Reduction of the eikonal exchange amplitude

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It is pointed out that the magnitude of the nuclear-scattering term in the eikonal exchange amplitude is smaller than but not negligible as compared with that of the electronic-scattering term at intermediate energies. It is, therefore, concluded that any approximation scheme which bypasses completely the nuclear-scattering term cannot provide a good approximate value for the eikonal exchange amplitude at intermediate energies especially at larger scattering angles. Comparison is made between these terms (electronic and nuclear scattering) using their exact eikonal forms as well as their various approximate expressions.

Although one has succeeded in representing the "exact" eikonal exchange amplitude in e-H scatterings by a two-dimensional integral,[1] the calculation of these amplitudes[1,2] is still quite tedious and hence consumes a great deal of time as well as demands a great deal of computation effort. Therefore, the interest in the reduction of these exchange amplitudes to simpler forms by considering some appropriate approximation still remains fully alive. In some previous reduction,[3] an expansion of the Ochkur-Bonham type[4] was considered and a reduced form, called the Glauber-Ochkur amplitude, was obtained. Aside from the lack of consistency in its derivation,[5] the eikonal-Ochkur exchange amplitude also has an unwanted feature, namely, it contains an undeterminate phase factor which impairs any attempt of including the exchange effect into the direct scattering amplitude through this formula. Recently,[6] Franco and Halpern showed that the formulation used to obtain the Glauber-Ochkur approximate exchange amplitude is not valid and developed an appropriate mathematical treatment which yields a new approximate amplitude with a well-defined unambiguous phase.

In these approximations, the nuclear-scattering term of the eikonal exchange amplitude has always been ignored. The neglect of this term has been based on a presumption that the magnitude of this term is quite small in comparison to that of the electronic scattering term. In this paper we wish, therefore, to carry out the separate calculations of these two terms (in both exact and approximate forms) and show that the magnitude of the nuclear-scattering term is actually significant in comparison to that of the electronic term. It is, thereby, concluded that any approximation scheme which completely bypasses the nuclear-scattering term cannot provide a good approximate value for the eikonal exchange amplitude in some significant ranges of energy and angle. Since the approximate amplitudes available in the literature are usually those of the electronic-scattering term only, it is, therefore, perhaps more appropriate to make a comparison of these approximate amplitudes with the exact electronic-scattering term, rather than with the total eikonal exchange amplitude. Through the process of calculating these two terms of the exact eikonal exchange amplitude, we also discovered that the calculation of the electronic-scattering term is, actually, quite simple and does not require that much computational effort. It is the nuclear-scattering term itself which is the source of all those computational difficulties. The need for a good analytic approximation is thus driven most strongly by the trickiness of the nuclear term numerical integration.

The exact "post" and "prior" exchange $T^{(\pm)}$ matrix for e-H collision can be written as the sum of $t^{(\pm)}(r_{12})$ and $t^{(\pm)}(r_2)$ which are due to the scattering by the electron and by the nucleus of the atom, respectively. The analytic expressions of these terms for post scattering can be put in the following forms:

$$t^{(+)}(r_{12})=\int d\vec{r}_1 d\vec{r}_{12}\exp[i(\vec{q}\cdot\vec{r}_1+\vec{k}_f\cdot\vec{r}_{12})]\phi_f^*(\vec{r}_1)\phi_i(\vec{r}_1-\vec{r}_{12})r_{12}^{-1}(r_{12}-z_{12})^{i\eta_+}(r_1-z_1)^{-i\eta_+}\ , \tag{1}$$

$$t^{(+)}(r_2)=-\int d\vec{r}_1 d\vec{r}_2\exp[i(\vec{k}_i\cdot\vec{r}_1-\vec{k}_f\cdot\vec{r}_2)]\phi_f^*(\vec{r}_1)\phi_i(\vec{r}_2)r_2^{-1}(r_{12}-z_{12})^{i\eta_+}(r_1-z_1)^{-i\eta_+}\ . \tag{2}$$

Both these terms have successfully been reduced to two-dimensional integrals.[1] The separate calculations of $t^{(+)}(r_{12})$ and $t^{(+)}(r_2)$ are performed for elastic e-H scattering at various intermediate and high energies, using the conventional z direction as the one perpendicular to the momentum transfer $\vec{q}=\vec{k}_i-\vec{k}_f$. As is well known, approximate forms are now available in the literature for both electronic- and nuclear-scattering terms.[7] These approximate forms are also evaluated and the values obtained also indicate that the magnitude of the nuclear-scattering term is quite significant. First, a brief review on the systematic derivations of these approximate forms is made. For the electronic-scattering term, if $t^{(+)}(r_{12})$ is approximated by setting r_{12} and z_{12} in

$$(r_{12}-z_{12})^{i\eta_+}\phi(\vec{r}_1-\vec{r}_{12})$$

to be zero, then one obtains[3] the Glauber-Ochkur approximate exchange amplitude. If, furthermore, the factor $(r_1-z_1)^{-i\eta_\pm}$ is expanded in terms of $k_\mp^{-1}$ and only the first-order term is kept, then one will obtain the Ochkur exchange amplitude. If in Eq. (1) above, one expands $\phi_i(\vec{r}_1-\vec{r}_{12})$ around $\vec{r}_1$, then one obtains[7] for the factor $h^{(+)}(r_{12})$ of $t^{(+)}(r_{12})$,

$$h^{(+)}(r_{12})=\int d\vec{r}_{12}\exp(i\vec{k}_f\cdot\vec{r}_{12})r_{12}^{-1}(r_{12}-z_{12})^{i\eta_+}(r_1-z_1)^{-i\eta_+}[\phi_i(\vec{r}_1)-\vec{r}_{12}\cdot\vec{\nabla}_{\vec{r}_1}\phi_i(\vec{r}_1)+\cdots] \;. \tag{3}$$

If only the first term of the expansion is kept,[6] then the "zeroth order" of the approximate eikonal exchange amplitudes by Franco and Halpern[6] is obtained,

$$\begin{aligned}(T_{fi}^{(\pm)})_{\text{FH}}=&16\pi^2k_\mp^{-2}k_\mp^{-i\eta_\pm}\pi\eta_\pm\sinh^{-1}\pi\eta_\pm\exp(\pi\eta_\pm/2)\\ &\times D_{\beta\vec{\lambda}}\{[\beta_\mp i(\vec{q}-\vec{\lambda})\cdot\hat{z}]^{-i\eta_\pm}[\beta^2+(\vec{q}-\vec{\lambda})^2]^{i\eta_\pm-1}\}\,|\,_{\vec{\lambda}=0}\;.\end{aligned} \tag{4}$$

The next order term of the electron-scattering term has also been recently included by Halpern and Franco.[7] By remarking that only the term $-z_{12}(\partial/\partial z_1)\phi_i(\vec{r}_1)$ of $-\vec{r}_{12}\cdot\vec{\nabla}_{\vec{r}_1}\phi_i(\vec{r}_1)$ in Eq. (3) survives the integration over $\vec{r}_{12}$ and that $\phi_f^*(\vec{r}_1)[\partial\phi_i(\vec{r}_1)/\partial z]$ in Eq. (1) may then be set equal to the form

$$r_1^{-1}D_{\beta\vec{\lambda}}^{(1,+)}\{\exp[-(\beta r_1+i\vec{\lambda}\cdot\vec{r}_1)]\}\;,$$

the next order contribution to the electron-scattering term can be put in closed form with no great difficulty. The following expression was found for this term:

$$\begin{aligned}[t^{(\pm)}(r_{12})]_{\text{1st order}}=&\mp16\pi^2\pi\eta_\pm\sinh^{-1}\pi\eta_\pm\exp(\pi\eta_\pm/2)i\frac{\partial}{\partial\mu}(k_\mp-\mu)^{-2-i\eta_\pm}\Big|_{\mu=0}\\ &\times D_{\beta\vec{\lambda}}^{(1,\pm)}\{[\beta_\mp i(\vec{q}-\vec{\lambda})\cdot\hat{z}]^{-i\eta_\pm}[\beta^2+(\vec{q}-\vec{\lambda})^2]^{i\eta_\pm-1}\}_{\vec{\lambda}=0}\;.\end{aligned} \tag{5}$$

In the case of 1s-1s e-H scattering, $D_{\beta\vec{\lambda}}^{(1,\pm)}=-(i/\pi)(\partial/\partial\lambda_{k_\mp})$ and $\beta=2$. Note that the present formula [Eq. (5)] is slightly different from the one given in Eq. (3) of Ref. 7 for e-H elastic scattering. The same formula as in Eq. (3) of Ref. 7 will be obtained if in the post scattering, an expansion of the integrand is made around $\vec{r}_2$ (instead of $\vec{r}_1$) and then an integration by parts is performed (vice versa for prior scattering). As for the nuclear-scattering term, if one expands $\phi_i(\vec{r}_{12})(r_{12}-z_{12})^{i\eta_+}$ around $\vec{r}_2=0$ and keeps only the zeroth-order term, then one will obtain the Glauber-Ochkur approximation of this term. This approximation form yields a rather poor result in comparison to the exact form. A better approximation due to Franco and Halpern[7] can be achieved by expanding $\phi_i(\vec{r}_2)$ around $\vec{r}_1$ (instead of zero), i.e.,

$$r_2^{-1}\phi_i(\vec{r}_2)=\vec{r}_1^{\,-1}\phi_i(\vec{r}_1)+(\vec{r}_2-\vec{r}_1)\cdot\vec{\nabla}_{\vec{r}_1}[r_1^{-1}\phi_i(\vec{r}_1)]+\cdots\;. \tag{6}$$

If only the first-order term of the expansion is kept, one obtains the following closed form for $t^{(\pm)}(r_2)$ [with $\phi_f^*(\vec{r})\phi_i(\vec{r})=D_{\beta\vec{\lambda}}^{(N,+)}(e^{-(\beta r+i\vec{\lambda}\cdot r)})$],

$$\begin{aligned}t^{(\pm)}(r_{2,1})=&-16\pi^2k_\mp^{-3}k_\pm\exp(\pi\eta_\pm/2)\pi\eta_\pm\sinh^{-1}(\pi\eta_\pm)k_\mp^{-i\eta_\pm}\\ &\times D_{\beta\vec{\lambda}}^{(N,\pm)}\{[\beta_\mp i(\vec{q}-\vec{\lambda})\cdot\hat{z}]^{-i\eta_\pm}[\beta^2+(\vec{q}-\vec{\lambda})^2]^{i\eta_\pm-1}\}_{\vec{\lambda}=0}\;.\end{aligned} \tag{7}$$

The corresponding expression for 1s-1s e-H scattering are found with $D_{\beta\vec{\lambda}}^{(N,\pm)}=1/\pi$ and $\beta=2$.

TABLE I. Values of electronic- and nuclear-scattering terms of the "exact" Glauber exchange amplitude ($\hat{z}\perp\vec{q}$) in 1*s*-1*s* *e*-H collision.

Angles in degrees	Energy = 100 eV Real parts Nuclear	Energy = 100 eV Real parts Electronic	Energy = 100 eV Imaginary parts Nuclear	Energy = 100 eV Imaginary parts Electronic	Energy = 1600 eV Real parts Nuclear	Energy = 1600 eV Real parts Electronic	Energy = 1600 eV Imaginary parts Nuclear	Energy = 1600 eV Imaginary parts Electronic
1	0.588(−1)[a]	−0.352	−0.144(−1)	0.124	0.164(−3)	−0.186(−1)	−0.288(−4)	0.379(−2)
10	0.565(−1)	−0.319	−0.130(−1)	0.103	0.896(−4)	−0.535(−2)	−0.120(−4)	0.555(−3)
40	0.368(−1)	−0.109	−0.380(−2)	−0.206(−2)	0.143(−4)	−0.802(−4)	−0.192(−5)	−0.593(−4)
80	0.200(−1)	−0.199(−1)	−0.190(−2)	−0.161(−1)	0.590(−5)	−0.310(−5)	−0.121(−5)	−0.187(−4)

[a]Numbers in parentheses represent powers of ten.

TABLE II. Values of electronic- and nuclear-scattering terms in various approximation schemes of the Glauber exchange amplitude ($\hat{z}\perp\vec{q}$) of elastic 1*s*-1*s* *e*-H collision at 100 eV. [Value of the nuclear-scattering term in the Glauber-Ochkur approximation is constant and equal to 0.312(−1).]

Angles in degrees	Ochkur Real	Glauber-Ochkur Real	Glauber-Ochkur Imaginary	Franco-Halpern (electronic-scattering term) Zeroth order Real	Franco-Halpern (electronic-scattering term) Zeroth order Imaginary	Franco-Halpern (electronic-scattering term) First order Real	Franco-Halpern (electronic-scattering term) First order Imaginary	Franco-Halpern (nuclear scattering) Real	Franco-Halpern (nuclear scattering) Imaginary
1	−0.272(+0)	−0.248(+0)	−0.299(−2)	−0.381(+0)	0.115(+0)	−0.327(+0)	0.119(+0)	0.530(−1)	−0.596(−2)
10	−0.244(+0)	−0.222(+0)	−0.929(−2)	−0.344(+0)	0.933(−1)	−0.299(+0)	0.944(−1)	0.503(−1)	−0.465(−2)
40	−0.787(−1)	−0.652(−1)	−0.273(−1)	−0.113(+0)	−0.103(−1)	−0.115(+0)	−0.646(−3)	0.285(−1)	0.334(−2)
80	−0.167(−1)	−0.772(−2)	−0.140(−1)	−0.186(−1)	−0.177(−1)	−0.310(−1)	−0.170(−1)	0.121(−1)	0.517(−2)

Some of the results of these calculations are tabulated in Tables I and II. It is found that at intermediate energy (100 eV), the values of both real and imaginary parts of the nuclear-scattering term are comparable to those of the electronic-scattering term at the larger but still interesting angles. Even at high energy (1600 eV) at the largest angles shown, the magnitude of the two sets of values (nuclear and electronic scatterings) are of the same order while their signs are opposite. The magnitude of the nuclear-scattering term becomes more and more significant (in comparison to the electronic-scattering term) when the scattering energy gets lower and lower. It is, therefore, concluded that this nuclear-scattering term contributes quite significantly to the eikonal exchange amplitude and cannot thereby be neglected. Thus, any approximation scheme which bypasses the nuclear-scattering term completely cannot provide a good approximate value for the exact eikonal exchange amplitude. We also believe that it would be more appropriate to make the comparison between the approximate values of the electronic- and nuclear-scattering terms with their exact ones, separately. This has not been done in the literature. Among the approximate forms considered, the ones by Halpern and Franco[6,7] yield a remarkably good agreement with the corresponding exact electronic- and nuclear-scattering terms if one sticks to the region of small-scattering angles and high-scattering energy (which the Glauber approximation is essentially designed for). In practice, the Glauber approximation in atomic collision seems to work reasonably well at much lower energies as well as at larger scattering angles. However, under these circumstances, the degree of agreement of the approximate values of Halpern and Franco with the exact Glauber ones decreases somewhat. The inclusion of the first-order correction of the electronic-scattering term in the Halpern-Franco approximation improves the values of the imagniary part at smaller scattering angles, but does not seem to improve very much the values of its real part. Note that the values of the Halpern-Franco approximate form for the electronic-scattering term, as expected, agree better with the exact values of the electronic-scattering term than with those of the total eikonal exchange amplitude. This is merely the reflection of the fact that the values of the nuclear-scattering term are quite large and thereby non-negligible, especially at lower intermediate energies. Although other approximate forms considered here provide a very poor agreement with the exact electronic- and nuclear-scattering terms, their values all indicate that the magnitude of the nuclear-scattering term is quite significant in comparison to that of the electronic-scattering term.

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