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Comment on the Glauber-Ochkur exchange amplitude*

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It is pointed out that the reason originally used by Ochkur to justify the need for performing the Ochkur reduction no longer remains valid in the Glauber case.

In recent years, there have been a lot of research activities going on in the application of the Glauber eikonal theory[1] to the study of atomic and molecular collisions.[2] In all these Glauber calculations, however, the success of the eikonal method appears to fail gradually at lower scattering energy. For instance, at an energy lower than 30–40 eV in an electron-atom scattering, the integrated cross sections calculated with various eikonal models all seem not to fit well with experimental data.[2] This failure could be viewed as due to the unsuitability of the eikonal method at low energy, but also probably as due to the neglect of the exchange effect which may become more significant at lower energy and, thereby, no longer negligible. The reason for the neglect of the exchange effect in the Glauber calculations is mainly because one does not at that time know exactly how to reduce the dimension of the integral involved in the calculation to a lesser order. On the other hand, some processes such as the $1\,^1S$-$2\,^3S$ in e-He scattering can occur only through the exchange of electrons. Thus, a simple method of calculation of the Glauber exchange effect must definitely be found.

Obviously, one thinks of extending to the Glauber case the well-known Ochkur method of reduction[3] which was initially designed to obtain for the first-order Born-Oppenheimer amplitude a reduced form free from terms of higher order in k_0^{-1}. These terms will make this amplitude become meaningless when extrapolated to the low-energy domain. The extension of the Ochkur reduction to the Glauber exchange amplitude has been carried out, and a reduced form without any discrepancy for "post" and "prior" elastic scattering has been obtained.[4] We wish, however, to point out in this note that the logic used by Ochkur to back up the need for the performance of this kind of reduction no longer remains valid for the Glauber case. Before doing so, it is preferable to mention that recently, through an elegant application of a similar method used by Gau and Macek[5] for the direct scattering amplitude, Madan[6] and then Foster and Williamson[7] have been successful in transforming the Glauber exchange amplitude to an exact simplified expression which can easily be accessed to numerical computation. These authors, however, still use the so-called "Glauber-Ochkur" amplitude in a part of calculations in their works. We, therefore, believe that it is still worthwhile to raise this point here.

To start with, one should be reminded again that the Ochkur's reduction was initially introduced just to remove terms of the *first-order* scattering amplitude which are considered as unwanted at low energy. The reason used by Ochkur to justify the need for performing this kind of reduction may be summarized as follows (see the introductory part of Ref. 3 for details). It is well known that the Born-Oppenheimer amplitude is the first-order term in the Born series of the exchange amplitude. By considering the Born-Oppenheimer amplitude as an approximate form for the exchange scattering, one has already neglected all these higher-order Born terms. As a result, terms of higher-order in k_0^{-1} have been cut off from the exact amplitude through the drop of these higher-order Born terms. Ochkur,[3] however, pointed out that the Born-Oppenheimer amplitude actually still contains higher-order terms in k_0^{-1}, which, within the first-order approximation theory, will make the exchange amplitude become meaningless when extrapolated to lower-energy domain. It is only because of this reason that Ochkur has proposed to perform a reduction of the Born-Oppenheimer amplitude in order to remove completely the remnant of higher-order terms in k_0^{-1} still contained in this first-order amplitude. This kind of reduction is later known as the Ochkur reduction.

Obviously, this idea is perfectly logical and valid for an exchange amplitude of *first-order approximation only*. In the Glauber case, however, the exchange amplitude is now composed of scattering amplitudes of higher orders. As a result, terms of higher orders in k_0^{-1} are always contained in the exchange amplitude through these higher-order scattering terms. Since the purpose of the Ochkur reduction is just to eliminate superfluous higher-order terms in k_0^{-1} still existing in the *first-order* scattering amplitude, it is, therefore, quite obvious that there is not any more sound basis for the need of performing the same kind of reduction here. In other words, one could ask the following question: Within the spirit of the Ochkur reduction, why does one need to perform this kind of reduction for the Glauber exchange amplitude at all? As a matter of fact, one can easily show that if the Ochkur reduction is performed for the Glauber exchange amplitude, the reduced form obtained still implicitly contains terms of higher-order in k_0^{-1}.

The well-known Glauber exchange amplitude for the "post" scattering of e-H is

$$f_{0n}^{\text{post}}(r_{12}) = -\frac{1}{2\pi}\int d\vec{r}_1\, d\vec{r}_2\, \varphi_n^*(\vec{r}_2) \times e^{i\vec{q}\cdot\vec{r}}\left(-\frac{1}{r_2}+\frac{1}{r_{12}}\right)\varphi_0(\vec{r}_1)e^{i\vec{k}_0\cdot\vec{r}_{12}}e^{-i\chi} \tag{1}$$

where

$$e^{-i\chi} = \left(\frac{r_{12}+z_{12}}{r_2+z_2}\right)^{-i\eta_0}\frac{(\vec{b}_2-\vec{b}_1)^2}{b_2^2}, \tag{2}$$

where $Z_{12}=Z_1-Z_2$, $r_{12}=|\vec{r}_1-\vec{r}_2|$, and $\eta=k_0^{-1}$. It has been shown[4] that if only the first-order term of the so-called Ochkur expansion[3] is kept, the Glauber exchange amplitude for the "post" scattering of e-H is reduced to

$$f_{\text{post}}^{(1)}(r_{12}) = -\frac{2}{k_0^2}e^{i\eta_0\ln\epsilon} \times\int d\vec{r}_1\, e^{i\vec{q}\cdot\vec{r}_1}\varphi_n^*(\vec{r}_1) \times\varphi_0(\vec{r}_1)\exp\{-i\eta_0\ln[r_1(1-\cos\theta_1)]\}. \tag{3}$$

φ_0 and φ_n are initial and final states of the hydrogen atom. Other notations are as usual.

This reduced exchange amplitude has an indeterminate phase, but one may treat it as a free parameter and when $|f_{\text{post}}^{(1)}|^2$ is calculated, this indeterminate phase just disappears in the process of calculation. Thus, one may ignore the factor $e^{i\eta_0\ln\epsilon}$, although when this amplitude is used to estimate the contribution of the exchange effect in an atomic process where a direct amplitude is already present, one may run into the problem of choosing the phase for this reduced form. At first sight, this reduced amplitude seems to be of order k_0^{-2} only, but a close analysis of this expression shows that this is actually not the case. In fact, one should always bear in mind that the Ochkur expansion was introduced at small k_0^{-1} just for the purpose of making terms of different orders in k_0^{-1} appear explicitly in a series so that one can then drop higher-order terms from the exchange amplitude since they will eventually become "bad terms" at low energy, if left untouched. However, with small k_0^{-1} and conformed to this procedure, there is no reason why one cannot again expand $\exp\{-i\eta_0\ln[r_1(1-\cos\theta_1)]\}$ to obtain

$$\exp\{-i\eta_0\ln[r_1(1-\cos\theta_1)]\} = 1 - i\eta_0\ln(r_1-z_1)+[(-i\eta_0)^2/2!]\ln^2(r_1-z_1)+\cdots. \tag{4}$$

When this expansion is replaced in Eq. (3) for $\exp[-i\eta_0\ln(r_1-z_1)]$, one obtains again a series in inverse powers of k_0 for $f_{\text{post}}^{(1)}$

$$f_{\text{post}}^{(1)} \approx -\frac{2}{k_0^2}e^{i\eta_0\ln\epsilon}\left(\int d\vec{r}_1\,\varphi_n^*(\vec{r}_1)e^{i\vec{q}\cdot\vec{r}_1}\varphi_0(\vec{r}_2) - \frac{i}{k_0}\int d\vec{r}_1\,\varphi_n^*(\vec{r}_1)e^{i\vec{q}\cdot\vec{r}_1}\varphi_0(\vec{r}_1)\ln(r_1-z_1) - \frac{1}{k_0^2}\int d\vec{r}_1\,\varphi_n^*(\vec{r}_1)e^{i\vec{q}\cdot\vec{r}_1}\varphi_0(\vec{r}_1)\ln^2(r_1-z_1)+\cdots\right). \tag{5}$$

If one believes that at low energy, higher-order terms in the Ochkur series would cause trouble for the calculation of exchange effect (and this is why one needs to remove them from the exchange amplitude), then to be consistent one must abandon all these terms of order higher than k_0^{-2} in the latter expansion as well. But if one does so, the reduced Glauber exchange amplitude simply becomes the conventional Ochkur term obtained previously.[3] The presence of higher-order terms in k_0^{-1} in the reduced Glauber-Ochkur form clearly violates the spirit of the Ochkur's method which, as evidenced by our discussions above, is only valid for exchange amplitudes of first order of approximation.

In summary, while in the Born-Oppenheimer case, one needs to perform the Ochkur reduction in order to remove terms of higher orders in k_0^{-1} which will become bad when this amplitude is extrapolated to the low-energy domain, in the Glauber case however, because of the permanent presence of these higher-order terms in k_0^{-1} in this amplitude (these terms remain present there even after the Ochkur reduction has been performed), there cannot be any more sound reason why we still need to perform the Ochkur reduction here at all. Beside the lack of a clear basis for the performance of the Ochkur reduction for the Glauber exchange amplitude, if one analyzes closely all the higher-order terms of the Ochkur expansion, one will find that they are all divergent. On the other hand, if the Ochkur expansion is not used at all for the reduction, the reduced form, as was obtained, obviously cannot be regarded as the result of a sound approximation. Because of these two deficiencies, we believe that one should seriously reconsider the application of the Ochkur reduction to the Glauber amplitude or to any other kind of exchange amplitude which is composed of higher orders of scattering. Perhaps, one should only use the exact simplified form of the eikonal exchange amplitude obtained in a recent fine work by Madan[6] and by Foster and Williamson[7] for the estimate of exchange effect in the calculations of atomic scattering within the eikonal theory.

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[2]See for instance a clear and complete review article by E. Gerjuoy and B. K. Thomas, Rep. Phys. 37, 1345 (1974), and references therein.

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[6]R. N. Madan, Phys. Rev. A 12, 2631 (1975).

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