PHYSICAL REVIEW A VOLUME 19, NUMBER 4 APRIL 1979

High-energy higher-order Born approximations: Theoretical development

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(Received 21 August 1978)

The second and third terms of the generalized Born series are analyzed in an attempt to gain a series approximation to the differential cross section, valid through $O(1/k^2)$, which treats all Born terms analogously. The resulting expressions for the second and third Born terms, derived from assumptions similar to those of Glauber theory, are compared with other analyses for the case of small-angle elastic scattering of electrons by hydrogen atoms. A most notable result is that, in addition to the Glauber-like term, there is a second term of $O(1/k^2)$ which contributes to the real part of the third Born term. In addition, the angular range of maximum validity of the Glauber assumptions is established for inelastic collisions.

I. INTRODUCTION

In recent years numerous calculations, corresponding to nearly as many theoretical descriptions, have been made of amplitudes of high-energy collisions of charged particles with atomic targets. Because of the enormous complexity in describing and predicting the results of associated experiments, most of the cited works have had as their objective the determination of accurate and computationally feasible theoretical procedures. Included among the more successful methods are variations of traditional impact-parameter studies,[1] the simplified second Born approximation,[2] Glauber[3] and modified Glauber[4] approaches, Coulomb-projected Born calculations,[5] and the eikonal-Born series approach.[6,7]

Two factors provide the motivation for the present study—aimed at suggesting yet another description of high-energy collisions. The first is prompted by the work—and success—of Byron and Joachain in their eikonal-Born series approach to medium- to high-energy electron-atom collisions, and constitutes an extension of earlier work of the present author.[8] Without in any way implying criticism of the eikonal-Born series work, the primary purpose of the current analysis is to develop an alternative high-energy expansion of the differential scattering cross section in terms of reciprocal powers of k_i (where $\hbar\vec{k}_i$ is the momentum of the incident particle), through $O(k^{-2})$, which is computationally tractable, yet derived from analogously treated second and third Born terms. A second consideration has been the suggestion of anomalous behavior of the small-angle high-energy differential cross secion in electron-atom collisions.[9]

In Sec. II the well-known generalized Born series description of the collision process is introduced and then transformed into a more convenient form. Section III concerns the development of approximate formulas through a "partial" expansion of the free-particle Green's function. Section IV applies the results of Sec. III to an analysis of the second and third Born terms. Section V contains a brief discussion of limiting forms of present estimates of the second and third Born terms as applied to the elastic scattering of electrons by hydrogen atoms.

II. EXACT FORMULAS

In this and the remaining sections, attention is confined to the specific case of an electron colliding with a neutral N-electron atom. The results nonetheless are easily generalizable to other collision types. Additionally, though the analysis proceeds similarly for the exchange amplitude, only the direct amplitude is considered below.

Atomic units are used throughout and, correspondingly, $\vec{k}_i$, $\vec{k}_f$, and $\vec{q}=\vec{k}_i-\vec{k}_f$ will denote, respectively, the initial and final momenta of the scattering electron, and the momentum transferred to the target as a result of the collision. Considering the position of the atomic nucleus as the coordinate origin, the space ($\vec{r}$) and spin (σ) coordinates of the incident and bound electrons will be written as $\vec{\tau}\equiv(\vec{r},\sigma)$, though spin integrations are generally suppressed.

The generalized Born series for the scattering amplitude, which describes the collision of an electron with an N-electron atom with initial and final atomic states and energies given by (ψ_i,E_i) and (ψ_f,E_f), respectively, is written[10]

$$f_{i\to f}=\sum_{n=1}^{\infty}f_{i\to f}^{(n)}, \tag{2.1}$$

where

$$f_{i\to f}^{(1)}=-\frac{1}{2\pi}\int d\vec{r}_0\, e^{i\vec{q}\cdot\vec{r}_0}V_{fi}(\vec{r}_0) \tag{2.2a}$$

and

$$f_{i\to f}^{(n)}=\frac{(-2)^{n-2}}{\pi}\sum_{m_1,m_2,\ldots,m_{n-1}}\int d\vec{r}_0\, e^{-i\vec{k}_f\cdot\vec{r}_0}V_{fm_1}(\vec{r}_0)\int d\vec{r}_0^{\,1}\,G_{m_1}(\vec{r}_0-\vec{r}_0^{\,1})V_{m_1m_2}(\vec{r}_0^{\,1})\cdots\int d\vec{r}_0^{\,n-1}\,G_{m_{n-1}}(\vec{r}_0^{\,n-2}-\vec{r}_0^{\,n-1})\times V_{m_{n-1}i}(\vec{r}_0^{\,n-1})e^{i\vec{k}_i\cdot\vec{r}_0^{\,n-1}}\,. \tag{2.2b}$$

In the preceding,

$$V_{nm}(\vec{r}_0)=\langle\psi_n(\vec{r}_1,\ldots,\vec{r}_N)\,|\,V(\vec{r}_0,\vec{r}_1,\ldots,\vec{r}_N)\,|\,\psi_m(\vec{r}_1,\ldots,\vec{r}_N)\rangle \tag{2.3}$$

and

$$G_m(\vec{r}_0-\vec{r}_0^{\,\prime})=\frac{1}{(2\pi)^3}\int\frac{d\vec{k}'\,e^{i\vec{k}'\cdot(\vec{r}_0-\vec{r}_0^{\,\prime})}}{k'^2-k_m^2-i\varepsilon}\,,\quad \varepsilon\to 0^+. \tag{2.4}$$

Also, V is the interaction between the incident electron and the atom, and is given by

$$V(\vec{r}_0,\ldots,\vec{r}_N)=-\frac{N}{r_0}+\sum_{i=1}^{N}\frac{1}{|\vec{r}_0-\vec{r}_i|}\,. \tag{2.5}$$

A more convenient form for $f_{i\to f}^{(2)}$ is obtained by transforming from the integration variables $(\vec{r}_0,\vec{r}_0^{\,\prime})$ to the set $(\vec{r}_0,\vec{\rho})$, $\vec{\rho}=\vec{r}_0-\vec{r}_0^{\,\prime}$; the result is

$$f_{i\to f}^{(2)}=\frac{1}{\pi}\sum_n\int d\vec{r}_0\,e^{i\vec{q}\cdot\vec{r}_0}V_{fn}(\vec{r}_0)\times\int d\vec{r}_0^{\,\prime}\,G_n(\vec{r}_0^{\,\prime})V_{ni}(\vec{r}_0-\vec{r}_0^{\,\prime})e^{-i\vec{k}_i\cdot\vec{r}_0^{\,\prime}}\,, \tag{2.6}$$

where $\vec{\rho}$ has been relabelled $\vec{r}_0^{\,\prime}$. In similar fashion,

$$f_{i\to f}^{(3)}=-\frac{2}{\pi}\sum_{n,n'}\int d\vec{r}_0\,e^{i\vec{q}\cdot\vec{r}_0}V_{fn}(\vec{r}_0)\int d\vec{r}_0^{\,\prime}e^{-i\vec{k}_i\cdot\vec{r}_0^{\,\prime}}G_n(\vec{r}_0^{\,\prime})V_{nn'}(\vec{r}_0-\vec{r}_0^{\,\prime})\int d\vec{r}_0^{\,\prime\prime}\,e^{-i\vec{k}_i\cdot\vec{r}_0^{\,\prime\prime}}G_{n'}(\vec{r}_0^{\,\prime\prime})V_{n'i}(\vec{r}_0-\vec{r}_0^{\,\prime}-\vec{r}_0^{\,\prime\prime})\,. \tag{2.7}$$

Equations (2.6) and (2.7) represent the desired results and form the basis of the analysis of the succeeding sections.

III. HIGH-ENERGY APPROXIMATION

As noted in the introductory paragraphs, the aim of the present work is to obtain a consistent approximation to the differential cross section, valid through order k_i^{-2}, i.e., for high-energy collisions. The procedure adopted here develops partial expansions of the second and third Born terms in reciprocal powers of k_i, parallels the method of Glauber,[11] and is most akin to the high-energy small-angle potential scattering analysis of Schiff.[12]

The basic approximations are introduced by considering the integral

$$I_n=\int d\vec{r}_0^{\,\prime}\,e^{-i\vec{k}_i\cdot\vec{r}_0^{\,\prime}}V_{ni}(\vec{r}_0-\vec{r}_0^{\,\prime})G_n(\vec{r}_0^{\,\prime})$$
$$=\frac{1}{(2\pi)^3}\int d\vec{r}_0^{\,\prime}\,e^{-i(\vec{k}_i-\vec{k}_n)\cdot\vec{r}_0^{\,\prime}}V_{ni}(\vec{r}_0-\vec{r}_0^{\,\prime})\times\int\frac{d\vec{s}\,e^{i\vec{s}\cdot\vec{r}_0^{\,\prime}}}{s^2+2\vec{s}\cdot\vec{k}_n-i\varepsilon}\,, \tag{3.1}$$

where the variable transformation $\vec{s}=\vec{k}'-\vec{k}_n$ has been made. If it is assumed that V_{ni} is slowly varying over the distance of a wavelength of the scattering electron, i.e., $k_na>1$, where a is the range of V_{ni}, and that $\vec{k}_n$ does not differ greatly from $\vec{k}_i$ in either magnitude or direction, then the principal contribution to the $\vec{r}_0^{\,\prime}$ integral occurs for small s. This then suggests that the integrated expansion of $(s^2+2\vec{s}\cdot\vec{k}_n-ie)^{-1}$ in powers of s^2 should be rapidly convergent. One obtains

$$I_n=\frac{1}{(2\pi)^3}\int d\vec{r}_0^{\,\prime}\,e^{-i(\vec{k}_i-\vec{k}_n)\cdot\vec{r}_0^{\,\prime}}V_{ni}(\vec{r}_0-\vec{r}_0^{\,\prime})\int\frac{d\vec{s}}{2\vec{s}\cdot\vec{k}_n-i\varepsilon}\left(1+\frac{\nabla^2_{\vec{r}_0^{\,\prime}}}{2\vec{s}\cdot\vec{k}_n-i\varepsilon}+\cdots\right)e^{i\vec{s}\cdot\vec{r}_0^{\,\prime}}$$
$$=\frac{i}{2k_n}\int d\vec{r}_0^{\,\prime}\,e^{-i(\vec{k}_i-\vec{k}_n)\cdot\vec{r}_0^{\,\prime}}V_{ni}(\vec{r}_0-\vec{r}_0^{\,\prime})\left(\delta(\vec{b}_0^{\,\prime})H(z_0^{\prime})+\frac{i}{2k_n}\nabla^2_{\vec{r}_0^{\,\prime}}[\delta(\vec{b}_0^{\,\prime})z_0^{\prime}H(z_0^{\prime})]+O(k_n^{-2})\right), \tag{3.2}$$

where $H(z)$ is the Heaviside function, and the $\vec{s}$ integration has been performed in cylindrical polar coordinates by choosing $\vec{k}_n$ as the polar axis and writing $\vec{r}_0' = \vec{b}_0' + z_0'\hat{k}_n$. Integrating the second term in Eq. (3.2) by parts twice permits writing I_n as

$$I_n = \frac{i}{2k_n}\int_{-\infty}^{\infty} dz_0' e^{-i(\vec{k}_i-\vec{k}_n)\cdot\hat{k}_n z_0'} H(z_0') \times\left[\left(1+\frac{iz_0'}{2k_n}\hat{O}_{in}\right) V_{ni}(\vec{r}_0-\vec{r}_0')\bigg|_{\vec{b}_0'=0} + O(k_n^{-2})\right], \tag{3.3}$$

with

$$\hat{O}_{in} = \nabla^2_{\vec{r}_0'} - 2i(\vec{k}_i-\vec{k}_n)\cdot\vec{\nabla}_{\vec{r}_0'} - |\vec{k}_i-\vec{k}_n|^2 .$$

Further simplification of I_n, consistent with the original assumptions, is possible on noting that

$$(\vec{k}_i-\vec{k}_n)\cdot\hat{k}_n = k_i\cos\theta_{in} - k_n = k_i - k_n + O(k_i\theta_{in}^2) \simeq k_i - k_n ,$$

which also leads to $\hat{k}_n \simeq \hat{k}_i$, and $k_n^{-1} = k_i^{-1} + O(k_i^{-3})$. I_n may now be written as

$$I_n \simeq \frac{i}{2k_i}\int_{-\infty}^{\infty} dz_0' e^{-i\beta_{in}z_0'} H(z_0') \times\left(1+\frac{iz_0'}{2k_i}\nabla^2_{\vec{r}_0'}\right) V_{ni}(\vec{r}_0-\vec{r}_0')\bigg|_{\vec{b}_0'=0}, \tag{3.4}$$

where $\beta_{in} = k_i - k_n \simeq \Delta E_{in}/k_i$, on using the energy-conservation condition. Equation (3.4) embodies the central approximations.

Before closing this section, comment regarding the expansion which led to Eq. (3.4) seems worthwhile. Because of the appearance of β_{in}, Eq. (3.4) represents only a partial expansion of I_n in reciprocal powers of k_i. If, instead of using the substitution $\vec{s} = \vec{k}' - \vec{k}_n$, $\vec{s}$ had been set equal to $\vec{k}' - \vec{k}_i$ in Eq. (3.1), the result would have been a true expansion in inverse powers of k_i. Such an expansion yields the leading term of the real part of the second Born term as proportional to $1/k_i^2$, suggesting that recovery of the known energy dependence is regained only through analysis (and possibly resummation) of higher-order terms of the expansion. The results of the succeeding sections seem ample justification of Eq. (3.4) as the more appropriate choice.

Finally, it is a simple task to show that if β_{in} is set equal to zero and only the first term in Eq. (3.4) is retained, substitution into Eq. (2.1) via Eq. (2.2b) gives *precisely* the Glauber eikonal series.

IV. ANALYSIS OF THE SECOND AND THIRD BORN TERMS

In view of the approximations of Sec. III, the evaluation of the scattering amplitude appears best performed in cylindrical polar coordinates. The orientation of the coordinate system is chosen such that the z-axis is always perpendicular to the vector $\vec{q}$. Thus $\vec{q}$ is two dimensional, and the position coordinates of the $N+1$ electrons will be written as $\vec{r}_i = \vec{b}_i + z_i\hat{\xi}$, $i = 0, \ldots, N$, where ξ is a unit vector in the z direction. It is noted that this choice of coordinate system leaves the first Born term $f_{i\to f}^{(1)}$ invariant for all scattering angles, i.e., no approximations are introduced for this term.

Equation (3.4) of Sec. III has a special dependence on the direction $\hat{k}_i$ through the argument of V_{ni} and its derivatives. In subsequent development of this Section, $\hat{k}_i$ is replaced by $\hat{\xi}$. As will be now shown, this replacement is wholly consistent with the earlier small-angle assumptions and is equivalent to the Glauber small-angle approximation.[11]

Suppose $\hat{\xi}$ is chosen so that, on requiring $\hat{\xi}$, $\vec{k}_i$, $\vec{k}_f$, and $\vec{q}$ to be coplanar, $\hat{\xi}$ points along $\vec{k}_i$ when $\vec{q}$ becomes perpendicular to $\vec{k}_i$.[13] It is then found that

$$\hat{k}_i = (\sin\alpha)\hat{q} + (\cos\alpha)\hat{\xi}, \quad \alpha = \tan^{-1}\left(\frac{k_i/k_f - \cos\theta}{\sin\theta}\right), \tag{4.1}$$

where θ is the scattering angle and $\alpha = \cos^{-1}(\hat{k}_i\cdot\hat{\xi})$. For elastic scattering this gives

$$\hat{k}_i = \sin(\tfrac{1}{2}\theta)\,\hat{q} + \cos(\tfrac{1}{2}\theta)\,\hat{\xi} ,$$

which is the well-known result that the best choice of the polar axis is along $\vec{k}_i + \vec{k}_f$.

Glauber's small-angle approximation [and also the implications of $\hat{k}_i \simeq \hat{\xi}$ in Eq. (3.4)] is obtained from

$$\sin\alpha = \hat{q}\cdot\hat{k}_i \simeq 0 \text{ and } \cos\alpha \simeq 1. \tag{4.2}$$

For elastic scattering these conditions are satisfied for $\theta = 0$, but can never be quite satisfied for inelastic collisions, where, for θ approaching zero, $\cos\alpha \to 0$. However, it is readily seen that for $\theta = \theta_G \equiv \cos^{-1}(k_f/k_i)$, $\cos\alpha$ is a maximum, indicating that for scattering angles $\theta \simeq \theta_G$ (and $q \simeq q_G \equiv 2\Delta E_{if}$), the Glauber conditions of Eq. (4.2) are most valid. This result provides an additional criterion for assessing the results of Glauber calculations and does not appear to have been noted previously.

In simplifying the present approximations to the second and third Born terms, it will prove useful to express the interaction potential of Eq. (2.5) in Fourier form as

$$V(\vec{r}_0, \ldots, \vec{r}_N) = \int d\vec{p}\, e^{-i\vec{p}\cdot\vec{b}_0} \times\int_{-\infty}^{\infty} dp_z e^{-ip_z z_0}\bar{V}(\vec{p}+p_z\hat{\xi}, \vec{r}_1, \ldots, \vec{r}_N) , \tag{4.3}$$

where

$$\overline{V}(\vec{p}+p_z\hat{\xi},\vec{r}_1,\ldots,\vec{r}_N) = \frac{1}{2\pi^2(p^2+p_z^2)}\sum_{j=1}^{N}(e^{i\vec{p}\cdot\vec{b}_j}e^{ip_z z_j}-1)\,. \quad (4.4)$$

A. Second Born term

Substitution of Eq. (3.4) into Eq. (2.6), and calling the result $f^{(2)}_{\rm HEA}$, gives the following high-energy approximation to the second Born term:

$$f^{(2)}_{\rm HEA}=\frac{i}{2\pi k_i}\sum_n\int d\vec{r}_0\, e^{i\vec{q}\cdot\vec{r}_0}V_{fn}(\vec{r}_0)\int_{-\infty}^{\infty}dz_0'\,e^{-i\beta_{in}z_0'}H(z_0')\left(V_{ni}(\vec{r}_0-z_0'\hat{\xi})+\frac{iz_0'}{2k_i}\nabla^2_{\vec{r}_0'}V_{ni}(\vec{r}_0-\vec{r}_0')\Big|_{\vec{b}_0'=0}\right). \quad (4.5)$$

The infinite summation over atomic states can be treated, with varying degrees of accuracy, by any one of several approximate methods. For the purpose of the present paper—which is to demonstrate a theoretical procedure—the simple method of defining an average excitation energy[14] and then employing closure is adopted. Specifically, it is assumed that $\beta_{in}\simeq\beta_i=\Delta E/k_i$, where ΔE is the average energy transferred to intermediate atomic states during the course of the collision. We may now write $f^{(2)}_{\rm HEA}$ in the somewhat simpler form,

$$f^{(2)}_{\rm HEA}=\frac{i}{2\pi k_i}\int d\vec{r}_0\, e^{i\vec{q}\cdot\vec{r}_0}\langle\psi_f|V(\vec{r}_0,\ldots,\vec{r}_N)\int_{-\infty}^{\infty}dz_0'\,H(z_0')e^{-i\beta_i z_0'}\Big(V(\vec{r}_0-z_0'\hat{\xi},\vec{r}_1,\ldots,\vec{r}_N)$$
$$+\frac{iz_0'}{2k_i}\nabla^2_{\vec{r}_0'}V(\vec{r}_0-\vec{r}_0',\vec{r}_1,\ldots,\vec{r}_N)\Big|_{\vec{b}_0'=0}\Big)|\psi_i\rangle\,. \quad (4.6)$$

Now, on using Eq. (4.3) and carrying out the ∇^2 operation, the preceding result can be rewritten

$$f^{(2)}_{\rm HEA}=\frac{i}{2\pi k_i}\int d\vec{p}\int_{-\infty}^{\infty}dp_z\int d\vec{p}'\int_{-\infty}^{\infty}dp_z'\langle\psi_f|\overline{V}(\vec{p}+p_z\hat{\xi},\ldots,\vec{r}_N)\overline{V}(\vec{p}'+p_z'\hat{\xi},\ldots,\vec{r}_N)|\psi_i\rangle$$
$$\times\int d\vec{b}_0\,e^{i(\vec{q}-\vec{p}-\vec{p}')\cdot\vec{b}_0}\int_{-\infty}^{\infty}dz_0\,e^{-i(p_z+p_z')z_0}\left(1+\frac{p'^2+p_z'^2}{2k_i}\frac{\partial}{\partial\beta_i}\right)\int_{-\infty}^{\infty}dz_0'\,e^{-i(p_z'-\beta_i)z_0'}H(z_0')$$
$$=\frac{4\pi^3}{k_i}\Big[i\int d\vec{p}\left(1+\frac{1}{2k_i}\frac{\partial}{\partial\beta_i}(p^2+\beta_i^2)\right)U^{(2)}_{fi}(\vec{q}-\vec{p}-\beta_i\hat{\xi},\vec{p}+\beta_i\hat{\xi})$$
$$-\frac{1}{\pi}\mathcal{P}\int d\vec{p}\int_{-\infty}^{\infty}dp_z\left(1+\frac{p^2+p_z^2}{2k_i}\frac{\partial}{\partial\beta_i}\right)\frac{1}{p_z-\beta_i}U^{(2)}_{fi}(\vec{q}-\vec{p}-p_z\hat{\xi},\vec{p}+p_z\hat{\xi})\Big]\,, \quad (4.7)$$

where $\mathcal{P}$ means the principal value and

$$U^{(2)}_{fi}(\vec{p}+p_z\hat{\xi},\vec{p}'+p_z'\hat{\xi})=\langle\psi_f|\overline{V}(\vec{p}+p_z\hat{\xi},\vec{r}_1,\ldots,\vec{r}_N)\overline{V}(\vec{p}'+p_z'\hat{\xi},\vec{r}_1,\ldots,\vec{r}_N)|\psi_i\rangle\,.$$

In arriving at the final form of Eq. (4.7), it has been necessary to use the usual integral representations of the one- and two-dimensional δ functions, and the additional result[15]

$$\int_{-\infty}^{\infty}dx\,e^{-i\alpha x}H(x)=\pi\delta(\alpha)-i\mathcal{P}\left(\frac{1}{\alpha}\right).$$

Recall that a high-energy approximation to the differential cross section, valid through $O(k_i^{-2})$, is sought. Since the first Born term is real and of zeroth order in $1/k_i$, the imaginary part of the scattering amplitude is required only through $O(k_i^{-1})$, whereas the real part is needed through $O(k_i^{-2})$. Further, it should be apparent from Eq. (3.4) and the definition of β_i that the leading k_i dependence of the various terms of Eq. (4.7) will be of order no lower than that explicitly given. Also, except for a possible complex phase factor common to all terms of the Born series, $U^{(2)}_{fi}$ is effectively real. Consistent with these comments, the real and imaginary parts of $f^{(2)}_{\rm HEA}$ are

$$\mathrm{Re}_{p}f^{(2)}_{\rm HEA}=-\frac{4\pi^2}{k_i}\mathcal{P}\int d\vec{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i}U^{(2)}_{fi}(\vec{q}-\vec{p}-p_z\hat{\xi},\vec{p}+p_z\hat{\xi})$$
$$-\frac{2\pi^2}{k_i^2}\frac{\partial}{\partial\beta_i}\mathcal{P}\int d\vec{p}\int_{-\infty}^{\infty}\frac{dp_z(p^2+p_z^2)}{p_z-\beta_i}U^{(2)}_{fi}(\vec{q}-\vec{p}-p_z\hat{\xi},\vec{p}+p_z\hat{\xi})\,, \quad (4.8a)$$

and

$$\mathrm{Im}f_{\mathrm{HEA}}^{(2)}=\frac{4\pi^3}{k_i}\int d\vec{p}\,U_{fi}^{(2)}(\vec{q}-\vec{p}-\beta_i\hat{\xi},\vec{p}+\beta_i\hat{\xi})\,. \quad (4.8\mathrm{b})$$

Equations (4.8) constitute the present approximation to the second Born term. If β_i is set equal to zero in Eqs. (4.8), the first term of Eq. (4.8a) vanishes, and the leading term of the real part of $f_{\mathrm{HEA}}^{(2)}$ is then proportional to $1/k_i^2$. Similarly, the imaginary part of $f_{\mathrm{HEA}}^{(2)}$ identically becomes Glauber's estimate of the second Born term.[8] These equations are discussed further in Sec. V in the context of elastic scattering of electrons by hydrogen atoms.

B. Third Born term

The treatment of the third Born term parallels that of Sec. IV A, except that only the first term of Eq. (3.4) is required. Substitution of the first term of Eq. (3.4) into Eq. (2.7) yields the result

$$f_{\mathrm{HEA}}^{(3)}=\frac{1}{2\pi k_i^2}\sum_{n,n'}\int d\vec{r}_0\,e^{i\vec{q}\cdot\vec{r}_0}V_{fn}(\vec{r}_0)\int_{-\infty}^{\infty}dz_0'e^{-i\beta_{in}z_0'}H(z_0')V_{nn'}(\vec{r}_0-z_0'\hat{\xi})\times\int_{-\infty}^{\infty}dz_0''\,e^{-i\beta_{in'}z_0''}H(z_0'')V_{n'i}(\vec{r}_0-z_0'\hat{\xi}-z_0''\hat{\xi})\,, \quad (4.9)$$

where as before, $\beta_{in}=\Delta E_{in}/k_i$ and $\beta_{in'}=\Delta E_{in'}/k_i$. If, as in the treatment of the second Born term, an average excitation energy ΔE in introduced such that $\Delta E_{in}=\Delta E_{in'}=\Delta E$, the sum may be carried out by invoking closure. If, in addition, Eq. (4.3) is used, one gets

$$\begin{aligned}f_{\mathrm{HEA}}^{(3)}=&\frac{1}{2\pi k_i^2}\int d\vec{p}\int_{-\infty}^{\infty}dp_z\int d\vec{p}\,'\int_{-\infty}^{\infty}dp_z'\int d\vec{p}\,''\int_{-\infty}^{\infty}dp_z''\,U_{fi}^{(3)}(\vec{p}+p_z\hat{\xi},\vec{p}\,'+p_z'\hat{\xi},\vec{p}\,''+p_z''\hat{\xi})\\&\times\int d\vec{b}_0\,e^{i(\vec{q}-\vec{p}-\vec{p}\,'-\vec{p}\,'')\cdot\vec{b}_0}\int_{-\infty}^{\infty}dz_0\,e^{-i(p_z+p_z'+p_z'')z_0}\\&\times\int_{-\infty}^{\infty}dz_0'\,e^{-i(\beta_i-p_z'-p_z'')z_0'}H(z_0')\\&\times\int_{-\infty}^{\infty}dz_0''\,e^{-i(\beta_i-p_z'')z_0''}H(z_0'')\\=&f_1^{(3)}+f_2^{(3)}+f_3^{(3)}+f_4^{(3)}\,,\end{aligned} \quad (4.10)$$

where

$$f_1^{(3)}=\frac{4\pi^4}{k_i^2}\int d\vec{p}\int d\vec{p}\,'U_{fi}^{(3)}(\vec{p}-\beta_i\hat{\xi},\vec{p}\,',\vec{q}-\vec{p}-\vec{p}\,'+\beta_i\hat{\xi})\,,$$

$$f_2^{(3)}=-\frac{4\pi^2}{k_i^2}\mathcal{P}\int d\vec{p}\int_{-\infty}^{\infty}\frac{dp_z}{p_z-\beta_i}\int d\vec{p}\,'\int_{-\infty}^{\infty}\frac{dp_z'}{p_z'-\beta_i}U_{fi}^{(3)}(\vec{p}-p_z\hat{\xi},\vec{q}-\vec{p}-\vec{p}\,'+p_z\hat{\xi}-p_z'\hat{\xi},\vec{p}\,'+p_z'\hat{\xi})\,,$$

$$f_3^{(3)}=\frac{4\pi^3 i}{k_i^2}\mathcal{P}\int d\vec{p}\int d\vec{p}\,'\int_{-\infty}^{\infty}\frac{dp_z'}{p_z'-\beta_i}U_{fi}^{(3)}(\vec{p}-\beta_i\hat{\xi},\vec{q}-\vec{p}-\vec{p}\,'+\beta_i\hat{\xi}-p_z'\hat{\xi},\vec{p}\,''+p_z'\hat{\xi})\,,$$

$$f_4^{(3)}=-\frac{4\pi^3 i}{k_i^2}\mathcal{P}\int d\vec{p}\int d\vec{p}\,'\int_{-\infty}^{\infty}\frac{dp_z'}{p_z'+\beta_i}U_{fi}^{(3)}(\vec{p}+p_z'\hat{\xi},\vec{p}\,'-\beta_i\hat{\xi}-p_z'\hat{\xi},\vec{q}-\vec{p}-\vec{p}\,'+\beta_i\hat{\xi})\,,$$

and

$$U_{fi}^{(3)}(\vec{p}+p_z\hat{\xi},\vec{p}\,'+p_z'\hat{\xi},\vec{p}\,''+p_z''\hat{\xi})=\langle\psi_f|\,\overline{V}(\vec{p}+p_z\hat{\xi},\vec{r}_1,\ldots,\vec{r}_N)\overline{V}(\vec{p}\,'+p_z'\hat{\xi},\vec{r}_1,\ldots,\vec{r}_N)\overline{V}(\vec{p}\,''+p_z''\hat{\xi},\vec{r}_1,\ldots,\vec{r}_N)\,|\psi_i\rangle\,.$$

The last form of Eq. (4.10) is obtained by straightforward use of the integral representation of the one- and two-dimensional δ functions and the Fourier transform of the Heaviside function.

For the present purposes, only the real part of $f_{\mathrm{HEA}}^{(3)}$ is needed, which is given as

$$\mathrm{Re}f_{\mathrm{HEA}}^{(3)}=f_1^{(3)}+f_2^{(3)}\,. \quad (4.11)$$

Now if β_i is set equal to zero, it is found that $f_{\mathrm{HEA}}^{(3)}(\beta_i=0)=f_1^{(3)}(\beta_i=0)$, which, as expected, is precisely Glauber's approximation to the third Born term. Thus the most notable result of this subsection is that, apart from the Glauber-like term $f_1^{(3)}$, there is a second term of $O(k_i^{-2})$ which contributes to the real part of the third Born term. In Sec. V, Eq. (4.11) is briefly considered for elastic scattering of electrons by hydrogen atoms in the forward direction.

V. LIMITING FORMS OF $f_{\text{HEA}}^{(2)}$ AND $f_{\text{HEA}}^{(3)}$

In this section, the results of the previous sections are applied to the elastic scattering of electrons by hydrogen atoms for the purpose of determining the behavior of $f_{\text{HEA}}^{(2)}$ and $f_{\text{HEA}}^{(3)}$ as q goes to zero for large k_i. Here, it is convenient to write the product of the initial and final wave functions in the form

$$\psi_f^*\psi_i=\frac{1}{\pi}\left(-\frac{\partial}{\partial\lambda}\right)\frac{e^{-\lambda(b^2+z^2)^{1/2}}}{(b^2+z^2)^{1/2}}\bigg|_{\lambda=2}, \tag{5.1}$$

where in the following, it is understood that λ is set equal to two at the end of the calculation.

Using Eqs. (4.8) (A4), the real and imaginary parts of $f_{\text{HEA}}^{(2)}$ can be written

$$\operatorname{Re}f_{\text{HEA}}^{(2)}=\frac{4}{\pi^2k_i}\frac{\partial}{\partial\lambda}\left[\frac{1}{\lambda^2}\left(2I_2(\beta_i,\lambda^2)-\frac{q^2}{\lambda^2+q^2}I_2(\beta_i,0)\right)+\frac{1}{2k_i}\frac{\partial}{\partial\beta_i}\left(\frac{1}{\lambda^2+q^2}I_3(\beta_i,0)+\frac{1}{\lambda^2}I_3(\beta_i,\lambda^2)-I_2(\beta_i,\lambda^2)\right)\right] \tag{5.2}$$

and

$$\operatorname{Im}f_{\text{HEA}}^{(2)}=\frac{-4}{\pi k_i}\frac{\partial}{\partial\lambda}\frac{1}{\lambda^2}\left(2I_1(\beta_i^2,\lambda^2)-\frac{q^2}{\lambda^2+q^2}I_1(\beta_i^2,0)\right), \tag{5.3}$$

where the I_j's are given in the Appendix.

Using Eq. (A1) of the Appendix, and assuming that both q and β_i are small, i.e., $q\to0$ and k_i is large,

$$\operatorname{Im}f_{\text{HEA}}^{(2)}=\frac{32}{k_i\lambda^3(q^2+\lambda^2)^2}\left[(q^2+2\lambda^2)\left(\ln\frac{q^2+\lambda^2}{\lambda\beta_i}-\frac{q}{(q^2+4\beta_i^2)^{1/2}}\ln\frac{q+(q^2+4\beta_i^2)^{1/2}}{2\beta_i}+\frac{1}{2}(q^2-\lambda^2)\right]. \tag{5.4}$$

Equation (5.4) is seen to be in exact agreement with the large-k_i limit of the imaginary part of the simplified second Born approximation as given by Byron and Joachain,[7] and behaves as $(\ln k_i)/k_i$ for q approaching zero. If β_i is set equal to zero in Eq. (5.4), the corresponding term in the Glauber eikonal series is obtained, and diverges as $\ln q$ as q goes to zero.

Using Eq. (A2) for $\lambda^2>q^2$, and Eq. (A3), the real part of $f_{\text{HEA}}^{(2)}$ can be written as[16]

$$\begin{aligned}\operatorname{Re}f_{\text{HEA}}^{(2)}=&\frac{16\pi}{k_i\lambda^3}\frac{q^2+2\lambda^2}{(\lambda^2+q^2)^2}\left(1-\frac{q}{(q^2+4\beta_i^2)^{1/2}}\right)\\&+\frac{12}{k_i^2\lambda^4}-\frac{4\lambda^2-48\Delta E}{k_i^2\lambda^4(\lambda^2+q^2)}-\frac{16}{k_i^2(\lambda^2+q^2)^2}\\&+\frac{32\lambda^2-128\Delta E}{k_i^2(\lambda^2+q^2)^3}+O(1/k_i^3),\end{aligned} \tag{5.5}$$

where the definition $\beta_i=\Delta E/k_i$ has been used. Again, the terms in Eq. (5.5) proportional to $1/k_i$ are in exact agreement with the corresponding results of Byron and Joachain. Differences between the simplified second Born approximation and the present approach begin to manifest themselves in their predictions of terms proportional to $1/k^2$. Clearly, a detailed analysis of $1/k^2$ terms should include a discussion of the pertinent third Born terms; nonetheless, it is expected that for decreasing q, similarities between the two descriptions should be enhanced. For $q=0$, Eq. (5.5) reduces to

$$\operatorname{Re}f_{\text{HEA}}^{(2)}=\frac{\pi}{k_i}+\frac{3}{2k_i^2}-\frac{5\Delta E}{4k_i^2}\ (\lambda=2,\ q=0), \tag{5.6}$$

which agrees with the corresponding result of Ref. 7. From the preceding argument in light of the successes of the comparative methods, we conclude that the present approximation should provide an accurate description of the second Born term, particularly so for small q. Turning briefly to the third Born term, it is found that on substituting Eq. (A5) into the expression for $f_i^{(3)}$, one gets

$$f_1^{(3)}=\frac{2\pi}{k_i^2}\left(-\frac{\partial}{\partial\lambda}\right)\int d\vec{p}\int\frac{d\vec{p}\,'}{(p^2+\beta_i^2)p'^2(|\vec{q}-\vec{p}-\vec{p}\,'|^2+\beta_i^2)}\left(-\frac{q^2}{\lambda^2(q^2+\lambda^2)}+\frac{2}{p^2+\beta_i^2+\lambda^2}-\frac{2}{|\vec{p}+\vec{p}\,'|^2+\beta_i^2+\lambda^2}+\frac{1}{p'^2+\lambda^2}-\frac{1}{|\vec{q}-\vec{p}\,'|^2+\lambda^2}\right). \tag{5.7}$$

From the definition of $f_2^{(3)}$ it should be obvious that an analogous expression, with identical symmetry properties, can be written; hence, $f_2^{(3)}$ can be treated similarly. If q is set equal to zero in Eq. (5.7), $f_1^{(3)}$ vanishes. Thus, one gets the result

$$\mathrm{Re} f_{\mathrm{HEA}}^{(3)} = f_1^{(3)} + f_2^{(3)} = 0 , \quad q = 0 , \tag{5.8}$$

which is valid for all β_i. This result is not particularly surprising if one notes that if $\beta_i = 0$ in Eq. (5.7), then $f_1^{(3)}(\beta_i = 0) = f_{G3}$, i.e., the third term in the Glauber eikonal series, which has been evaluated in closed form.[8]

The intent of this section has been to illustrate, by simple example, the potential usefulness and computational feasibility of the present approach, and to speak briefly of its relationship to established procedures. In closing this section, one final observation is worth noting. In recent months there has been considerable interest in the theoretical description of high-energy small-angle scattering of electrons by atomic targets. Notably, the work of Konaka and Kohl,[17] Bonham and Konaka,[18] and Byron and Joachain,[19] has focused on the characteristics of channel coupling in the second Born approximation and its impact on the small-angle cross section. Though all speak of non-negligible contributions of polarization effects, particularly for dipole-allowed transitions, none has predicted the precipitous increase found by Mohr.[9] It had been thought that Mohr's predicted behavior of the cross section could be explained through investigation of higher Born terms. Though it is conceded that in-depth analysis of the third Born term is needed, Eq. (5.8) hardly supports the notion of spectacularly anomalous behavior in the forward direction.

VI. SUMMARY

As stated in the introductory paragraphs, this work has been concerned with the elucidation of the character of the second and third Born terms for short-wavelength collisions and for small momentum transfers. Specifically, the general integral I_n, defined by Eq. (3.1), has been partially expanded in reciprocal powers of k_i in an effort to ensure treatment of all portions of these Born terms which contribute to the differential cross section through order $1/k_i^2$. The partial expansion was necessitated by a desire to include a plausible and reasonably accurate description of virtual excitations, i.e., target polarization; hence, the intermediate energy loss ΔE_{in} explicitly appears. The usual high-energy assumptions were made, along with the small-angle approximation of Glauber.

To avoid approximating the first Born term and possibly to extend the validity of the results to larger values of the momentum transfer, the z axis is chosen perpendicular to $\vec{q}$ for all values of $\vec{q}$. Discussion of the coordinate system leads to the result that $\theta_G = \cos^{-1}(k_f/k_i)$ is the scattering angle for which the Glauber-angle approximations are most valid. For elastic scattering $\theta_G = 0$; note, however, that for excitation of the $n = 2$ states of hydrogen, $\theta_G = 2.59°$ for 5-keV and $\theta_G = 26.8°$ for 50-eV incident electrons.

The central results are given by Eqs. (4.8) (4.11). An unfortunate feature of these results, generally common to all approximate second Born theories (for arbitrary $\vec{q}$), is the implicit k_i dependence through the appearance of β_i. This point has been discussed in some detail by Byron and Joachain.[18] One is, nonetheless, assured of the inclusion of all terms which contribute to the differential cross section through order $1/k_i^2$. This leads to the definition of the high-energy higher-order Born direct amplitude as

$$f_{\mathrm{HH}}^{d} = f_{i\to f}^{(1)} + \mathrm{Re} f_{\mathrm{HEA}}^{(2)} + \mathrm{Re} f_{\mathrm{HEA}}^{(3)} + i\, \mathrm{Im} f_{\mathrm{HEA}}^{(2)} , \tag{6.1}$$

which represents a wholly consistent approximation, treating all terms equivalently. In the next paper of the series, Eq. (6.1) will form the basis of an analysis of elastic and inelastic scattering of electrons by hydrogen atoms.

One of the most attractive aspects of the proposed high-energy higher-order Born theory is its computational simplicity. As demonstrated in Sec. V, $f_{\mathrm{HEA}}^{(2)}$ can be evaluated with relative ease for ground-state hydrogen; few additional complications arise for atomic wave functions written as antisymmetrized products of one-electron orbitals. Both of the third Born terms, though straightforward to analyze, are algebraically tedious. Using the integration procedures introduced in Ref. 8, $f_1^{(3)}$ can, in essence, be reduced to closed form for elastic (e^-, H) collisions. After evaluating the double principal-value integral appearing in the expression for $f_2^{(3)}$, it appears that this term is reducible to a single numerical integration. These results will be explicitly demonstrated in a later paper.

ACKNOWLEDGMENTS

The author is grateful to Professor R. A. Bonham for numerous discussions throughout the course of this work. Acknowledgment is also made to the donors of the Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research.

APPENDIX

In this brief appendix, several results pertinent to Sec. V are tabulated. All integrals are easily evaluated by standard integration techniques.

$$I_1(\beta_i^2,\lambda^2)=\int\frac{d\vec{p}}{(|\vec{q}-\vec{p}|^2+\beta_i^2)(p^2+\beta_i^2+\lambda^2)}$$
$$=\frac{\pi}{\xi}\ln\left(\frac{(q^2+\beta_i^2)(\xi+q^2+\lambda^2)+2\beta_i^2(q^2-\lambda^2)}{(\beta_i^2+\lambda^2)(\xi-q^2-\lambda^2)}\right), \tag{A1}$$

where $\xi^2=(\lambda^2+q^2)^2+4q^2\beta_i^2$.

$$I_2(\beta_i,\lambda^2)=\mathcal{P}\int d\vec{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-\beta_i)(|\vec{q}-\vec{p}|^2+p_z^2)(p^2+p_z^2+\lambda^2)}$$
$$=-\frac{\pi^3}{\xi}\left\{1-\text{sgn}(\lambda^2-q^2)\left[\frac{1}{2}-\frac{1}{\pi}\sin^{-1}\left(1-\frac{2\beta_i^2(\lambda^2-q^2)^2}{(\lambda^2+q^2)^2(\beta_i^2+\lambda^2)}\right)\right]\right\}, \tag{A2}$$

where the contour for the principal-value integral has been chosen as a semicircle in the upper-half complex plane.

$$I_3(\beta_i,\lambda^2)=\mathcal{P}\int d\vec{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-\beta_i)(p^2+p_z^2+\lambda^2)}=-\pi^3\left(1-\frac{2}{\pi}\tan^{-1}\frac{\lambda}{\beta_i}\right). \tag{A3}$$

$$U_{fi}^{(2)}(\vec{q}-\vec{p}-X\hat{\xi},\vec{p}+X\hat{\xi})=\langle 1S|\overline{V}(\vec{q}-\vec{p}-X\hat{\xi},\vec{r})\overline{V}(\vec{p}+X\hat{\xi},\vec{r})|1S\rangle$$
$$=\frac{1}{\pi^4(|\vec{q}-\vec{p}|^2+X^2)(p^2+X^2)}\left(-\frac{\partial}{\partial\lambda}\right)\left(\frac{q^2+2\lambda^2}{\lambda^2(q^2+\lambda^2)}-\frac{1}{|\vec{q}-\vec{p}|^2+X^2+\lambda^2}-\frac{1}{p^2+X^2+\lambda^2}\right). \tag{A4}$$

$$U_{fi}^{(3)}(\vec{p}-\beta_i\hat{\xi},\vec{p}\,',\vec{q}-\vec{p}-\vec{p}\,'+\beta_i\hat{\xi})=\langle 1S|\overline{V}(\vec{p}-\beta_i\hat{\xi},\vec{r})\overline{V}(\vec{p}\,',\vec{r})\overline{V}(\vec{q}-\vec{p}-\vec{p}\,'+\beta_i\hat{\xi},\vec{r})|1S\rangle$$
$$=\frac{1}{2\pi^3(p^2+\beta_i^2)p'^2(|\vec{q}-\vec{p}-\vec{p}\,'|^2+\beta_i^2}\left(-\frac{\partial}{\partial\lambda}\right)$$
$$\times\left(-\frac{q^2}{\lambda^2(q^2+\lambda^2)}+\frac{1}{p^2+\beta_i^2+\lambda^2}+\frac{1}{p'^2+\lambda^2}+\frac{1}{|\vec{q}-\vec{p}-\vec{p}\,'|^2+\beta_i^2+\lambda^2}\right.$$
$$\left.-\frac{1}{|\vec{p}+\vec{p}\,'|^2+\beta_i^2+\lambda^2}-\frac{1}{|\vec{q}-\vec{p}\,'|^2+\lambda^2}-\frac{1}{|\vec{q}-\vec{p}|^2+\beta_i^2+\lambda^2}\right). \tag{A5}$$

Equation (5.1) has been used in obtaining the results of Eqs. (A4) and (A5).

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