Eikonal exchange amplitudes and the inclusion of exchange in elastic (e, H) scattering

Rabinder N. Madan
Department of Physics, North Carolina A & T State University, Greensboro, North Carolina 27411
(Received 7 July 1975)

The six-dimensional integral involved in the eikonal (e,H) rearrangement amplitudes is reduced to a two-dimensional form. When the Glauber condition $\vec{q}\cdot\hat{z}=0$ is imposed, there is no post-prior discrepancy in the elastic rearrangement amplitudes. The Ochkur reduction of the rearrangement amplitudes is obtained in a closed form. Application is made to the inclusion of the exchange effect in the Glauber calculation of elastic (e,H) scattering at 50 eV.

In an earlier paper[1] (hereafter referred to as paper I) this author had given the "post" and "prior" forms of the rearrangement amplitudes for the process $e_1^- + \mathrm{H}(i) \to e_2^- + \mathrm{H}(f)$. For an infinitely heavy proton, the eikonal approximation to the prior on-shell exchange amplitude is given by

$$g_{fi}^{(-)} = -\frac{1}{2\pi}\int d\vec{r}_1 d\vec{r}_2 \exp(-i\vec{k}_f\cdot\vec{r}_2)\,\phi_f^*(\vec{r}_1)\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right) \times \exp(i\vec{k}_i\cdot\vec{r}_1)\,\phi_i(\vec{r}_2)\left(\frac{\vec{r}_2+\hat{z}\cdot\vec{r}_2}{r_{12}+z_{21}}\right)^{-i\eta_f}, \tag{1}$$

where $\eta_f = 1/k_f$ and $z_{21}=\hat{z}\cdot(\vec{r}_2-\vec{r}_1)$. $\phi_i(\vec{r}_2)$ is the wave function of the initial ground state of the hydrogen atom and $\phi_f(\vec{r}_1)$ of the final bound hydrogenic state. The multidimensional integral in Eq. (1) occurs in the eikonal approximation to several other atomic rearrangement processes, like $e^+ + \mathrm{H} \to \mathrm{H}^+ + (e^+e^-)$, $\mathrm{H}^+ + \mathrm{H} \to \mathrm{H} + \mathrm{H}^+$, and, in general, (heavy charged particle) + (atom) → (atom) + (heavy charged particle), with differences in kinematics and dimensions.

We are able to reduce the above integral to a compact two-dimensional form for numerical integration. To evaluate the integral for exchange excitation to any arbitrary state of the hydrogen atom, we replace $\phi_f^*(\vec{r}_1)$ by $N_f\exp(-\beta r_1 + i\vec{\lambda}\cdot\vec{r}_1)$ and the initial state $\phi_i(\vec{r}_2)$ by $N_i\exp(-\mu r_2)$. The wave function of any arbitrary hydrogenic state can be generated by operating with a differential operator $\mathfrak{D}(\beta,\vec{\lambda})$ with $\vec{\lambda}$ set equal to zero, ultimately. Employing a parametrization technique [demonstrated below for the integral in Eq. (3)] the imaginary exponent of the factor $r_{12}+z_{21}$ is separated. Then one is able to replace the factors containing $\vec{r}_{21}$ by their Fourier transform. The integrations over $\vec{r}_1, \vec{r}_2$, and the intermediate momentum are easily carried out, and one obtains

$$g_{fi}^{(-)} = i\pi\eta_f 2^{3-i\eta_f} N_i N_f\,\mathfrak{D}(\beta,\vec{\lambda})\left\{\int_0^\infty dt\, t^{-i\eta_f}\int_0^1 du\left[t^{-1}\frac{d}{d\beta}\frac{d}{d\rho^2}-2(1-u)\left(\frac{d}{d\rho^2}\right)^2\right] \times[(\mu+\rho)^2+Q^2]^{i\eta_f-1}(\mu+\rho-i\vec{Q}\cdot\hat{z})^{-i\eta_f}\right\}_{\vec{\lambda}=0}, \tag{2}$$

where

$$\rho^2 = \beta^2 u + (\vec{k}_i+\vec{\lambda})^2 u - [(\vec{k}_i+\vec{\lambda})u + it(1-u)\hat{z}]^2,$$

$$\vec{Q} = -\vec{q} + \vec{k}_i(1-u) - it(1-u)\hat{z} - \vec{\lambda}u.$$

The post form of the eikonal rearrangement amplitude leads to a similar reduction and can be obtained from Eq. (2) by changing $\eta_f \to \eta_i$, $\mu \leftrightarrow \beta$ and $\vec{k}_i + \vec{\lambda} \leftrightarrow \vec{k}_f$ in all terms except the operator $\mathfrak{D}(\beta,\vec{\lambda})$. For the elastic rearrangement case $\mu=\beta=1$, $N_i = N_f = 1/\sqrt{\pi}$, and $\mathfrak{D}(\beta,\vec{\lambda})=1$. For this case $|\vec{k}_i| = |\vec{k}_f| = k$, $\eta_i = \eta_f = \eta$, and it can be easily verified that, with the condition $\vec{q}\cdot\hat{z}=0$ imposed, which implies $\hat{z} = (\vec{k}_i+\vec{k}_f)/|\vec{k}_i+\vec{k}_f|$, the post and the prior forms of Eq. (2) are identical, thus there is *no* discrepancy between the *two* forms of the Glauber exchange amplitudes.

We have employed Eq. (2) to include the exchange effect in the Glauber "straight-line" calculation[2] of elastic (e, H) scattering at $E = 50$ eV. The symmetrized differential cross section is at most 12% above the Glauber straight-line value for forward scattering angles. Typically at $\theta = 30°$, the symmetrized value is 9% above the Glauber, and at $\theta = 45°$, it is 12% above the Glauber. Still, the result obtained remains much below the experimental data of Lloyd *et al.*[3]

In view of the above, one might conclude that the Glauber exchange approximation is essentially valid at $k_i \gg 1$ a.u., and as the exchange contribution to the collision cross section decreases rapidly with the increase in collision energy, the extrapolation of the Glauber exchange amplitude, Eq. (2) with $\vec{q}\cdot\hat{z}=0$, to lower energies (typically $E=50$ eV, $k_i=1.917$ a.u.) is not physically valid. One possible way around this difficulty is to follow the Ochkur[4] idea. The Ochkur term of the prior form of the eikonal exchange amplitude, Eq. (1), has been obtained in paper I [Eq. (2.10)] and is given by

$$g^{(-)}(r_{12}) = -\frac{2}{k_i^2}\lim_{\epsilon\to 0}\exp(i\eta_f \ln\epsilon) \times \int d\vec{r}\,\phi_f^*(\vec{r})\phi_i(\vec{r})\exp(i\vec{q}\cdot\vec{r})(r+\vec{r}\cdot\hat{z})^{-i\eta_f}. \tag{3}$$

To demonstrate the parametrization technique involved in the reduction of the integral in Eq. (1) to the two-dimensional form of Eq. (2), we perform the integration in Eq. (3) explicitly. With no initial restriction on the spatial direction of the momentum transfer $\vec{q}$, we are able to reduce Eq. (3) to a simple algebraic expression. The imaginary exponent of the factor $r+\vec{r}\cdot\hat{z}$ is separated out by employing a representation of the beta function,[5] and Eq. (3) becomes

$$g^{(-)}(r_{12}) = -\frac{2}{k_i^2}\lim_{\epsilon\to 0}\exp(i\eta_f\ln\epsilon)N_iN_f\mathfrak{D}(\beta,\vec{\lambda})[B(i\eta_f,1-i\eta_f)]^{-1} \times\left(\int d\vec{r}\exp[i(\vec{q}+\vec{\lambda})\cdot\vec{r}-(\mu+\beta)r]\int_0^1 ds\, s^{i\eta_f-1}(1+sr+\vec{r}\cdot\hat{z}s)^{-1}\right)_{\vec{\lambda}=0}. \tag{4}$$

Reversing the order of integrations, the integration over $\vec{r}$ is performed by introducing a parameter t and the integration over s is carried out by employing the same representation of the beta function as in Eq. (4), and is a reversal of the operation introduced at that stage. One gets

$$g^{(-)}(r_{12}) = 2^{3-i\eta_f}\frac{\pi}{k_i^2}\lim_{\epsilon\to 0}\exp(i\eta_f\ln\epsilon)N_iN_f\,\mathfrak{D}(\beta,\vec{\lambda})\frac{d}{d\beta}\bigg([(\mu+\beta)^2+(\vec{q}+\vec{\lambda})^2]^{i\eta_f-1}[\mu+\beta+i\hat{z}\cdot(\vec{q}+\vec{\lambda})]^{-i\eta_f} \times\int_0^\infty dt\,t^{-i\eta_f}\exp(-t)\bigg)_{\vec{\lambda}=0}. \tag{5}$$

The integral over t is recognized to be the Euler integral of the gamma function $\Gamma(1-i\eta_f)$. Instead of employing the integral representation of the beta function to separate the imaginary exponent in Eq. (3), one could have employed the Euler integral of the gamma function with the same effect. But a noteworthy feature about employing the beta function is that the step is reversed during the course of the evaluation. The Ochkur term of the post form of the eikonal exchange amplitude can be obtained from Eq. (5) by changing $\eta_f\to\eta_i$ and $\hat{z}\to-\hat{z}$. As an application of Eq. (5), we evaluate the differential exchange cross section for elastic (e, H) collisions and get

$$|g^{(\pm)}(r_{12})|^2 = \frac{256}{k_i^4}(4+q^2)^{-4}\left(\frac{2\mp i\vec{q}\cdot\hat{z}}{2\pm i\vec{q}\cdot\hat{z}}\right)^{i\eta}\frac{\pi\eta}{\sinh\pi\eta}\left(4+4\eta^2+\eta^2\frac{(4+q^2)^2}{16+4(\vec{q}\cdot\hat{z})^2}-\frac{4\eta^2\mp 2\eta\vec{q}\cdot\hat{z}}{4+(\vec{q}\cdot\hat{z})^2}(4+q^2)\right), \tag{6}$$

where the upper and lower signs refer to the post and prior forms, respectively. With the Glauber condition $\vec{q}\cdot\hat{z}=0$ imposed, there is no post-prior discrepancy in the Ochkur reduced eikonal cross section in Eq. (6); otherwise, it does exist. The numerical results obtained from Eq. (6) are identical with our earlier work in paper I. We hope that this derivation of the Ochkur reduced eikonal exchange amplitudes will clear the understanding about the choice of direction of $\vec{q}$.[6]

There are several justifications for the Glauber choice $\vec{q}\cdot\hat{z}=0$ for direct collisions.[7] We find that there are some physical justifications for the choice $\vec{q}\cdot\hat{z}=0$ in rearrangement collisions also. There is *no* post-prior discrepancy in the Glauber exchange amplitudes, and of course the same result carries through in the Ochkur reduction. Furthermore, the Ochkur-reduced Glauber exchange amplitudes are invariant under the reversal of directions of $\vec{k}_i$ and $\vec{k}_f$.

The indeterminate phase in Eq. (6) does not play any role, in case one is interested, in optically-forbidden exchange-allowed collisions, but it makes the expression unsuitable for the inclusion of exchange effect in calculations of symmetrized differential cross sections. But we notice that in the limit $\eta_f=0$, the indeterminate phase in Eq. (5) vanishes and the expression reduces to the Ochkur approximation of the Born-Oppenheimer amplitude. This amplitude is real and is known to give meaningful results at $E=50$ eV. Thus to include the exchange effect in the Glauber "straight-line" approximation in the simplest possible way, the limiting value of Eq. (5) at $\eta_f=0$ appears to be the only choice. We have done this calculation and the result is displayed in Fig. 1.

In Fig. 1, we have also plotted for comparison the differential cross section in the Glauber straight-line approximation, the experimental points, and a calculation in the first Born approximation with the exchange effect included by the Ochkur term. The inclusion of the exchange effect at $E = 50$ eV leads to a considerable improvement in the Glauber approximation. For instance, at scattering angle $\theta = 30°$ the Glauber with exchange is 66% above the Glauber, and at $\theta = 50°$ it is 71% above. The Glauber with exchange is in agreement with the experimental points, within the normalization and statistical errors quoted in Ref. 3, for angles $\leq 50°$. In the comparison of the experimental data with various theories, Teubner *et al.*[3(b)] find that the close-coupling calculation agrees very well with the measured values for angles greater than 50°. We are able to make the same observation with reference to our calculation of the symmetrized differential cross section in the first Born approximation with Ochkur exchange. We

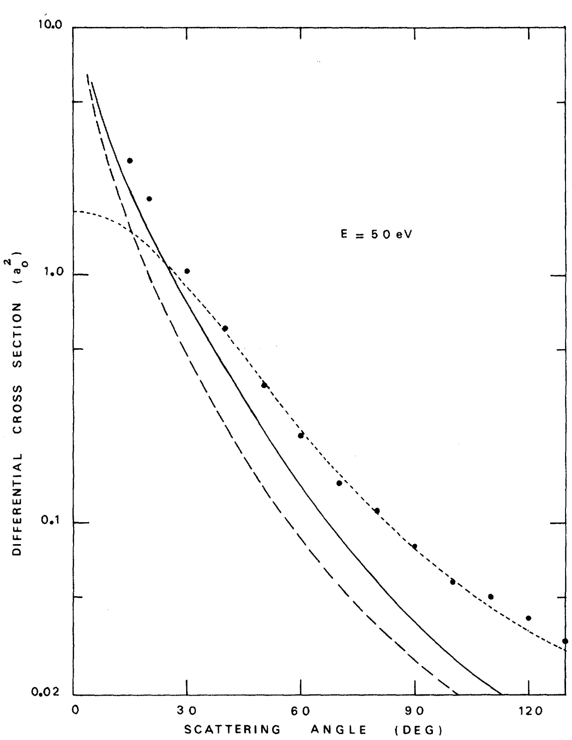

FIG. 1. Differential cross sections for elastic e^--H collisions. Dots are experimental points of Ref. 4; solid line denotes Glauber straight-line with Ochkur exchange; long-dashed line, Glauber straight line of Franco (Ref. 2); short-dashed line, first Born approximation with Ochkur exchange.

notice that the result in this calculation is almost identical with the close coupling result for angles $>15°$ and $<130°$. To see this, one must compare the plot of the close-coupling calculation in Fig. 2 of Teubner *et al.*[3(b)] with our plot in Fig. 1. It is a noteworthy result in the sense that the first Born approximation with Ochkur exchange is a trivial calculation and can be done by hand, whereas the close-coupling (1*s* -2*s* -2*p* projection) calculation of Burke *et al.*[8] is extremely arduous.

From the experimental data of Teubner *et al.*, Gerjuoy and Thomas[9] estimate the integrated elastic e^--H(1*s*) cross section (σ) at 50 eV to be $1.20\pi a_0^2$. For comparison, we have calculated the integrated cross sections at 50 eV, and the values are as follows: Glauber straight-line approximation, $0.598\pi a_0^2$; Glauber straight-line symmetrized with Glauber exchange, $0.609\pi a_0^2$; Glauber straight-line symmetrized with Ochkur exchange, $0.669\pi a_0^2$; first Born approximation symmetrized with Ochkur exchange, $0.908\pi a_0^2$. The integrated cross section in the close-coupling method is known to be $0.80\pi a_0^2$. Thus the first Born symmetrized value is in better agreement with the estimated experimental value than the close-coupling integrated cross section at 50 eV.

One must mention the eikonal-Born series method of Byron and Joachain.[10] A critical discussion on the comparison of this method with the Glauber approximation is available in the review article of Gerjuoy and Thomas.[9] This method includes the exchange effect by the Ochkur approximation and the prediction of this method in the case of elastic (*e*, H) scattering is in good agreement with the experimental data *only* at $E = 50$ eV. Our calculation shows that the inclusion of exchange by the Ochkur term makes a significant correction to the Glauber calculation and also to the first Born approximation at lower intermediate energies. To make corrections to the Glauber at higher intermediate energies, it would be worthwhile to look at the next term in the eikonal expansion of the amplitude.

In conclusion, we make the following comments: The six-dimensional integral involved in the eikonal (*e*, H) rearrangement amplitude can be reduced to a two-dimensional form which can be accurately evaluated numerically. For the case that the Glauber condition on the momentum transfer, e.g., $\vec{q} \cdot \hat{z} = 0$, is imposed, there is *no* post-prior discrepancy in the elastic rearrangement amplitudes. For the inelastic rearrangement amplitudes the discrepancy does exist, but diminishes with the increase in projectile energy. Ochkur reduction of the eikonal rearrangement amplitudes is obtained in a closed form and would be useful for calculations of optically-forbidden exchange allowed transitions due to electron impact at the lower values (~ 50 eV) of intermediate energies. To include the exchange effect in Glauber straight-line approximation, it is found that one must consider the Ochkur approximation to the Born-Oppenheimer amplitude. This leads to a substantial correction in the Glauber calculation. One may note that at $E=50$ eV, the symmetrized differential cross section in the first Born approximation, with exchange included by the Ochkur term, is almost identical with the close-coupling result of Burke *et al.*[8] for angles $>15°$ and $<130°$, and the integrated cross section is closer to the experimental value than the close-coupling result.

[1]R. N. Madan, Phys. Rev. A 11, 1968 (1975); this paper will henceforth be referred to as paper I. In Eq. (2.9) of paper I, we should have had z_{21} instead of z_{12}.
[2]V. Franco, Phys. Rev. Lett. 20, 709 (1968).
[3](a) C. R. Lloyd, P. J. O. Teubner, E. Weigold, and B. R. Lewis, Phys. Rev. A 10, 175 (1974); (b) the results at incident energy $E=50$ eV were reported earlier by P. J. O. Teubner, C. R. Lloyd, and E. Weigold, J. Phys. B 6, L134 (1973).
[4]V. I. Ochkur, Zh. Eksp. Teor. Fiz. 45, 734 (1963) [Sov. Phys.—JETP 18, 503 (1964)].
[5]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, Natl. Bur. Std. Spec. Pub. No. 55 (U.S. GPO, Washington, D.C., 1964), formula 6.2.1.
[6]A. Tenney and A. C. Yates, Chem. Phys. Lett. 17, 324 (1972). These authors performed the integration in Eq. (3) by choosing the polar axis along $\vec{q}$ (as in the Born approximation, and obtained a post-prior discrepancy for the elastic case). We have discussed their work in paper I. One can get the result of Tenney and Yates from Eq. (6) by choosing $\vec{q}\cdot\hat{z}=q$, but there is no physical basis for this choice.
[7]R. J. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1959), Vol. I.
[8]P. G. Burke, H. M. Schey, and K. Smith, Phys. Rev. 129, 1258 (1963).
[9]E. Gerjuoy and B. K. Thomas, Rep. Prog. Phys. 37, 1345 (1974).
[10]F. W. Byron, Jr., and C. J. Joachain, J. Phys. B 7, L212 (1974); Phys. Rev. A 8, 1267 (1973).