i.e., f_{G6}, f_{G8}, etc. As expected, the difference between the two values decreases with the increase of energy and is about 10% at 100 eV, which further reduces to about 2% at 500 eV.

In Table II we have shown the values of $Q_T(e^{\mp})$ for the hydrogen atom obtained from different approximations. All the calculations have utilized optical theorem. The values shown in the last column are the adopted cross sections of de Heer *et al.*[17] for electron impact which we take as reference values. The values obtained in the present investigation through (16), (27), (28), and (29) are denoted by $P1$, $P2$, $P3$, and $P4$, respectively. As remarked earlier the values obtained by the application of (17) and (19) are exactly the same as given by the EBS method. From the table we notice that the $P1$ values for electron impact do not show even a qualitative agreement with those of de Heer *et al.* and are in general too small. $P1$ shows unrealistically large differences between $Q_T(e^-)$ and $Q_T(e^+)$. Even at 500 eV, $Q_T(e^-)$ is larger than $Q_T(e^+)$ by a factor of about 2.8. The Das method also utilizes the same input trial function as employed in (16), but a different procedure has been adopted to obtain the multiplying factor (a^D+ib^D). Such a difference has led to the increase in the values of $Q_T(e^{\mp})$. The Das values for $Q_T(e^-)$, although better than $P1$, also do not compare favorably with those of de Heer *et al.* The Das method overestimates the cross sections. Thus it is evident that the representation of $\psi_{\mathbf{k}_i}^+$ and $\psi_{\mathbf{k}_f}^-$ by plane waves in variational (Schwinger) as well as nonvariational (Das) methods is not adequate. This is in agreement with the conclusions of the previous investigators.

TABLE I. Variation of $f_{G4}(0)$ and $\mathrm{Im}[f_G(0)-f_{G2}(0)]$ (in a_0) with energy for $e^{\mp}$-H elastic scattering. The numbers within the parentheses indicate the power of ten by which the entries must be multiplied; e.g., $-7.342(-1)=-7.342\times10^{-1}$.

E (eV)	f_{G4} (0)	$\mathrm{Im}[f_G(0)-f_{G2}(0)]$
20	−1.349	−8.701(−1)
30	−7.342(−1)	−5.339(−1)
50	−3.412(−1)	−2.745(−1)
100	−1.206(−1)	−1.075(−1)
200	−4.266(−2)	−4.019(−2)
300	−2.322(−2)	−2.232(−2)
400	−1.509(−2)	−1.464(−2)
500	−1.079(−2)	−1.054(−2)

Improvement of the wave function $\psi_{\mathbf{k}_i}^+$ from the plane wave to the scattered wave function correct up to first order leads to the EBS and KL methods. These two methods yield much better values for Q_T in comparison of those given by $P1$ and the Das method. However, these methods do not distinguish between $Q_T(e^-)$ and $Q_T(e^+)$. Further, whereas the EBS method overestimates the cross sections, Khare and Lata's method underestimates them. As expected, the values obtained by these two methods approach each other with the increase of impact energy and the magnitudes of underestimation and overestimation are also reduced.

$P2$ values are obtained by a further improvement of the scattering wave functions. Such a change leads to different values for $Q_T(e^-)$ and $Q_T(e^+)$, both being lower than those given by the EBS method. $P2$ underestimates the cross sections but the overestimation by EBS is always higher than the underestimation by (27) at all the impact energies except 20 eV. The difference between $Q_T(e^-)$ and $Q_T(e^+)$ obtained in $P2$ is also quite reasonable. Except at 20 eV the differences between $P2$ and those obtained from [2,2] Padé approximant (denoted by $P3$) are small (less than 1%). The table shows highly satisfactory agreement between $P2$ and $P3$ values and the adopted cross sections of de Heer *et al.*[17] for $E\geq50$ eV. At 30 eV the difference between them is about 20% which increases to a rather large value at 20 eV. This trend is according to the expectation. Since the cross sections given by $P2$ and $P3$ are correct only up to k_i^{-3}, they are, hence, not likely to be satisfactory at low impact energies. It seems from Table II that 30 eV is a lower limit for the application of (27) and (28). We also note that the above equations are obtained from (25) and (26), respectively, after replacing $\bar{f}_{B4I}$ by f_{G4}. This replacement is also likely to introduce additional error. A comparison of $\bar{f}_{B2I}$ with f_{G2} for $\theta\geq10°$ at 30 eV shows that the difference between their values varies from 6% to 30%. Due to the divergence of f_{G2} in the forward direction a comparison at smaller angles is not useful. We may expect a similar difference between $\bar{f}_{B4I}$ and f_{G4}. In our investigation the ratio $f_{G4}/\bar{f}_{B2I}$ is always less than unity and it decreases with energy. Hence Q_T is not likely to be very sensitive to the value of f_{G4}. We have noticed that a change of 50% in the value of f_{G4} changes Q_T by about 25% and 10% at

TABLE II. Total collision cross section (in a_0^2) for the scattering of electrons and positrons by the hydrogen atoms.

E (eV)	$P1$[a]		D[b]		EBS[c]	KL[b]
	e^-	e^+	e^-	e^+	$e^{\mp}$	$e^{\mp}$
20	2.476	0.919	23.71	0.655	17.89	8.736
30	2.847	1.035	19.84	1.573	15.84	9.00
50	2.983	1.050	15.25	2.281	11.86	7.942
100	2.850	0.965	8.453	2.585	7.343	5.778
200	2.465	0.826	4.828	2.285	4.315	3.774
300	2.238	0.721	3.440	1.955	3.119	2.821
400	1.913	0.665	2.695	1.699	2.466	2.295
500	1.720	0.613	2.226	1.501	2.051	1.935

E (eV)	$P2$[a]		$P3$[a]		$P4$[a]	MGA[c]	H[d]
	e^-	e^+	e^-	e^+	$e^{\pm}$	$e^{\pm}$	e^-
20	6.151	8.147	4.793	7.280	3.916	8.878	14.36
30	10.27	10.97	10.18	10.89	9.627	11.32	12.72
50	9.78	9.958	9.757	10.08	9.650	10.09	10.30
100	6.773	6.823	6.796	6.824	6.785	6.845	6.850
200	4.177	4.180	4.177	4.181	4.176	4.183	4.180
300	2.926	2.927	2.926	2.928	2.926	3.059	3.060
400	2.432	2.432	2.432	2.432	2.431	2.432	2.430
500	2.029	2.029	2.029	2.029	2.019	2.029	

[a] $P1$, $P2$, $P3$, and $P4$ denote the results obtained in the present investigation by the use of (16), (27), (28), and (29), respectively.
[b] D and KL are the result of the Das and Khare-Lata methods (Ref. 1).
[c] EBS and MGA are the results of Jhanwar *et al.* (Ref. 21).
[d] H are the adopted values of de Heer *et al.* (Ref. 17).

30 and 50 eV, respectively. The percent change further decreases with the increase of energy. The contribution of $\bar{f}_{B3}$ is expected to be small, which is equal to zero when evaluated through closure. Due to these reasons we obtain a satisfactory agreement between the values of the cross sections represented by $P2$, $P3$, and H in Table II down to 30 eV. The agreement between theoretical and adopted cross sections is likely to be further improved when the effects of exchange in the electron scattering and positronium formation in the positron scattering are included. The table further shows that $Q_T(e^+)$ as given by (27) and (28) is greater than $Q_T(e^-)$ at all the impact energies. A similar trend has been observed in the experimental investigations of Hoffmann *et al.*[22] and Deuring *et al.*[23] for $e^{\pm}$-H_2 scattering in 30—300-eV energy range. However, they observed that at 20 eV $Q_T(e^-)$ is greater than $Q_T(e^+)$, whereas in our investigation even at this energy $Q_T(e^+)$ is greater than $Q_T(e^-)$. As already discussed, our theoretical values at 20 eV are not reliable. Finally, we note that MGA values are slightly greater than $P2$ and $P3$ values and are in better agreement with the adopted cross sections of de Heer *et al.*[17] This may be due to a fortunate situation for the hydrogen atom. All the terms present in the Born series and missing from the modified Glauber series are zero in the forward direction when evaluated through closure.[19] However, like other approximations, the MGA also yields a value at 20 eV which is not in satisfactory agreement with the adopted cross section of de Heer *et al.* Furthermore, unlike (27) and (28) MGA does not distinguish between $Q_T(e^+)$ and $Q_T(e^-)$.

Finally, we conclude that out of all the methods discussed in the present paper Eq. (18), obtained from the Schwinger variational principle, and the [2,2] Padé approximant look quite attractive for the investigation of $e^{\pm}$ scattering by atoms and molecules in the intermediate-energy range. Evaluation (18) and (20), for other targets and even for the hydrogen atom in oblique directions, will require the evaluation of $\bar{f}_{B3}$ and $\bar{f}_{B4}$. An attempt in this direction would be progress. At present their replacement by f_{G3} and f_{G4} may not be too bad.

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